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polarons

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Zusammenfassung

Polarone sind Quasiteilchen, die durch die Wechselwirkung von Elektronen mit Gitterschwingungen entstehen. In der Physik der kondensierten Materie spielen Polarone für viele Systeme eine zentrale Rolle, da sie sowohl Transporteigenschaften als auch optische und supraleitende Eigenschaften maßgeblich beeinflussen können. Es ist deshalb von großer Bedeutung für die theoretische Festkörperphysik, das Verhalten von Polaronen in unterschiedlichen Kopplungsregimen und für verschiedene Wechselwirkungsmechanismen zu verstehen. Die vorliegende Dissertation untersucht verschiedene Polaronmodelle mit Hilfe von analytischen Herleitungen und numerischen Simulationen basierend auf der diagrammatischen Monte-Carlo-Methode (DiagMC). Die Arbeit konzentriert sich dabei auf drei repräsentative Modelle in der Elektron-Phonon-Physik: (i) das historisch wichtige große Fröhlich-Polaron, (ii) das akustische Gitterpolaron, und (iii) das quadratische Polaron. Für das zwei- und dreidimensionale Fröhlich-Polaron werden Grundzustandsenergien, effektive Massen und Dispersionsrelationen präsentiert. Die Ergebnisse werden sowohl mit dem Pfadintegralansatz von Feynman als auch mit bekannten Störungstheorien für das schwache und starke Wechselwirkungsregime verglichen und zur Überprüfung exakter Skalierungsrelationen verwendet. Der zweite Teil dieser Dissertation untersucht das akustische Gitterpolaron, bei dem das Elektron über ein Deformationspotential mit einem akustischen Phononenzweig wechselwirkt. Die Simulationen zeigen eine Selbstlokalisierungsregion, die das schwache und starke Kopplungsregime trennt und durch eine quantenmechanische Resonanz verschiedener Gitterverzerrungen gekennzeichnet ist. Das resultierende Quasiteilchen besitzt eine zusammengesetzte Phononenwolke, welche aus dem Zusammenspiel lang- und kurzwelliger Gitterschwingungen entsteht. Dies führt zur Ausbildung mehrerer konkurrierender Polaronzustände sowie zu einer komplexen spektralen und optischen Antwort, die sich deutlich von zuvor untersuchten Polaronmodellen unterscheidet. Abschließend werden Polarone mit quadratischer Kopplung an Gitterauslenkungen untersucht. Im Gegensatz zu linearen Modellen reagiert das Quasiteilchen weitgehend unempfindlich auf starke quadratische Wechselwirkungen, außer in der Nähe der Instabilitätsschwelle. Die Polaroneigenschaften hängen hauptsächlich vom adiabatischen Verhältnis ab und kaum von der Elektronendispersion oder der räumlichen Dimension des Modells. Außerdem sind die Gitterverzerrungen nur schwach ausgeprägt,

selbst nahe der Instabilitätsschwelle. Zusammenfassend liefern die Ergebnisse dieser Dissertation neue Referenzwerte für verschiedene Polaronmodelle und tragen zum Verständnis der Elektron-Phonon-Physik in polarisierbaren Materialien bei.

Abstract

Polarons, quasiparticles formed by electrons interacting with lattice vibrations, play a central role in determining transport, optical, and superconducting properties of many condensed matter systems. Understanding their behavior across different coupling regimes and interaction mechanisms remains a major challenge in theoretical condensed matter physics. This thesis presents theoretical and numerical investigations of several polaron models based on the Diagrammatic Monte Carlo (DiagMC) method. The research focuses on three representative models in electron-phonon physics: (i) the historically well-known Fröhlich large polaron, (ii) an acoustic lattice polaron, and (iii) the quadratic polaron. For the two- and three-dimensional Fröhlich model, ground state energies, effective masses, and dispersion relations are presented. The results are benchmarked against Feynman's path-integral approach, compared to known weak- and strong-coupling expansions, and used to verify exact scaling relations. In the second part of the thesis, we investigate the acoustic lattice polaron, where the electron interacts with an acoustic phonon branch through deformation-potential coupling. The simulations reveal a self-trapping region separating weak and strong coupling regimes, characterized by quantum resonance between various lattice distortions. The resulting quasiparticle exhibits a composite phonon cloud arising from the interplay of long- and short-wavelength lattice vibrations, leading to multiple competing polaron states and a complex spectral and optical response distinct from previously studied models. Finally, the thesis presents a study on polarons with quadratic coupling to lattice displacements. In contrast to linear models, the quasiparticle's behavior is largely insensitive to strong quadratic interactions, except near the instability threshold. Its properties depend mainly on the adiabatic ratio rather than the electron dispersion or dimensionality, and it exhibits weak lattice deformations even at the point of instability. Overall, the results shown in this work provide new benchmarks for the polaron community and contribute to the understanding of electron-phonon physics in polarizable materials.

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Publications

List of Publications Produced During the PhD:

1. T. Hahn, S. Klimin, J. Tempere, J.T. Devreese, C. Franchini, *Diagrammatic Monte Carlo study of Fröhlich polaron dispersion in two and three dimensions*, [Physical Review B 97 \(13\), 134305 \(2018\)](#)
2. T. Hahn, N. Nagaosa, C. Franchini, A.S. Mishchenko, *Diagrammatic quantum Monte Carlo study of an acoustic lattice polaron*, [Physical Review B 104 \(16\), L161111 \(2021\)](#)
3. S. Ragni, T. Hahn, Z. Zhang, N. Prokof'ev, A. Kuklov, S. Klimin, M. Houtput, B. Svistunov, J. Tempere, N. Nagaosa, C. Franchini, A. S. Mishchenko, *Polaron with quadratic electron-phonon interaction*, [Physical Review B 107 \(12\), L121109 \(2023\)](#)
4. S.N. Klimin, J. Tempere, M. Houtput, S. Ragni, T. Hahn, C. Franchini, A. S. Mishchenko, *Analytic method for quadratic polarons in nonparabolic bands*, [Physical Review B 110 \(7\), 075107 \(2024\)](#)
5. S. Ragni, T. Mišić, T. Hahn, N. Prokof'ev, O.S. Barišić, N. Nagaosa, C. Franchini, A. S. Mishchenko, *Polarons with arbitrary nonlinear electron-phonon interaction*, [Physical Review Research 7 \(4\), 043304 \(2025\)](#)
6. S.N. Klimin, J. Tempere, M. Houtput, I. Zappacosta, S. Ragni, T. Hahn, L. Celiberti, C. Franchini, and A.S. Mishchenko, *Analytic treatment of a polaron in a nonparabolic conduction band*, [arXiv:2603.09609 \(2026\)](#)

Although all publications are thematically connected to the scope and title of this thesis, space constraints limit the discussion to the results presented in the first three papers, to which I contributed most significantly, as explicitly stated in the respective chapters.

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List of Abbreviations

1D	one-dimensional, one dimension
2D	two-dimensional, two dimensions
3D	three-dimensional, three dimensions
AL	atomic limit
ARPES	angle-resolved photoemission spectroscopy
BCS	Bardeen-Cooper-Schrieffer
BEC	Bose-Einstein condensate
BvK	Born-von Kármán
BZ	(first) Brillouin zone
CC	consistent constraints
DFT	density functional theory
DiagMC / DMC	diagrammatic Monte Carlo
EPI	electron phonon interaction
FES	first excited state
GS	ground state
LSF	Lehmann spectral function
MC	Monte Carlo
MCC	method of consistent constraints
MCMC	Markov chain Monte Carlo
NAC	numerical analytic continuation
OC	optical conductivity
SC	(BvK) super cell
SCR	strong coupling regime
SOCC	stochastic optimization with consistent constraints
SOM	stochastic optimization method
SSH	Su-Schrieffer-Heeger
ST	self-trapping
UC	(real space) unit cell
WCR	weak coupling regime

Chapter 1

Introduction

Condensed matter physics is the study of macroscopic and microscopic properties of matter in its liquid and solid phase. Over the last decades, it has arguably become the largest and most active discipline within all of physics. Its popularity might be attributed to the fact that it overlaps with several other branches of physics and related sciences like atomic physics, particle physics, biophysics, chemistry or material science. Another reason could be the large number of applications and the enormous impact it has on our everyday lives. Many of the groundbreaking and even Nobel Prize-winning breakthroughs of recent times have been made in the field of condensed matter physics. Examples include the discoveries of conventional [1, 2] and high-temperature [3] superconductivity, the explanation of the former in terms of BCS theory [4], the detection of giant magnetoresistance on Fe/Cr films [5, 6], the discoveries of the quantum [7] and fractional quantum Hall effects [8] (as well as their various derivatives [9]) and the closely related theory of topological order and phase transitions [10].

Despite such great achievements, there remain many open problems and challenges, especially from a theoretical point of view. Looking only at the above-mentioned examples, we do not yet have an accepted microscopic theory of high-temperature superconductivity or a satisfactory understanding of the mechanisms behind the fractional quantum Hall effect. To be able to answer such interesting questions, one has to study the individual constituents of matter and their interactions at a quantum mechanical level.

In condensed matter physics, the fundamental microscopic building blocks are atoms and the dominant force is the electromagnetic interaction between the positively charged atomic nuclei and the negatively charged electrons. If relativistic effects can be neglected and no external forces are present, the corresponding Hamilton operator takes on the following form [11]:

$$\hat{H} = \hat{T}_e + \hat{V}_{e-e} + \hat{T}_n + \hat{V}_{n-n} + \hat{V}_{e-n} , \quad (1.1)$$

where

$$\hat{T}_e = \sum_{i=1}^{N_e} \frac{\hat{\mathbf{p}}_i^2}{2m_e} \quad (1.2)$$

is the kinetic energy of the electrons,

$$\hat{V}_{e-e} = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N_e} v_{e-e}(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j) = \frac{1}{2} \frac{1}{4\pi\epsilon_0} \sum_{\substack{i,j=1 \\ i \neq j}}^{N_e} \frac{e^2}{|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|} \quad (1.3)$$

is the potential energy between the electrons,

$$\hat{T}_n = \sum_{i=1}^{N_n} \frac{\hat{\mathbf{P}}_i^2}{2M_i} \quad (1.4)$$

is the kinetic energy of the nuclei,

$$\hat{V}_{n-n} = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N_n} v_{n-n}(\hat{\mathbf{R}}_i, \hat{\mathbf{R}}_j) = \frac{1}{2} \frac{1}{4\pi\epsilon_0} \sum_{\substack{i,j=1 \\ i \neq j}}^{N_n} \frac{Z_i Z_j e^2}{|\hat{\mathbf{R}}_i - \hat{\mathbf{R}}_j|} \quad (1.5)$$

is the potential energy between the nuclei and

$$\hat{V}_{e-n} = \sum_{i=1}^{N_e} \sum_{j=1}^{N_n} v_{e-n}(\hat{\mathbf{r}}_i, \hat{\mathbf{R}}_j) = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^{N_e} \sum_{j=1}^{N_n} \frac{-Z_j e^2}{|\hat{\mathbf{r}}_i - \hat{\mathbf{R}}_j|} \quad (1.6)$$

is the potential energy between the electrons and nuclei. Here, $\hat{\mathbf{r}}_i$ ($\hat{\mathbf{R}}_i$) and $\hat{\mathbf{p}}_i$ ($\hat{\mathbf{P}}_i$) are the position and momentum operators of an electron (nucleus), m_e is the electron mass, e is the elementary charge, ϵ_0 is the vacuum permittivity and M_i and Z_i denote the mass and atomic number of the i^{th} nucleus.

Equations 1.1-1.6 can be applied to any system consisting of N_e electrons and N_n nuclei, e.g. crystalline and non-crystalline solids, liquids or individual molecules. They may also describe the situation where one distinguishes between tightly bound core and valence electrons. In this case, an atomic nucleus together with its core electrons constitute a single entity, an ion, and the bare Coulomb potentials, $v_{n-n}(\hat{\mathbf{R}}_i, \hat{\mathbf{R}}_j)$ and $v_{e-n}(\hat{\mathbf{r}}_i, \hat{\mathbf{R}}_j)$, are replaced by effective potentials to account for screened interactions. In the following, we will not make such a distinction and use the terms “nucleus”, “atom” and “ion” interchangeably. Furthermore, it will be assumed that we are dealing with a crystalline solid, where each atom has an equilibrium position, $\mathbf{R}_i^{(0)}$, and its motion is confined to a small volume around $\mathbf{R}_i^{(0)}$.

The difficulty in solving the corresponding Schrödinger equation, $\hat{H}\Psi = E\Psi$,

is due to the large number of strongly interacting particles, which in any macroscopic sample is of the order of $\approx 10^{23} - 10^{24}$ [12]. One of the most useful and widespread simplifications is provided by the so-called *Born-Oppenheimer* or *adiabatic* approximation [13]. It is based on the fact that atomic nuclei are much heavier than electrons, $m_e/M < 1/1800$, and that their dynamics take place on different time scales. This justifies an initial decoupling of electronic and ionic degrees of freedom and allows us to introduce the following two independent subsystems:

(i) The electronic structure problem considers interacting electrons in an external potential created by immobile ions. It tries to solve the following Schrödinger equation:

$$\begin{aligned}\hat{H}_e(\underline{\mathbf{r}}; \underline{\mathbf{R}})\Phi_\alpha(\underline{\mathbf{r}}; \underline{\mathbf{R}}) &= \left(\hat{T}_e + \hat{V}_{e-e}(\underline{\mathbf{r}}) + \hat{V}_{e-n}(\underline{\mathbf{r}}; \underline{\mathbf{R}})\right) \Phi_\alpha(\underline{\mathbf{r}}; \underline{\mathbf{R}}) \\ &= E_\alpha(\underline{\mathbf{R}})\Phi_\alpha(\underline{\mathbf{r}}; \underline{\mathbf{R}}) .\end{aligned}\tag{1.7}$$

Here, α is some quantum number and the vector notation $\underline{\mathbf{r}} = (\mathbf{r}_1, \dots, \mathbf{r}_{N_e})$ and $\underline{\mathbf{R}} = (\mathbf{R}_1, \dots, \mathbf{R}_{N_n})$ is used to denote the positions of all electrons and nuclei, respectively. Since the heavy ions are assumed to be stationary, their positions $\underline{\mathbf{R}}$ only enter the equation as fixed parameters. Despite ignoring the motion of ions, Eq. 1.7 still poses one of the biggest challenges in condensed matter physics to this day. The most successful approach for computing the ground state (GS) electronic structure of real materials is without doubt density functional theory (DFT) [14, 15]. DFT works incredibly well for many materials but can fail in certain situations, for example when correlations between electrons are strong. Such strongly correlated systems are instead often studied by approximating Eq. 1.7 with an effective model Hamiltonian. A famous example is the Hubbard model [16], which displays various interesting phenomena ranging from metal-insulator transitions to high-temperature superconductivity.

(ii) The ionic subsystem, on the other hand, is governed by the general Hamiltonian

$$\hat{H}_{\text{ph}} = \hat{T}_n + \hat{V}_{\text{eff}}(\underline{\mathbf{R}}) .\tag{1.8}$$

The effective potential, $V_{\text{eff}}(\underline{\mathbf{R}})$, is usually either given as a parameterized, analytic expression, e.g. as the Lennard-Jones potential to model van der Waals interactions, or it can be calculated within the adiabatic approximation from first principles. In the latter case, $V_{\text{eff}}(\underline{\mathbf{R}}) = V_{n-n}(\underline{\mathbf{R}}) + E_0(\underline{\mathbf{R}})$, where $E_0(\underline{\mathbf{R}})$ is the electronic GS energy from Eq. 1.7. Irrespective of its origin, the standard approach to study Eq. 1.8 is to employ the so-called *harmonic approximation* [17, 18]. It makes the assumption that the ions move only slightly away from their equilibrium positions, $\underline{\mathbf{R}}^{(0)}$, at which the potential energy exhibits a minimum. $V_{\text{eff}}(\underline{\mathbf{R}})$

is then written as a Taylor expansion around $\underline{\mathbf{R}}^{(0)}$ and only terms up to second order are taken into account. The approximate Hamiltonian can easily be diagonalized leading to independent harmonic oscillators with well-known properties from basic quantum mechanics. A single quantum of vibration is called a *phonon* and represents a *collective excitation* of all ions [12]. Note that although a phonon is a stable excitation within the harmonic approximation, it will acquire a finite lifetime due to phonon-phonon interactions when higher-order (anharmonic) terms of the Taylor expansion are included.

The electronic and ionic Hamiltonians from Eqs. 1.7 and 1.8 form the basis of modern calculations in materials physics. However, they completely neglect any coupling between the two independent subsystems, which can have a significant influence on various physical properties. It is therefore often necessary to go beyond the adiabatic approximation by considering corrections in the form of *electron-phonon interactions* (EPIs) [19]. EPIs have played a key role in all of condensed matter physics over the last century. For example, the resistivity of metals, the carrier mobility in semiconductors or the temperature dependence of electronic band structures and optical spectra can only be explained when EPIs are taken into account [20, 21]. Additionally, EPIs give rise to conventional superconductivity and they constitute the driving force behind *polaron* formation in many materials [22].

Polarons are the central objects of the current thesis. They are fermionic *quasi-particles* consisting of an electron surrounded by a cloud of phonons. Due to EPIs, the *bare* electron gets dressed with phonons resulting in a new bound state with lower energy compared to the non-interacting system. The physical properties of a polaron, e.g. its energy dispersion, effective mass or quasiparticle weight, as well as its response to external perturbations, e.g. its optical absorption or mobility, can differ drastically from the bare particle. The main goal of this thesis is to calculate how EPIs renormalize various physical quantities for selected polaron models.

In order to properly set the stage, Section 1.1 introduces the general polaron Hamiltonian used throughout the present work. Since many textbooks [11, 17, 19] and review articles [20] already contain detailed derivations, we will only highlight the most important aspects and use the opportunity to establish specific notations. Section 1.2 gives a short summary on the history of polarons and some basic polaron models, before Sec. 1.3 outlines the rest of this thesis.

1.1 Polaron Hamiltonian

From now on, it will be assumed that the atoms form a crystalline solid with an underlying D -dimensional Bravais lattice spanned by basis vectors $\{\mathbf{a}_1, \dots, \mathbf{a}_D\}$.

An arbitrary lattice vector $\mathbf{R}_{\mathbf{n}}$ can then be decomposed as

$$\mathbf{R}_{\mathbf{n}} = \sum_{i=1}^D n_i \mathbf{a}_i, \quad \mathbf{n} = (n_1, \dots, n_D), \quad n_i \in \mathbb{Z}, \quad (1.9)$$

and the volume of a primitive unit cell is $V_{\text{UC}} = |\det(\mathbf{a}_1 \dots \mathbf{a}_D)|$.

Associated with the real space Bravais lattice is a corresponding reciprocal lattice defined by the primitive basis vectors $\{\mathbf{b}_1, \dots, \mathbf{b}_D\}$. They fulfill the relations $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$ for all $i, j = 1, \dots, D$ and enclose a volume of size $V_{\text{BZ}} = |\det(\mathbf{b}_1 \dots \mathbf{b}_D)| = (2\pi)^D/V_{\text{UC}}$. Similar to Eq. 1.9, a reciprocal lattice vector is given by

$$\mathbf{G}_{\mathbf{m}} = \sum_{i=1}^D m_i \mathbf{b}_i, \quad \mathbf{m} = (m_1, \dots, m_D), \quad m_i \in \mathbb{Z}. \quad (1.10)$$

Since we are not interested in surface effects, we use Born-von Kármán (BvK) boundary conditions to describe the infinitely expanding crystal. This means we impose periodic boundary conditions on a large supercell (SC) consisting of N_i primitive unit cells in direction $\mathbf{a}_i$ such that their total number is $N = \prod_{i=1}^D N_i$ and its volume is $V = NV_{\text{UC}}$. A primitive unit cell in the BvK supercell can therefore be identified with a lattice vector $\mathbf{R}_{\mathbf{n}}$, whose n_i in Eq. 1.9 are restricted to integers between 0 and $N_i - 1$.

Furthermore, we define the Bloch wave vectors as

$$\mathbf{q} = \sum_{i=1}^D \frac{m_i}{N_i} \mathbf{b}_i, \quad m_i = 0, \dots, N_i - 1, \quad (1.11)$$

such that they form a uniform grid in the primitive unit cell situated at the origin in reciprocal space. It is clear from Eq. 1.11 that there are as many different Bloch wave vectors as primitive unit cells in the BvK supercell. In the thermodynamic limit, the discrete Bloch wave vectors become continuous quantities and $\mathbf{q}$ -sums are replaced with integrals over a primitive reciprocal unit cell:

$$\sum_{\mathbf{q}} \longrightarrow \frac{V}{(2\pi)^D} \int_{\text{BZ}} d\mathbf{q}. \quad (1.12)$$

The standard Hamiltonian describing a coupled electron-phonon system is usually comprised of three terms:

$$\hat{H}_{\text{pol}} = \hat{H}_{\text{e}} + \hat{H}_{\text{ph}} + \hat{H}_{\text{el-ph}}. \quad (1.13)$$

Here, $\hat{H}_{\text{e}}$ and $\hat{H}_{\text{ph}}$ correspond to the electronic and phonon subsystems and $\hat{H}_{\text{el-ph}}$

contains their interactions. In the following, all summations over $\mathbf{k}$, $\mathbf{k}'$ and $\mathbf{q}$ are restricted to Bloch wave vectors from Eq. 1.11 or equivalently to the first Brillouin zone.

For the electrons, we assume that they can be described in terms of well-defined quasiparticle excitations such that the electrostatic, periodic potential from the ions in their equilibrium positions and possible electron-electron interactions are already included in the single-particle energies $\varepsilon_{n\mathbf{k}}$ [20]. Then, the electronic Hamiltonian takes on the simple form

$$\hat{H}_e = \sum_{n\mathbf{k}} \varepsilon_{n\mathbf{k}} \hat{c}_{n\mathbf{k}}^\dagger \hat{c}_{n\mathbf{k}} , \quad (1.14)$$

where $\varepsilon_{n\mathbf{k}}$ is the energy of an electron in band n with wave vector $\mathbf{k}$ and $\hat{c}_{n\mathbf{k}}^\dagger$ ($\hat{c}_{n\mathbf{k}}$) creates (destroys) a particle in the Bloch state $|n\mathbf{k}\rangle$ [23]. The fermionic operators obey the usual anticommutation relations

$$\left\{ \hat{c}_{n\mathbf{k}}^\dagger, \hat{c}_{n'\mathbf{k}'}^\dagger \right\} = \left\{ \hat{c}_{n\mathbf{k}}, \hat{c}_{n'\mathbf{k}'} \right\} = 0 , \quad \left\{ \hat{c}_{n\mathbf{k}}, \hat{c}_{n'\mathbf{k}'}^\dagger \right\} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{nn'} . \quad (1.15)$$

Note that the spin variable σ has not been included to avoid a cluttered notation and because it won't play a role for our purposes.

To describe the phonon subsystem, suppose a primitive unit cell contains M nuclei or ions. The position of ion κ in the primitive cell $\mathbf{n}$ is specified as $\mathbf{R}_{n\kappa} = \mathbf{R}_{n\kappa}^{(0)} + \mathbf{u}_{n\kappa}$ and its D components as $R_{n\kappa i}$, where $\mathbf{R}_{n\kappa}^{(0)}$ denotes the ion's equilibrium position and $\mathbf{u}_{n\kappa}$ its displacement relative to $\mathbf{R}_{n\kappa}^{(0)}$. Within the harmonic approximation, the effective potential is expanded in a Taylor series up to second order around the ionic equilibrium positions:

$$V_{\text{eff}}(\underline{\mathbf{R}}) \approx V_{\text{eff}}(\underline{\mathbf{R}}^{(0)}) + \frac{1}{2} \sum_{\substack{n\kappa i \\ n'\kappa' i'}} \left. \frac{\partial^2 V_{\text{eff}}}{\partial R_{n\kappa i} \partial R_{n'\kappa' i'}} \right|_{\underline{\mathbf{R}}^{(0)}} u_{n\kappa i} u_{n'\kappa' i'} . \quad (1.16)$$

The zeroth order term is just a constant and has no influence on the lattice dynamics. After plugging the approximation from Eq. 1.16 into Eq. 1.8 and using the bosonic creation and destruction operators

$$\left[\hat{a}_{\mathbf{q}\nu}^\dagger, \hat{a}_{\mathbf{q}'\nu'}^\dagger \right] = \left[\hat{a}_{\mathbf{q}\nu}, \hat{a}_{\mathbf{q}'\nu'} \right] = 0 , \quad \left[\hat{a}_{\mathbf{q}\nu}, \hat{a}_{\mathbf{q}'\nu'}^\dagger \right] = \delta_{\mathbf{q}\mathbf{q}'} \delta_{\nu\nu'} , \quad (1.17)$$

the final, diagonalized phonon Hamiltonian can be written as (for details see e.g. Ref. [20])

$$\hat{H}_{\text{ph}} = \sum_{\mathbf{q}\nu} \hbar \omega_{\mathbf{q}\nu} \left(\hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu} + 1/2 \right) . \quad (1.18)$$

Here, $\omega_{\mathbf{q}\nu}$ is the phonon frequency corresponding to the wave vector $\mathbf{q}$ and branch ν .

For each Bloch wave vector $\mathbf{q}$, there are DM frequencies, of which D are assigned to acoustic branches with $\omega_{\mathbf{q}\nu} \rightarrow 0$ for $\mathbf{q} \rightarrow 0$ and $D(M-1)$ to optical branches. The following important equation relates the real displacements $u_{\mathbf{n}\kappa i}$ to the phonon creation and destruction operators [20]:

$$u_{\mathbf{n}\kappa i} = \sum_{\mathbf{q}\nu} \left(\frac{\hbar}{2M_\kappa N \omega_{\mathbf{q}\nu}} \right)^{1/2} e^{i\mathbf{q}\mathbf{R}_\mathbf{n}} e_{\kappa i, \nu}(\mathbf{q}) \left(\hat{a}_{\mathbf{q}\nu} + \hat{a}_{-\mathbf{q}\nu}^\dagger \right), \quad (1.19)$$

where M_κ is the mass of ion κ and $\mathbf{e}_\nu(\mathbf{q})$ is the normal mode of the lattice vibration, also called polarization vector. The normal modes are eigenvectors of the $DM \times DM$ (Hermitian) dynamical matrix and can therefore be chosen to be orthonormal for every $\mathbf{q}$:

$$\sum_{\nu} e_{\kappa i, \nu}^*(\mathbf{q}) e_{\kappa' i', \nu}(\mathbf{q}) = \delta_{ii'} \delta_{\kappa\kappa'}, \quad \sum_{\kappa i} e_{\kappa i, \nu}^*(\mathbf{q}) e_{\kappa i, \nu'}(\mathbf{q}) = \delta_{\nu\nu'}. \quad (1.20)$$

The electron-phonon interaction has its origin in the electron-ion potential from Eq. 1.6. Let $U(\mathbf{r}, \mathbf{R})$ be the general potential a single electron at position $\mathbf{r}$ feels due to all the ions. Using again a Taylor expansion around the ionic equilibrium positions up to linear order, we can write

$$U(\mathbf{r}, \mathbf{R}) \approx U(\mathbf{r}, \mathbf{R}^{(0)}) + \sum_{\mathbf{n}\kappa i} \left. \frac{\partial U}{\partial R_{\mathbf{n}\kappa i}} \right|_{\mathbf{R}^{(0)}} u_{\mathbf{n}\kappa i}. \quad (1.21)$$

Here, $U(\mathbf{r}, \mathbf{R}^{(0)})$ is just the static, lattice periodic potential when the ions are in their equilibrium positions and it is assumed to be already included in the electronic energies $\varepsilon_{n\mathbf{k}}$. The remaining term corresponds to the linear approximation to the electron-phonon interaction. Its second-quantized form is derived with the usual ansatz [17]:

$$\begin{aligned} \hat{H}_{\text{el-ph}} &= \sum_{\substack{n\mathbf{k} \\ n'\mathbf{k}'}} \left\langle n\mathbf{k} \left| \sum_{\mathbf{n}\kappa i} \left. \frac{\partial U}{\partial R_{\mathbf{n}\kappa i}} \right|_{\mathbf{R}^{(0)}} u_{\mathbf{n}\kappa i} \right| n'\mathbf{k}' \right\rangle \hat{c}_{n\mathbf{k}}^\dagger \hat{c}_{n'\mathbf{k}'} \\ &= \frac{1}{\sqrt{N}} \sum_{\substack{n\mathbf{k} \\ n'\mathbf{k}'}} \sum_{\mathbf{q}\nu} \langle n\mathbf{k} | e^{i\mathbf{q}\mathbf{r}} \Delta_{\mathbf{q}\nu} U(\mathbf{r}) | n'\mathbf{k}' \rangle \hat{c}_{n\mathbf{k}}^\dagger \hat{c}_{n'\mathbf{k}'} \left(\hat{a}_{\mathbf{q}\nu} + \hat{a}_{-\mathbf{q}\nu}^\dagger \right), \end{aligned} \quad (1.22)$$

where we used Eq. 1.19 and defined the variations $\Delta_{\mathbf{q}\nu}$ as

$$\Delta_{\mathbf{q}\nu} U(\mathbf{r}) = \sum_{\kappa i} \left(\frac{\hbar}{2M_\kappa \omega_{\mathbf{q}\nu}} \right)^{1/2} e_{\kappa i, \nu}(\mathbf{q}) \sum_{\mathbf{n}} e^{-i\mathbf{q}(\mathbf{r} - \mathbf{R}_\mathbf{n})} \left. \frac{\partial U}{\partial R_{\mathbf{n}\kappa i}} \right|_{\mathbf{R}^{(0)}}. \quad (1.23)$$

The partial derivative describes the change in potential an electron at position $\mathbf{r}$

feels if the ion κ in unit cell $\mathbf{n}$ is displaced in direction i . Due to the translational symmetry of the lattice, this change cannot explicitly depend on $\mathbf{R}_\mathbf{n}$, but only on the difference vector $\mathbf{r} - \mathbf{R}_\mathbf{n}$. Hence, $\Delta_{\mathbf{q}\nu}U(\mathbf{r})$ is a lattice periodic function of $\mathbf{r}$. To further simplify the electron-phonon Hamiltonian, let us use the following expression for the Bloch wave functions

$$\langle \mathbf{r} | n\mathbf{k} \rangle = \psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} e^{i\mathbf{k}\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) , \quad (1.24)$$

where $\psi_{n\mathbf{k}}(\mathbf{r})$ is normalized to unity over the BvK supercell and $u_{n\mathbf{k}}(\mathbf{r})$ has the periodicity of the lattice. The expectation value in Eq. 1.22 can then be written as

$$\begin{aligned} \langle n\mathbf{k} | e^{i\mathbf{q}\mathbf{r}} \Delta_{\mathbf{q}\nu} U | n'\mathbf{k}' \rangle &= \int_{\text{SC}} d\mathbf{r} \psi_{n\mathbf{k}}^*(\mathbf{r}) e^{i\mathbf{q}\mathbf{r}} \Delta_{\mathbf{q}\nu} U(\mathbf{r}) \psi_{n'\mathbf{k}'}(\mathbf{r}) \\ &= \frac{1}{N} \sum_{\mathbf{n}} e^{i(\mathbf{k}' + \mathbf{q} - \mathbf{k})\mathbf{R}_\mathbf{n}} \int_{\text{UC}} d\mathbf{r} u_{n\mathbf{k}}^*(\mathbf{r}) e^{i(\mathbf{k}' + \mathbf{q} - \mathbf{k})\mathbf{r}} \Delta_{\mathbf{q}\nu} U(\mathbf{r}) u_{n'\mathbf{k}'}(\mathbf{r}) \\ &= \sum_{\mathbf{m}} \delta_{\mathbf{k}' + \mathbf{q} - \mathbf{k}, \mathbf{G}_\mathbf{m}} \int_{\text{UC}} d\mathbf{r} u_{n\mathbf{k}}^*(\mathbf{r}) e^{i\mathbf{G}_\mathbf{m}\mathbf{r}} \Delta_{\mathbf{q}\nu} U(\mathbf{r}) u_{n'\mathbf{k}'}(\mathbf{r}) . \end{aligned} \quad (1.25)$$

In the second line, Eq. 1.24 and the lattice periodicity of the integrands were used to split the integral over the BvK supercell into a sum of integrals over all unit cells, while in the last line we explicitly performed the sum over lattice vectors with the help of

$$\sum_{\mathbf{n}} e^{i\mathbf{k}\mathbf{R}_\mathbf{n}} = N \sum_{\mathbf{m}} \delta_{\mathbf{k}, \mathbf{G}_\mathbf{m}} . \quad (1.26)$$

Combining Eqs. 1.25 and 1.22 results in the electron-phonon Hamiltonian

$$\hat{H}_{\text{el-ph}} = \frac{1}{\sqrt{N}} \sum_{\substack{\mathbf{k}, \mathbf{q}, \mathbf{m} \\ mn\nu}} g_{mn\nu}(\mathbf{k}, \mathbf{q}) \hat{c}_{m\mathbf{k} + \mathbf{q} + \mathbf{G}_\mathbf{m}}^\dagger \hat{c}_{n\mathbf{k}} \left(\hat{a}_{\mathbf{q}\nu} + \hat{a}_{-\mathbf{q}\nu}^\dagger \right) , \quad (1.27)$$

with the electron-phonon matrix element

$$g_{mn\nu}(\mathbf{k}, \mathbf{q}) = \int_{\text{UC}} d\mathbf{r} u_{m\mathbf{k} + \mathbf{q}}^*(\mathbf{r}) \Delta_{\mathbf{q}\nu} U(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) . \quad (1.28)$$

Figure 1.1 visualizes the two interaction terms. Their interpretation is pretty straightforward: The ionic motion breaks the discrete translational symmetry of the lattice such that an electronic Bloch state is no longer an eigenstate of the Hamiltonian. An electron in state $|n\mathbf{k}\rangle$ can therefore be scattered into a new state $|m\mathbf{k} + \mathbf{q} + \mathbf{G}_\mathbf{m}\rangle$ by either absorbing or emitting a phonon in state $|\mathbf{q}\nu\rangle$ or $|-\mathbf{q}\nu\rangle$, respectively. Both processes occur with probability amplitude $g_{mn\nu}(\mathbf{k}, \mathbf{q})$ and conserve crystal momentum. Note that $\mathbf{k} + \mathbf{q} + \mathbf{G}_\mathbf{m}$ is a valid Bloch wave

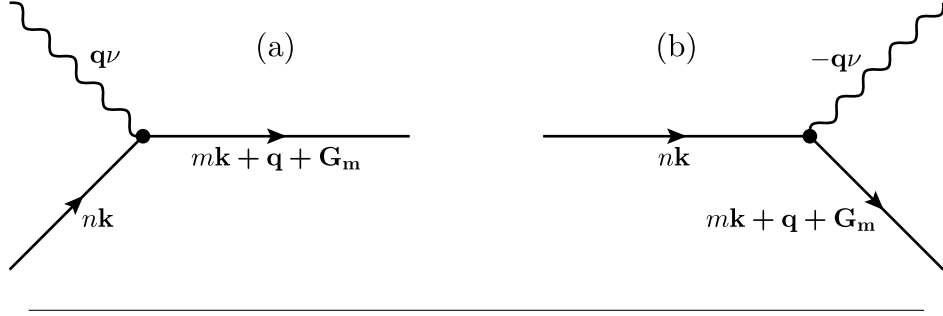


FIGURE 1.1: Feynman diagrams visualizing linear electron-phonon coupling. An electron is scattered from state $|n\mathbf{k}\rangle$ to $|m\mathbf{k} + \mathbf{q} + \mathbf{G}_m\rangle$ by either (a) absorbing a phonon in state $|\mathbf{q}\nu\rangle$ or (b) emitting a phonon in state $|-\mathbf{q}\nu\rangle$.

vector, whereas $\mathbf{k} + \mathbf{q}$ might not be, i.e. for a given $\mathbf{k}$ and $\mathbf{q}$ in Eq. 1.7, the sum over reciprocal lattice vectors only contributes one term to the Hamiltonian. Often this sum is not written explicitly and we will do the same from now on.

The full Hamiltonian of the electron-phonon system is given as

$$\hat{H}_{\text{pol}} = \sum_{n\mathbf{k}} \varepsilon_{n\mathbf{k}} \hat{c}_{n\mathbf{k}}^\dagger \hat{c}_{n\mathbf{k}} + \sum_{\mathbf{q}\nu} \hbar\omega_{\mathbf{q}\nu} \hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu} + \frac{1}{\sqrt{N}} \sum_{\substack{\mathbf{k}\mathbf{q} \\ m\nu}} g_{m\nu}(\mathbf{k}, \mathbf{q}) \hat{c}_{m\mathbf{k}+\mathbf{q}}^\dagger \hat{c}_{n\mathbf{k}} \left(\hat{a}_{\mathbf{q}\nu} + \hat{a}_{-\mathbf{q}\nu}^\dagger \right), \quad (1.29)$$

where we have ignored the zero-point energy of the lattice. $\hat{H}_{\text{pol}}$ is completely characterized by the electronic band structure $\varepsilon_{n\mathbf{k}}$, the phonon frequencies $\omega_{\mathbf{q}\nu}$ and the electron-phonon matrix elements $g_{m\nu}(\mathbf{k}, \mathbf{q})$. All three of these quantities can be readily calculated from first principles with modern DFT software packages [24, 25]. In fact, Reference [20] shows how Eq. 1.29 might be derived from the Kohn-Sham Hamiltonian and thus put into direct relation with DFT-accessible quantities. However, solving the Schrödinger equation for the polaron Hamiltonian requires sophisticated analytical or computational methods, which either fail to or cannot efficiently incorporate the complicated numerical data from ab initio calculations. Even though there have been recent advances towards a general treatment of Eq. 1.29 for real materials [26–29], the standard way of dealing with this difficulty is to use effective model Hamiltonians, in which $\varepsilon_{n\mathbf{k}}$, $\omega_{\mathbf{q}\nu}$ and $g_{m\nu}(\mathbf{k}, \mathbf{q})$ are derived from phenomenological arguments and take on simple analytic forms.

In this thesis, we use the latter approach and study different effective polaron models with the diagrammatic Monte Carlo (DiagMC) technique. Furthermore, we will restrict our calculations to the single polaron or low density limit of Eq. 1.29, i.e. to a system consisting of a single electron interacting with a bath of phonons. This simplifies the diagrammatic expansion and allows us to study in detail how $\hat{H}_{\text{el-ph}}$ changes various properties compared to the bare particle. Physically, such situation is realized in materials with low charge carrier densities, for example in

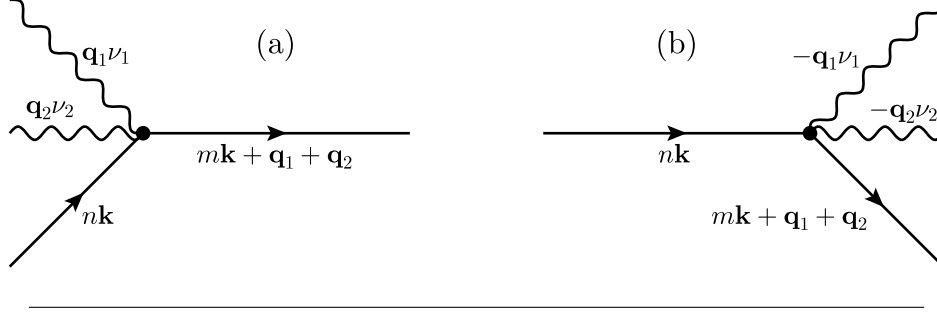


FIGURE 1.2: Feynman diagrams visualizing quadratic electron-phonon coupling. An electron is scattered from state $|\mathbf{n}\mathbf{k}\rangle$ to $|\mathbf{m}\mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2\rangle$ by either (a) absorbing two phonons in states $|\mathbf{q}_1\nu_1\rangle$ and $|\mathbf{q}_2\nu_2\rangle$ or (b) emitting two phonons in states $|\mathbf{-q}_1\nu_1\rangle$ and $|\mathbf{-q}_2\nu_2\rangle$. The remaining two processes, where one phonon is absorbed and the other emitted, are not depicted.

an insulator with an additional electron in the conduction band [30].

As a final remark, let us note a slight inconsistency in the derivation of $\hat{H}_{\text{el-ph}}$. While the electron-ion potential is only expanded up to the first order in the atomic displacements (Eq. 1.21), the total potential of the ions is expanded up to second order (Eq. 1.16). If the arguments for the truncation of the expansions are based on the smallness of $u_{\mathbf{n}\kappa i}$, why not also include the quadratic term into the interaction Hamiltonian? On paper, this can be done without any problems. The quadratic electron-phonon coupling term has the general form [20]

$$\hat{H}_{\text{el-ph}}^{(2)} = \frac{1}{N} \sum_{\substack{\mathbf{k}, \mathbf{q}_1, \mathbf{q}_2 \\ m, n, \nu_1, \nu_2}} g_{mn\nu_1\nu_2}^{(2)}(\mathbf{k}, \mathbf{q}_1, \mathbf{q}_2) \hat{c}_{m\mathbf{k}+\mathbf{q}_1+\mathbf{q}_2}^\dagger \hat{c}_{n\mathbf{k}} \left(\hat{a}_{\mathbf{q}_1\nu_1} + \hat{a}_{-\mathbf{q}_1\nu_1}^\dagger \right) \left(\hat{a}_{\mathbf{q}_2\nu_2} + \hat{a}_{-\mathbf{q}_2\nu_2}^\dagger \right), \quad (1.30)$$

with the electron-phonon-phonon matrix element

$$g_{mn\nu_1\nu_2}^{(2)}(\mathbf{k}, \mathbf{q}_1, \mathbf{q}_2) = \frac{1}{2} \int_{\text{UC}} d\mathbf{r} u_{m\mathbf{k}+\mathbf{q}_1+\mathbf{q}_2}^*(\mathbf{r}) \Delta_{\mathbf{q}_1\nu_1} \Delta_{\mathbf{q}_2\nu_2} U(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}), \quad (1.31)$$

where the variations $\Delta_{\mathbf{q}\nu}$ have been defined in Eq. 1.23. $\hat{H}_{\text{el-ph}}^{(2)}$ leads to two phonon processes, which are illustrated in Fig. 1.2. Their interpretation is the same as for linear coupling. Unfortunately, calculations with quadratic interactions become much more involved and they are usually restricted to smallest order in perturbation theory. In Chapter 6, we will come back to this problem to show how the DiagMC algorithm for linear coupling can be extended to include $\hat{H}_{\text{el-ph}}^{(2)}$ and to investigate its effects on a particle.

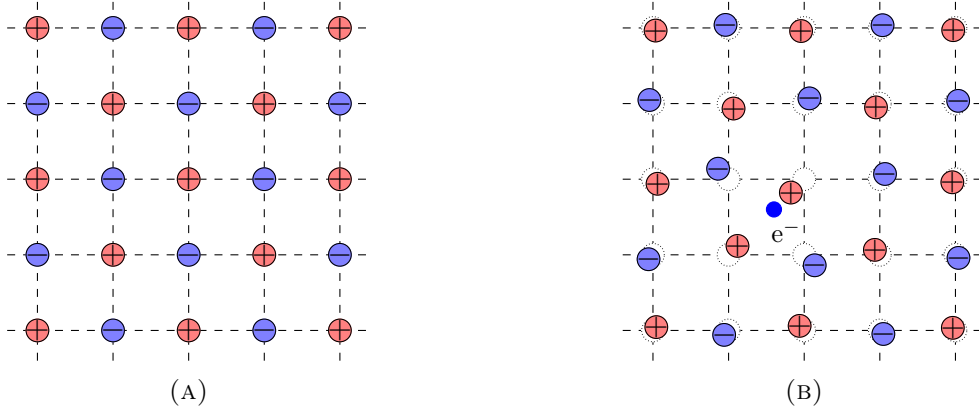


FIGURE 1.3: Artistic illustration of a polaron in an ionic crystal. (A) Ideal ionic crystal with all ions residing in their equilibrium positions. (B) An additional electron induces a lattice distortion. The positively charged ions are attracted to the additional electron while the negatively charged ions are repelled.

1.2 Polaron models

Polaron theory has its origins in the 1930s, when Lev Landau published a short paper on the possible self-trapping of an electron in a (strongly) distorted lattice [31]. Subsequently, Pekar performed quantitative, semiclassical calculations in which he considered a single electron interacting with a dielectric continuous medium. The situation is illustrated in Fig. 1.3, except that the dielectric continuum has been exchanged for an ionic crystal: When an electron is placed inside an otherwise undistorted lattice, it will attract positive and repel negative charges in its neighborhood. This creates a polarization around the electron, which in turn acts on the charge carrier and can so influence its energetics and dynamics. As the electron moves through the crystal, the polarization surrounding it follows along. The electron together with the induced lattice distortion can then be viewed as a single entity, for which Pekar coined the term *polaron* [32].

The first fully microscopic model of a polaron was formulated by Fröhlich, Pelzer and Zienau in the 1950s [33]. They quantized the classical polarization field of Pekar and derived an electron-phonon Hamiltonian in the form of Eq. 1.29. The Fröhlich model describes the long-range, polar interaction of an electron in a parabolic band with a longitudinal, optical phonon branch of constant frequency, i.e. $\varepsilon_{\mathbf{k}} \propto k^2$, $\omega_{\mathbf{q}} = \omega_{\text{LO}}$ and $g(\mathbf{q}) \propto \sqrt{\alpha} q^{-1}$. The strength of the electron-phonon coupling is determined by α , a dimensionless, material dependent quantity and the only important parameter of the Fröhlich model:

$$\alpha = \frac{1}{2\hbar\omega_{\text{LO}}} \frac{e^2}{4\pi\varepsilon_0} \sqrt{\frac{2m\omega_{\text{LO}}}{\hbar}} \left(\frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon} \right). \quad (1.32)$$

Here, m is the electron band mass, ε_0 is the vacuum permittivity and ε and ε_∞ are the static and high-frequency dielectric constants, respectively. A detailed derivation of the Hamiltonian can be found in Ref. [34].

The Fröhlich model is based on the *continuum approximation*, where the discrete crystal lattice is replaced with a continuous medium. In doing so, it assumes that the polaron wave function and the corresponding lattice distortions spread over multiple lattice sites, the defining feature of a *large* or *continuum polaron* [35]. On the other hand, if the size of the polaron is of the order of the lattice parameter $a = \sqrt[3]{V_{UC}}$, the crystal structure becomes important and has to be accounted for in the model. This leads to so-called *small* or *lattice polaron* theories. The oldest and most studied small polaron Hamiltonian is due to Holstein [36]. It describes a short-range (local) interaction of an electron in a tight-binding band with an optical phonon branch of constant frequency, i.e. $\varepsilon_{\mathbf{k}} = -2t \sum_{i=1}^D \cos(k_i a)$, $\omega_{\mathbf{q}} = \omega_{LO}$ and $g(\mathbf{q}) = g$. Here, t is the nearest-neighbor hopping amplitude and we assumed a hypercubic crystal structure. The two important parameters of the Holstein model are the ratio ω_{LO}/t and the electron-phonon coupling strength g , which is usually replaced with the dimensionless quantity $\lambda = g^2/(2tD\hbar\omega_{LO})$. Let us remark that Holstein based his original derivation of the Hamiltonian on a molecular crystal model, where at each lattice site resides a polar molecule with which the electron interacts locally [37].

In materials with covalent bonds between the atoms, e.g. non-polar semiconductors or metals, another type of electron-phonon interaction is expected to be dominant: the short-range coupling of acoustic phonons to the deformation potential [38, 39]. Similar to the Fröhlich polaron, this interaction is usually modelled in the continuum approximation, where $\varepsilon_{\mathbf{k}} \propto k^2$, $\omega_{\mathbf{q}} \propto sq$ and $V(\mathbf{q}) \propto \sqrt{\alpha q}$. The parameter α is again responsible for the coupling strength but now depends on the deformation potential constant D , the mass density ρ of the crystal and the sound velocity s of the longitudinal, acoustic phonon branch [40]:

$$\alpha = \frac{D^2 m^2}{8\pi \rho \hbar^3 s}. \quad (1.33)$$

Besides α , another important parameter, k_0 , has to be introduced to function as a wave vector cutoff in reciprocal space. It is naturally taken to be $k_0 \sim 1/a$, with a the lattice constant, and should mimic the discreteness of the lattice. This is in contrast to the Fröhlich Hamiltonian, in which all involved integrals converge for $k_0 \rightarrow \infty$ and no cutoff is necessary. Throughout the rest of the thesis, we will refer to this model as the acoustic continuum polaron.

Another noteworthy polaron theory is due to Su, Schrieffer and Heeger [41].

Their SSH model was derived to study soliton formation in polyacetylene and uses an EPI mechanism, where the ionic motion couples to the electron hopping instead of the electron density. This leads to $\mathbf{k}$ - and $\mathbf{q}$ -dependent electron-phonon matrix elements and to polaron properties quite different from the other models [42].

Over the years, the concept of polarons has been further generalized and applied to a wide variety of other physical systems. Examples include BEC-impurity polarons [43], exciton polarons [44], spin or magnetic polarons [45], ripplonic polarons [46], Fermi polarons [47] and the more “exotic” angulons [48], where the rotational (instead of the translational) degrees of freedom of a quantum impurity couple to a bosonic bath. They all describe the interaction of a particle with its environment and share the general form of the Hamiltonian from Eq. 1.29. Because of the ubiquity of polaron theory in condensed matter and other branches of physics, it is of major interest to have reliable and accurate numerical methods that are able to calculate various polaron properties for different models.

The list of numerical methods, which have been applied to at least some kind of polaron problem, is long and keeps extending to this day. A summary of the most important and successful techniques can be found in Ref. [22]. Many of those approaches are either based on approximations, e.g. variational methods, or they only have a limited range of applicability, e.g. weak- or strong coupling perturbation theory. In the former case, it is often difficult to distinguish between real, physical behavior and artifacts originating from the applied approximation, while in the latter case, it might not be clear in what parameter region the results are actually valid. It is therefore important to have techniques available, which are capable of producing accurate benchmarks. Ideally, they should be approximation-free and valid for all interesting parameter ranges. The diagrammatic Monte Carlo method is one of them.

DiagMC uses a stochastic sampling technique based on the Metropolis-Hastings algorithm to calculate quantities expressed as an infinite series of Feynman diagrams. It was first applied to the Fröhlich polaron problem by Nikolai Prokof'ev and Boris Svistunov in 1998 [49]. They computed the one-electron Green's function in imaginary time and extracted the GS energy and quasiparticle weight from its asymptotic, long- τ behavior. Since then, DiagMC has been extended and improved to obtain other polaron GS properties like effective mass, group velocity or phonon distribution functions. In combination with a numerical analytic continuation (NAC) method, e.g. stochastic optimization with consistent constraints (SOCC) [50], it is also possible to calculate quantities like the Lehmann spectral function (LSF), optical conductivity (OC) or the mobility of polarons. So far,

DiagMC together with NAC has been applied to a wide variety of polaron models including the Fröhlich model [50–53], Holstein model [54–56], Rashba-Pekar model [57], t - J model [58–60], $tt't''$ - J model [61, 62], acoustic continuum model [63] or the SSH model [42, 64]. Because of the approximation-free nature of the DiagMC algorithm, some of these results have been used as benchmarks for other numerical methods [28, 29, 42, 53–55, 65] or to clarify misinterpretations of non-physical artifacts due to previous approximate calculations [51, 63].

1.3 Outline

The present thesis aims to further increase our understanding of polarons by studying the effects of different electron-phonon interaction mechanisms using DiagMC and SOCC. To be more specific, we calculate accurate energy dispersion relations for the Fröhlich polaron in two (2D) and three dimensions (3D), we perform a detailed study of a novel acoustic lattice polaron model and we investigate the effects of quadratic electron-phonon coupling using a simple model Hamiltonian.

The outline of the rest of this work is as follows:

- Chapter 2 introduces the DiagMC and SOCC algorithms from a general point of view without any references to polaron Hamiltonians or many-body physics.
- Chapter 3 reviews the theory of many-body Green’s functions and Feynman diagrams, before discussing and reviewing DiagMC implementations for linear polaron Hamiltonians.
- Chapter 4 presents novel results for the Fröhlich polaron problem. First our DiagMC code is benchmarked against data obtained with another DiagMC implementation, then it is used to study energy dispersion relations in 2D and 3D.
- Chapter 5 introduces the acoustic lattice polaron model and shows results for GS properties, OC and LSFs. Emphasis is placed on the crossover region from the weak- to the strong-coupling regime and on the comparison with other model systems.
- Chapter 6 investigates the effects of quadratic EPIs by studying a simple Hamiltonian similar to the linear Holstein model with DiagMC and another MC technique based on a path integral formulation [66].

- Chapter 7 summarizes the work done in the current thesis and gives a short outlook for possible follow-up projects.

In addition to the work described above, the author has implemented two major scientific software libraries: (i) a generic Monte Carlo (MC) library that forms the basis for all MC simulations performed as part of this thesis, and (ii) a flexible DiagMC code for the general polaron Hamiltonian from Eq. 1.29. Even though the development of these two software projects has occupied a significant part of the author's PhD program, they are not part of the current dissertation. Instead, they will be released as open-source libraries in the near future or, if necessary, access can be granted upon request.

Chapter 2

Methodology

A lot of interesting phenomena in condensed matter physics occur because of the interactions and correlations between particles. Examples include high-temperature superconductivity [3], metal-insulator transitions [67], the fractional quantum Hall effect [68] or, most relevant to the current work, polaron formation in materials [22]. Understanding such systems requires the study of quantum many-body problems which are inherently difficult to solve and rely on sophisticated numerical techniques often based in quantum field theory. A direct solution of the corresponding Schrödinger equation is all but impossible, even for the simplest model systems. Instead, the calculation of many-body Green's functions is usually more practical. Their advantage is that they contain most of the relevant physical information of the system and, by treating the interaction between particles as a perturbation, can be written as an infinite series of Feynman diagrams (for more details see Ch. 3). Although the summation of such a diagrammatic series is not any easier than solving the original Schrödinger equation, it allows us to make use of diagrammatic Monte Carlo [49] methods which deal with the complicated series by sampling individual terms (Feynman diagrams) in a stochastic fashion. The calculated Green's function usually does not directly correspond to a physical observable quantity but is related to one via an integral equation, e.g. the imaginary time single-particle Green's function, $G_{n\mathbf{k}}(\tau)$, at zero temperature is related to its spectral function, $A_{n\mathbf{k}}(\omega)$, via

$$G_{n\mathbf{k}}(\tau) = \int_0^\infty d\omega A_{n\mathbf{k}}(\omega) e^{-\omega\tau} . \quad (2.1)$$

Here, $|n\mathbf{k}\rangle$ is a single-particle state and the quantum numbers, n and $\mathbf{k}$, refer to the particle's band and wave vector, respectively. To retrieve the physical relevant quantity, $A_{n\mathbf{k}}(\omega)$ in case of Eq. 2.1, we have to perform numerical analytic continuation [50].

This chapter introduces the two main numerical approaches used throughout the thesis: (i) diagrammatic Monte Carlo and (ii) stochastic optimization with consistent constraints analytic continuation. We start with a general review of Monte

Carlo (MC) methods in Sec. 2.1, including Markov chain Monte Carlo (MCMC) sampling with emphasis on the Metropolis-Hastings algorithm and basic error analysis. Section 2.2 explains the general idea behind diagrammatic Monte Carlo from a mathematical point of view without any reference to many-body physics or Green's functions. Using a simple toy example, we show how the previously introduced concepts work in practice and highlight the differences between “traditional” and diagrammatic MC. The final part of this chapter, Sec. 2.3, is dedicated to numerical analytic continuation, especially to SOCC.

2.1 Monte Carlo method

For the most part of this introductory section, we follow closely the excellent book by Gubernatis *et al.* [69] and the doctoral thesis of Marchand [70].

The first mention of the name “Monte Carlo method” can be found in a paper by Metropolis and Ulam from 1949 [71], in which they describe a general statistical approach to study integro-differential equations occurring in natural sciences.

A probably more familiar use case of MC comes from classical statistical mechanics. In 1953, Metropolis *et al.* [72] calculated thermodynamic properties of a system consisting of N interacting molecules. They were faced with the well-known problem of solving high-dimensional integrals of the form (in case of a canonical ensemble):

$$\langle F \rangle = \frac{\int_{\Gamma} d\mathbf{p} d\mathbf{q} F(\mathbf{p}, \mathbf{q}) e^{-E(\mathbf{p}, \mathbf{q})/(k_B T)}}{\int_{\Gamma} d\mathbf{p} d\mathbf{q} e^{-E(\mathbf{p}, \mathbf{q})/(k_B T)}} , \quad (2.2)$$

where F is the quantity of interest, Γ is the integration volume, $\mathbf{p}$ and $\mathbf{q}$ are the momenta and positions of the N particles, T is the temperature, k_B is the Boltzmann constant and $E(\mathbf{p}, \mathbf{q})$ is the energy corresponding to a certain state of the system specified by a point in phase space.

In order to obtain the thermodynamic average $\langle F \rangle$, one has to solve the $2DN$ -dimensional integrals, D being the number of dimensions. For many particles and non-trivial interactions, this quickly becomes an impossible task to do analytically. Deterministic numerical integration techniques are also not an option, since they suffer from the *curse of dimensionality*, referring to the fact that the number of function evaluations needed for such methods grows exponentially with the number of dimensions, i.e. as M^D , where M is the number of discrete points used in one dimension.

To overcome this issue, Metropolis *et al.* approached the problem stochastically. Instead of integrating over a regular grid in phase space, they generated points $(\mathbf{p}_i, \mathbf{q}_i)$ randomly from some probability distribution $p(\mathbf{p}, \mathbf{q})$. The numerator of

Eq. 2.2 (similar considerations apply to the denominator) can then be rewritten as:

$$\begin{aligned} \int_{\Gamma} d\mathbf{p} d\mathbf{q} F(\mathbf{p}, \mathbf{q}) e^{-E(\mathbf{p}, \mathbf{q})\beta} &= \int_{\Gamma} d\mathbf{p} d\mathbf{q} \frac{F(\mathbf{p}, \mathbf{q})}{p(\mathbf{p}, \mathbf{q})} e^{-\beta E(\mathbf{p}, \mathbf{q})} p(\mathbf{p}, \mathbf{q}) \\ &= \left\langle \frac{F(\mathbf{p}, \mathbf{q})}{p(\mathbf{p}, \mathbf{q})} e^{-\beta E(\mathbf{p}, \mathbf{q})} \right\rangle_p \\ &\approx \frac{1}{M} \sum_{i=1}^M \frac{F(\mathbf{p}_i, \mathbf{q}_i)}{p(\mathbf{p}_i, \mathbf{q}_i)} e^{-\beta E(\mathbf{p}_i, \mathbf{q}_i)}. \end{aligned} \quad (2.3)$$

Here we have introduced the common notation $\beta = 1/(k_B T)$ for the inverse temperature and $\langle \dots \rangle_p$ for an expectation value with respect to the probability distribution p . The last line in Eq. 2.3 employs the usual approximation of an expectation value with its arithmetic mean, where the M individual phase space samples $(\mathbf{p}_i, \mathbf{q}_i)$ are distributed according to $p(\mathbf{p}, \mathbf{q})$. As will be shown later in this section, the error of the approximation in Eq. 2.3 scales as $\mathcal{O}(M^{-1/2})$, i.e. it is independent of the dimensionality and only depends on the number of samples taken into account (see Eq. 2.29). The efficiency of this approach is determined by the choice of $p(\mathbf{p}, \mathbf{q})$.

Naively, one could simply use a uniform distribution defined on the phase space volume: $p(\mathbf{p}, \mathbf{q}) = \Gamma^{-1}$. In most cases, this would generate a large number of states with high energies or very small Boltzmann factors $\exp\{-\beta E(\mathbf{p}_i, \mathbf{q}_i)\}$, which only have a negligible contribution to the integral.

A much more efficient way is to sample directly the Boltzmann distribution. Let us define

$$p_B(\mathbf{p}, \mathbf{q}) = \frac{e^{-\beta E(\mathbf{p}, \mathbf{q})}}{\int_{\Gamma} d\mathbf{p} d\mathbf{q} e^{-\beta E(\mathbf{p}, \mathbf{q})}} = \frac{e^{-\beta E(\mathbf{p}, \mathbf{q})}}{\mathcal{Z}}, \quad (2.4)$$

where we have introduced the partition function $\mathcal{Z}$. Equation 2.2 now becomes

$$\langle F \rangle = \int_{\Gamma} d\mathbf{p} d\mathbf{q} F(\mathbf{p}, \mathbf{q}) p_B(\mathbf{p}, \mathbf{q}) = \langle F(\mathbf{p}, \mathbf{q}) \rangle_{p_B} \approx \frac{1}{M} \sum_{i=1}^M F(\mathbf{p}_i, \mathbf{q}_i), \quad (2.5)$$

with $(\mathbf{p}_i, \mathbf{q}_i) \sim p_B(\mathbf{p}, \mathbf{q})$. The difficulty of the original problem is thus shifted to the generation of random samples $(\mathbf{p}_i, \mathbf{q}_i)$ from the Boltzmann distribution.

Metropolis *et al.* already proposed a simple procedure on how to achieve this in their original publication [72], which would later be known as the famous *Metropolis* algorithm. In 1970, Hastings generalized the method, leading to the *Metropolis-Hastings* algorithm [73]. We will provide the details in Sec. 2.1.2.

Ever since then, the Monte Carlo method has been further developed, specialized and optimized. It has established itself as an indispensable tool in all fields of physics, mathematics, chemistry and various other branches of science. Nowadays, the term *Monte Carlo method* comprises a huge class of stochastic algorithms and

numerical techniques. Their main purpose is to provide solutions to problems for which deterministic methods fail or which are inherently stochastic by nature.

The rest of this section focuses on the necessary background knowledge needed to understand how MC methods work and how to implement them. This includes some general remarks about MC (Sec. 2.1.1), MCMC algorithms (Sec. 2.1.2) and basic error analysis (Sec. 2.1.3).

2.1.1 General remarks about MC

Let us start by generalizing the notation from the previous section: Suppose we are interested in the ensemble average of some quantity $X(C)$. Each possible state of the system is represented by a specific configuration $C = (x_1, \dots, x_N) \in \mathcal{C}$ and has an associated weight factor $\mathcal{W}(C)$. The average or expectation value of $X(C)$ can then be written as a weighted sum over all configurations

$$\langle X \rangle = \mathbb{E}(X) = \frac{\sum_C X(C) \mathcal{W}(C)}{\sum_C \mathcal{W}(C)} = \frac{\sum_C X(C) \mathcal{W}(C)}{\mathcal{Z}}, \quad (2.6)$$

where $\mathcal{Z}$ is the partition function or, more generally, the normalization of the weights. Depending on the nature of x_i , the sum over C includes integrals over continuous ($\int dx_i$) and summations over discrete ($\sum_{x_i}$) variables. The configuration space $\mathcal{C}$ is simply the set of all possible configurations and does not necessarily have any particular mathematical structure associated with it.

To make a connection to Eq. 2.2 from the previous section, consider the following transformations: $X(C) \rightarrow F(\mathbf{p}, \mathbf{q})$, $C = (x_1, \dots, x_N) \rightarrow (\mathbf{p}, \mathbf{q})$, $\mathcal{W}(C) \rightarrow e^{-E(\mathbf{p}, \mathbf{q})/(k_B T)}$ and $\sum_C \rightarrow \int_{\Gamma} d\mathbf{p} d\mathbf{q}$.

There it has already been established that the MC method is especially suited to evaluate complicated expectation values such as Eq. 2.6. The general idea is to interpret the normalized weights

$$p(C) = \frac{\mathcal{W}(C)}{\mathcal{Z}} \quad (2.7)$$

as probabilities (or a probability density) and approximate the exact average $\langle X \rangle$ with its so-called sample mean $\bar{X}$ by generating random configurations C_i from $p(C)$:

$$\langle X \rangle = \langle X \rangle_p = \sum_C X(C) p(C) \approx \frac{1}{M} \sum_{i=1}^M X(C_i) = \bar{X}. \quad (2.8)$$

This is only valid, as long as the normalized weights represent proper probabilities, i.e. if

$$\mathcal{W}(C) \in \mathbb{R} \wedge 0 \leq \mathcal{W}(C) < \infty \quad \forall C \in \mathcal{C}. \quad (2.9)$$

For the more general case, when $\mathcal{W}(C) < 0$ or $\mathcal{W}(C) \in \mathbb{C}$ for some $C \in \mathcal{C}$, Eq. 2.6 needs to be rewritten as

$$\langle X \rangle = \frac{\sum_C X(C) e^{i\phi(C)} |\mathcal{W}(C)|}{\sum_C |\mathcal{W}(C)|} \frac{\sum_C |\mathcal{W}(C)|}{\sum_C e^{i\phi(C)} |\mathcal{W}(C)|} . \quad (2.10)$$

Here, we have first factorized the complex weight $\mathcal{W}(C)$ into its modulus $|\mathcal{W}(C)|$ and its phase factor $\exp\{i\phi(C)\}$ and then introduced the new normalization $\mathcal{Z}_c = \sum_C |\mathcal{W}(C)|$. If the weights are known to be real, the complex phase may be replaced with the sign function $\text{sgn}\{\mathcal{W}(C)\}$. With these modifications, it is again possible to use the probability interpretation for

$$p_c(C) = \frac{|\mathcal{W}(C)|}{\mathcal{Z}_c} \quad (2.11)$$

and to approximate the exact averages in Eq. 2.10 with their sample means

$$\langle X \rangle = \frac{\langle X e^{i\phi(C)} \rangle_{p_c}}{\langle e^{i\phi(C)} \rangle_{p_c}} \approx \frac{\sum_{i=1}^M X(C_i) e^{i\phi(C_i)}}{\sum_{i=1}^M e^{i\phi(C_i)}} = \bar{X} . \quad (2.12)$$

Note that due to the linear property of expectation values, one can choose to measure the real and imaginary parts of a complex quantity separately, e.g.

$$\langle e^{i\phi(C)} \rangle_{p_c} = \langle \cos \phi(C) \rangle_{p_c} + i \langle \sin \phi(C) \rangle_{p_c} . \quad (2.13)$$

Although Eq. 2.12 enables us to use the MC method to evaluate $\langle X \rangle$ for complex (negative) weights, there is still a price we have to pay. If the average phase (sign) in the denominator goes to zero, the statistical error of the MC approximation will be much larger than its mean and it becomes practically impossible to get a meaningful result for $\langle X \rangle$ from Eq. 2.12. This is the famous *sign problem* plaguing many quantum Monte Carlo algorithms, especially those dealing with interacting fermions. Since we will mostly avoid such difficulty in the rest of the thesis, we refer the interested reader to Ref. [74] and assume from now on that the weights for all configurations satisfy $0 \leq \mathcal{W}(C) < \infty$, unless otherwise stated.

2.1.2 Markov chain Monte Carlo

As was already mentioned in the introductory part of this section, the most efficient way to evaluate Eq. 2.6 with a MC procedure is to generate configurations C according to their weight $\mathcal{W}(C)$ and approximate the expectation value with its sample mean. This simply implies that configurations with a larger weight are more likely to be sampled and therefore more likely to contribute to the right hand

sum in Eq. 2.8. The difficult part is the sampling of the non-trivial distribution $p(C)$.

MCMC methods provide a solution to this problem by constructing a Markov chain on the configuration space $\mathcal{C}$ with $p(C)$ as its stationary distribution. That means after reaching equilibrium, it will generate a sequence of configurations

$$C_0 \rightarrow C_1 \rightarrow C_2 \rightarrow \dots C_n \rightarrow C_{n+1} \rightarrow \dots , \quad (2.14)$$

where each C_i represents a random sample $\sim p(C)$.

A (time-homogeneous) Markov chain is defined by some arbitrary initial distribution $p^{(0)}(C)$ and transition probabilities $P(C'|C)$ from state C to C' . The transition probabilities are required to be normalized

$$\sum_{C'} P(C'|C) = 1 , \quad (2.15)$$

and they are used to construct the chain recursively [69]:

$$p^{(k+1)}(C') = \sum_C P(C'|C) p^{(k)}(C) . \quad (2.16)$$

Intuitively, the stationary distribution should satisfy

$$p(C') = \sum_C P(C'|C) p(C) . \quad (2.17)$$

We can derive this condition by considering the following master equation [75]

$$p^{(k+1)}(C) - p^{(k)}(C) = \sum_{C'} P(C|C') p^{(k)}(C') - \sum_{C'} P(C'|C) p^{(k)}(C) . \quad (2.18)$$

It describes the change in probability between two consecutive time steps, where the first and second term on the right-hand side represents the flow of probability into and out of state C , respectively. If we require that the stationary distribution does not change with time, i.e. $p^{(k+1)}(C) = p^{(k)}(C) = p(C)$, and if we use the normalization from Eq. 2.15, the master equation becomes

$$\sum_{C'} P(C|C') p(C') = \sum_{C'} P(C'|C) p(C) = p(C) , \quad (2.19)$$

which is equal to Eq. 2.17.

The following conditions are sufficient for the Markov chain to asymptotically converge to its stationary distribution $p(C)$ [76]:

- *Global balance*: If Eq. 2.19 is satisfied by $p(C)$ and $P(C|C')$ for all C , then the Markov chain is said to have global balance.
- *Ergodicity*: Any configuration C has to be reachable from any other configuration C' in a finite number of Markov steps.

It is common, but not necessary, to impose an even stronger condition on the transition probabilities such that Eq. 2.19 is automatically satisfied:

$$P(C|C')p(C') = P(C'|C)p(C) \quad \forall C, C' \in \mathcal{C}. \quad (2.20)$$

These are called *detailed balance* equations and they state that the probability flow from configuration C into C' and vice versa is balanced for all pairs $C, C' \in \mathcal{C}$.

Our task now is to find transition probabilities $P(C'|C)$ which obey the system of equations in Eq. 2.19 or Eq. 2.20 for a given (desired) target distribution $p(C)$. MCMC methods provide us with different solutions to this problem. Here, we will only focus on the one developed by Metropolis *et al.* [72] and Hastings [73].

The Metropolis-Hastings algorithm fulfills detailed balance and is based on the simple idea to split the transition probability $P(C'|C)$ into a proposal $T(C'|C)$ and an acceptance $A(C'|C)$ probability:

$$P(C'|C) = T(C'|C)A(C'|C). \quad (2.21)$$

For the proposal distribution we require $T(C'|C) \geq 0$ and $\sum_{C'} T(C'|C) = 1$ to hold. Plugging Eq. 2.21 into Eq. 2.20 yields the modified detailed balance equation

$$\frac{A(C|C')}{A(C'|C)} = \frac{T(C'|C)p(C)}{T(C|C')p(C')}. \quad (2.22)$$

Furthermore, the Metropolis-Hastings algorithm proposes the following acceptance probabilities:

$$A(C|C') = \min \left\{ 1, \frac{T(C'|C)p(C)}{T(C|C')p(C')} \right\}. \quad (2.23)$$

One can check that this choice satisfies Eq. 2.22.

In practice, the algorithm works as follows: Suppose the current configuration is C' . Use $T(C|C')$ to propose a new state C and calculate the acceptance probability $A(C|C')$ from Eq. 2.23. Accept the new configuration C with probability $A(C|C')$, otherwise stay in C' . Figure 2.1 depicts the pseudo-code of these steps [69].

A great advantage of the Metropolis-Hastings algorithm is that the normalization of the target distribution $p(C)$ does not need to be known, as can be seen from Eq. 2.23. However, it is advisable to be careful, when working with unnormalized

Input : Current configuration C_i
Target distribution $p(C)$
Proposal distribution $T(C|C_i)$

Output: New configuration C_{i+1}

Propose a new C from $T(C|C_i)$;
Calculate acceptance probability $R = A(C|C_i)$ using Eq. 2.23;
Generate a uniform random number $r \in [0, 1]$;
if $r \leq R$ **then**
| $C_{i+1} \leftarrow C$;
else
| $C_{i+1} \leftarrow C_i$;
end
return C_{i+1} ;

FIGURE 2.1: Metropolis-Hastings algorithm.

weights: Suppose one is interested in the weighted sum

$$S_X = \sum_C X(C) \mathcal{W}(C) , \quad (2.24)$$

for which $\mathcal{Z} = \sum_C \mathcal{W}(C) \neq 1$. Since $\mathcal{Z}$ is not needed for the Metropolis-Hastings algorithm, it is tempting to use the same MC strategy as if the weights were properly normalized. But this produces the maybe at first unexpected result $S_X/\mathcal{Z}$, instead of S_X . In Sec. 2.2, it will be shown how we can estimate $\mathcal{Z}$ and hence also S_X , regardless of the presence of $\mathcal{Z}$ in Eq. 2.24.

2.1.3 Error analysis in MC

Equipped with Eqs. 2.6–2.8 and the Metropolis-Hastings algorithm to efficiently sample $p(C)$, we are now in a position to perform actual calculations and obtain reasonable results for the ensemble average $\langle X \rangle$ of some observable $X(C)$. Due to the stochastic nature of the MC method, the approximation $\bar{X}$ will always have an associated statistical error. It is important to understand the origin of such error, its magnitude and how to confidently estimate it in applications. The rest of this section therefore tries to give a short overview of the most important concepts concerning error analysis in MC simulations.

In Sec. 2.1.1, we defined a specific configuration in terms of x_i . From a statistics point of view, each x_i represents a random variable such that $C = (x_1, \dots, x_N)$ and any other function of C , like $X(C)$, are themselves random variables. Knowing that the configurations are distributed according to $p(C)$, we can define the expectation

value of $X(C)$ as

$$\langle X \rangle = \sum_C X(C) p(C) \quad (2.25)$$

and its variance as

$$\text{Var}(X) = \sigma_X^2 = \langle (X - \langle X \rangle)^2 \rangle = \sum_C (X(C) - \langle X \rangle)^2 p(C) . \quad (2.26)$$

Typically, the standard deviation, $\sigma_X = \sqrt{\sigma_X^2}$, is used for reporting error bars, rather than the variance itself.

As already discussed previously, an unbiased estimator for the expectation value is given by the sample mean

$$\bar{X} = \frac{1}{M} \sum_{i=1}^M X(C_i) . \quad (2.27)$$

The variance, on the other hand, can be estimated with the sample variance

$$s_X^2 = \frac{1}{M-1} \sum_{i=1}^M (X(C_i) - \bar{X})^2 . \quad (2.28)$$

Unbiased implies that $\langle \bar{X} \rangle = \langle X \rangle$ and $\langle s_X^2 \rangle = \sigma_X^2$.

The sample mean itself can be regarded as a random variable with its own expectation value $\langle \bar{X} \rangle$ and variance $\sigma_{\bar{X}}^2$. In fact, the *central limit theorem* tells us that the distribution of $\bar{X}$ approaches a normal distribution with mean $\mu = \langle X \rangle$ and standard deviation $\sigma = \sigma_{\bar{X}} = \sigma_X / \sqrt{M}$ as $M \rightarrow \infty$ [69].

An obvious choice for estimating the error of a MC calculation of $\bar{X}$ is therefore

$$\sigma_{\bar{X}} = \frac{\sigma_X}{\sqrt{M}} \approx \frac{s_X}{\sqrt{M}} = \sqrt{\frac{1}{M(M-1)} \sum_{i=1}^M (X(C_i) - \bar{X})^2} . \quad (2.29)$$

This shows that the MC error indeed scales as $\mathcal{O}(M^{-1/2})$ and that it is possible to reduce the error by taking more samples into account or, equivalently, increasing the run time of the simulation.

So far we have implicitly assumed that the generated configurations C_i are statistically independent. However, samples taken from Markov chains are inherently correlated, since the probability of visiting state C_{i+1} depends explicitly on the current state C_i (see Fig. 2.1). Using Eq. 2.29 with correlated samples will

underestimate the error [69]:

$$\begin{aligned}
\text{Var}(\bar{X}) &= \text{Var}\left(\frac{1}{M} \sum_i x_i\right) = \left\langle \left(\frac{1}{M} \sum_i x_i\right)^2 \right\rangle - \left\langle \frac{1}{M} \sum_i x_i \right\rangle^2 \\
&= \frac{1}{M^2} \left\{ \sum_i \langle x_i^2 \rangle + 2 \sum_{j>i} \langle x_i x_j \rangle - \sum_i \langle x_i \rangle^2 - 2 \sum_{j>i} \langle x_i \rangle \langle x_j \rangle \right\} \\
&= \frac{1}{M^2} \left\{ \sum_i (\langle x_i^2 \rangle - \langle x_i \rangle^2) + 2 \sum_{j>i} (\langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle) \right\} \\
&= \frac{1}{M^2} \left\{ \sum_i \text{Var}(x_i) + 2 \sum_{j>i} \chi_{|j-i|} \right\} \\
&= \frac{1}{M} \left\{ \sigma_X^2 + 2 \sum_{i=1}^{M-1} \left(1 - \frac{i}{M}\right) \chi_i \right\} \\
&= \frac{\sigma_X^2}{M} (1 + 2\tau_X) .
\end{aligned} \tag{2.30}$$

Here, we have used $X(C_i) = x_i$ and assumed that the summation limits are clear from the context unless specifically stated. In line four, we introduced the correlation function $\chi_{|j-i|} = \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle$, which depends only on the distance $|j - i|$ and is equal to the variance σ_X^2 for $j = i$, i.e. $\chi_0 = \langle x_i^2 \rangle - \langle x_i \rangle^2 = \sigma_X^2$. The last line defines the important autocorrelation time

$$\tau_X = \sum_{i=1}^{M-1} \left(1 - \frac{i}{M}\right) \frac{\chi_i}{\chi_0} . \tag{2.31}$$

It takes on values $\tau_X \geq 0$ and indicates the degree of correlation between individual measurements $X(C_i)$.

If the samples are statistically independent, $\tau_X = 0$ and Eq. 2.30 reproduces the previous result $\sigma_{\bar{X}}^2 = \sigma_X^2/M$. On the other hand, correlations between the generated data reduce the effective sample size by a factor of $1 + 2\tau_X$ and the naive error estimation in Eq. 2.29 would produce error bars that are too small. In principle, it is possible to calculate σ_X^2 and τ_X directly and use Eq. 2.30 to compute $\sigma_{\bar{X}}^2$. This turns out to be rather cumbersome in practice. The so-called *blocking analysis* offers a more pragmatic approach.

The main idea behind blocking is to group individual samples together into N_B blocks of size M_B , i.e. $M = N_B M_B$, and use their average values as effective measurements. If M_B is big enough, the block averages become statistically independent and naive error estimation from Eq. 2.29 applies. Since the required block size is not known before the simulation, it is common practice to study how

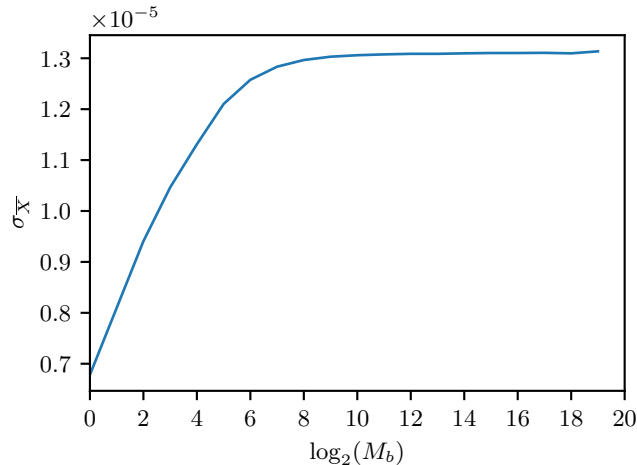


FIGURE 2.2: MC error $\sigma_{\bar{X}}$ as a function of the block size M_b . Block averages become statistically independent after $\approx 2^8 = 256$ measurements. The final error is $\approx 1.3 \times 10^{-5}$.

the calculated error changes with increasing M_B . Our considerations in the last paragraph have shown that for block sizes which are taken too small, the error will be underestimated. Therefore, as M_B gets larger and block averages become less correlated, the estimated error increases and gets closer to its true value derived in Eq. 2.30. At some point, it will level off as a function of the block size, indicating statistical independence of the block averages. The value the error assumes at this plateau will usually be a good estimate. Figure 2.2 shows an example taken from a real MC simulation.

In general, autocorrelation times, τ_X and τ_Y , of two different observables, $X(C)$ and $Y(C)$, do not coincide and blocking should be performed for each observable separately.

To complete this section, let us mention the important subject of error propagation. Suppose we are interested in a function of one or more ensemble averages: $f(\langle X \rangle, \langle Y \rangle, \dots)$. A frequently encountered example can be found in Eq. 2.12. The obvious approximation, $f(\bar{X}, \bar{Y}, \dots)$, is in most situations good enough, although it comes with a bias of order $\mathcal{O}(M^{-1})$ for non-linear functions [77]. Depending on the form of f , estimating the error σ_f can become more involved. Two general strategies dealing with error propagation are the *jackknife* [78, 79] and *bootstrap* [80] resampling techniques. A detailed description is outside the scope of the current thesis and we refer the interested reader to Refs. [69, 77].

2.2 Diagrammatic Monte Carlo

For many numerical problems, it is possible to write down a formal solution in terms of an infinite series of multi-dimensional integrals or summations. Because of the complexity of such a series, this is in most cases just a mere reformulation of the original problem without actually providing an answer. An important example is the calculation of various correlation functions for quantum many-body systems. In Chapter 3 it will be shown, how correlation functions can be written as an infinite series of Feynman diagrams using a perturbative expansion. Each term in the series contains complicated integrals or summations, which makes it impossible to provide an exact analytic solution.

Two standard approximations are (i) to truncate the series and focus only on the lowest order diagrams or (ii) to sum a specific class of diagrams up to infinity. In the former case, one can use MC techniques from the previous section and apply them to the pre-selected set of terms individually to calculate the multi-dimensional integrals. Either way, both approximations have to be justified depending on the situation.

Diagrammatic Monte Carlo offers a more generic and systematic approach to this problem. It generalizes the Metropolis-Hastings algorithm to sample the configuration space of all Feynman diagrams (or terms in the series) and is therefore not restricted to any order or specific class of diagrams. Lifting those restrictions is one of the most important aspects of the technique, because it makes DiagMC numerically exact, i.e. it does not have any bias or systematic errors attached to it.

The rest of this section introduces the basic theory of DiagMC (Sec. 2.2.1), with special attention given to the important concept of updates (Sec. 2.2.2), and shows how it works in practice by studying a very simple toy model with an analytic solution (Sec. 2.2.3).

2.2.1 General remarks about DiagMC

The following discussion is based on the lecture notes by Prokof'ev in Ref. [81].

Diagrammatic Monte Carlo is a numerical method first developed by Nikolai Prokof'ev, Boris Svistunov and Igor Tupitsyn in 1998 [49, 82]. Despite its name, DiagMC is not limited to problems in many-body physics dealing with Feynman diagrams. It is a generic MC sampling technique, based on the Metropolis-Hastings algorithm, that allows for an unbiased exploration of a configuration space with a varying number of continuous (or discrete) variables [81]. Unbiased in this context

means without introducing any systematic errors, e.g. when restricting the configuration space to some subspace or when discretizing the domain of an otherwise continuous variable.

DiagMC therefore generalizes the ideas and algorithms presented in Sec. 2.1, where it was implicitly assumed that the number of variables describing a configuration is fixed. For example, looking back at the thermal average in Eq. 2.2 for a three-dimensional system, each configuration C corresponds to a point in phase space specified by exactly $6N$ continuous variables, i.e. $C = (p_{1x}, \dots, p_{Nz}, q_{1x}, \dots, q_{Nz})$.

However, many problems are more naturally defined on a configuration space $\mathcal{C}$ with a varying number of degrees of freedom, e.g.

$$\mathcal{C} = \bigcup_{n=0}^{\infty} \mathcal{C}^n = \bigcup_{n=0}^{\infty} \{(x_1, \dots, x_n) : (x_1, \dots, x_n) \in \mathcal{C}^n\} , \quad (2.32)$$

where $\mathcal{C}^n$ is some n -dimensional subspace of $\mathcal{C}$. DiagMC provides us with the necessary tools to sample complicated spaces like Eq. 2.32. The main difference to “traditional” MCMC methods is that, in addition to the usual transitions,

$$\mathcal{C}^n \ni C = (x_1, \dots, x_n) \longleftrightarrow (x'_1, \dots, x'_n) = C' \in \mathcal{C}^n , \quad (2.33)$$

DiagMC also offers transitions between subspaces of different dimensionality

$$\mathcal{C}^n \ni C = (x_1, \dots, x_n) \longleftrightarrow (x'_1, \dots, x'_n, x'_{n+1}, \dots, x'_{n+m}) = C' \in \mathcal{C}^{n+m} . \quad (2.34)$$

In DiagMC terminology, transitions are called updates and they form the backbone of the algorithm. Their correct implementation decides on the success or failure of any DiagMC simulation.

Once a configuration space is defined and updates to explore it are established, the theory from Sec. 2.1 can be used to evaluate expectation values similar to Eq. 2.6. To be more precise, DiagMC is able to calculate averages $\langle X \rangle$ of the following form

$$\langle X \rangle = \sum_C X(C) p(C) = \sum_{n=0}^{\infty} \int dx_1 \cdots \int dx_n X(x_1, \dots, x_n) p(x_1, \dots, x_n) . \quad (2.35)$$

Here, $X(C)$ and $p(C)$ are some known functions defined on $\mathcal{C}$ and integrals indicate integration over continuous and summation over discrete variables. The probability (density) $p(C)$ can be further factorized into a weight function $\mathcal{W}(C)$ and a

normalization factor $\mathcal{Z}$

$$p(C) = p(x_1, \dots, x_n) = \frac{\mathcal{W}(C)}{\mathcal{Z}} = \frac{\mathcal{W}(x_1, \dots, x_n)}{\mathcal{Z}}, \quad (2.36)$$

where

$$\mathcal{Z} = \sum_C \mathcal{W}(C) = \sum_{n=0}^{\infty} \int dx_1 \cdots \int dx_n \mathcal{W}(x_1, \dots, x_n). \quad (2.37)$$

In case of complex or non-positive weights, considerations from Sec. 2.1 apply.

Note that $p(C)$ is normalized over the whole configuration space $\mathcal{C}$. The restricted function $p(C)|_{\mathcal{C}^n}$ is therefore not a proper probability (density) on $\mathcal{C}^n$ because it does not integrate to unity, i.e.

$$\sum_{C \in \mathcal{C}^n} p(C) = \int dx_1 \cdots \int dx_n p(x_1, \dots, x_n) \neq 1. \quad (2.38)$$

This shows that DiagMC is fundamentally different from simply going through each order $n \leq N$ separately and using “traditional” MC to evaluate the multi-dimensional integrals [81]. While the former treats all possible states $C \in \mathcal{C}$ on equal footing, which allows it to incorporate information from the whole configuration space $\mathcal{C}$ into its sampling routine, the latter is always restricted to some subspace $\mathcal{C}^n$ without being even aware of all the other configurations $C \notin \mathcal{C}^n$.

For a simple example of these abstract concepts, we refer the reader to Sec. 2.2.3.

2.2.2 DiagMC updates

Similar to “traditional” MC methods, DiagMC is based on a Markov process, which generates new states $C = (x_1, \dots, x_n) \in \mathcal{C}^n$ according to their weight $\mathcal{W}(C) = \mathcal{W}(x_1, \dots, x_n)$. However, since the configuration space is not restricted to $\mathcal{C}^n$, the Markov chain needs to be able to move from $\mathcal{C}^n$ to $\mathcal{C}^m$ and back for $n \neq m$. We can distinguish between two types of updates:

- *Type-I* updates do not change the number of variables of a configuration. They belong to transitions described in Eq. 2.33. If the Markov chain is in the current state $C \in \mathcal{C}^n$, it will be in some state $C' \in \mathcal{C}^n$ after the update. In this case, the standard Metropolis-Hastings algorithm from Fig. 2.1 can be used without modification.

For completeness, we provide the detailed balance equation and acceptance probability for the simplest update which changes a single x_i :

$$C = (x_1, \dots, x_i, \dots, x_n) \longleftrightarrow (x_1, \dots, x'_i, \dots, x_n) = C' \quad (2.39)$$

Let $T(x'_i|C)$ be the proposal distribution. Detailed balance tells us that

$$\mathcal{W}(C) T(x'_i|C) A(C'|C) = \mathcal{W}(C') T(x_i|C') A(C|C') , \quad (2.40)$$

such that the acceptance probability for the transition $C \rightarrow C'$ is given as

$$A(C'|C) = \min \left\{ 1, \frac{\mathcal{W}(C') T(x_i|C')}{\mathcal{W}(C) T(x'_i|C)} \right\} , \quad (2.41)$$

and for the inverse transition $C' \rightarrow C$ as

$$A(C|C') = \min \left\{ 1, \frac{1}{A(C'|C)} \right\} . \quad (2.42)$$

- *Type-II* updates change the number of variables of a configuration. They belong to transitions described in Eq. 2.34 and they distinguish DiagMC from “traditional” MC methods. In order for the Markov chain to sample configuration spaces like Eq. 2.32, it needs to be able to move between different subspaces $\mathcal{C}^n$ and $\mathcal{C}^m$. Type-II updates make these transitions possible.

Consider an update, which adds/removes m variables while keeping all others fixed:

$$C = (x_1, \dots, x_n) \quad \longleftrightarrow \quad (x_1, \dots, x_n, x_{n+1}, \dots, x_{n+m}) = C' , \quad (2.43)$$

where $C \in \mathcal{C}^n$ and $C' \in \mathcal{C}^{n+m}$. Let $T(x_{n+1}, \dots, x_{n+m}|C)$ be a probability distribution which is used to propose values for the m variables $x_{n+1}, \dots, x_{n+m}$. In this case, the detailed balance equation is

$$\begin{aligned} u(C'|C) \mathcal{W}(C) T(x_{n+1}, \dots, x_{n+m}|C) A(C'|C) \\ = u(C|C') \mathcal{W}(C') A(C|C') . \end{aligned} \quad (2.44)$$

Here, we have included implementation specific probabilities $u(C'|C)$ and $u(C|C')$. They need to be chosen correctly, depending on how the addition/removal of the new variables is performed (see Sec. 2.2.3 for an illustrative example). Following the Metropolis-Hastings algorithm, the acceptance probability for the transition $C \rightarrow C'$ is

$$A(C'|C) = \min \left\{ 1, \frac{u(C|C') \mathcal{W}(C')}{u(C'|C) \mathcal{W}(C) T(x_{n+1}, \dots, x_{n+m}|C)} \right\} , \quad (2.45)$$

and for the inverse transition $C' \rightarrow C$

$$A(C|C') = \min \left\{ 1, \frac{1}{A(C'|C)} \right\} . \quad (2.46)$$

Before looking at a practical example in the next section, let us make a few final remarks.

In Ref. [81] it is shown, how to make the detailed balance equation 2.44 for type-II updates plausible by reducing them to type-I. The idea is to rewrite the n^{th} -order term of the original series in Eq. 2.35 as

$$\begin{aligned} \int dx_1 \cdots \int dx_n X(x_1, \dots, x_n) p(x_1, \dots, x_n) \\ \times \int dx_{n+1} \cdots \int dx_{n+m} T(x_{n+1}, \dots, x_{n+m}|C) , \end{aligned} \quad (2.47)$$

which is possible because the proposal distribution is required to be properly normalized, i.e.

$$\int dx_{n+1} \cdots \int dx_{n+m} T(x_{n+1}, \dots, x_{n+m}|C) = 1 . \quad (2.48)$$

In this way, any transition of type-II can be reduced to type-I.

The set of updates needed to explore a specific configuration space with DiagMC is not unique. One can choose from an infinite number of possible updates. The only requirements are (i) detailed balance and (ii) ergodicity.

The latter has the same meaning as in Sec. 2.1.2: Any configuration $C \in \mathcal{C}$ should be reachable from any other configuration $C' \in \mathcal{C}$ with a finite number of Markov steps. For most systems, it is straightforward to design a set of updates which is ergodic.

Detailed balance, on the other hand, requires updates to come in pairs: If one transition is able to move the Markov chain from state C to C' , then a corresponding inverse transition should be able to move the chain back to its original state C . While type-I updates are usually their own inverses, it is common to split type-II updates into additions and removals, which increase and decrease the number of variables, respectively.

Closely related to detailed balance are the probabilities $u(C'|C)$ and $u(C|C')$ of type-II updates. Their values are implementation dependent and can be a source of subtle and hard to catch errors. We will therefore mention them explicitly in the next section when introducing type-II updates for our practical example.

2.2.3 DiagMC in practice

The previous sections have introduced the most important topics needed to run successful DiagMC simulations including the “traditional” MC method, error analysis, MCMC sampling as well as the Metropolis-Hastings algorithm and its extension to DiagMC. For readers, who are unfamiliar with these abstract concepts, it might not be clear how everything fits together and how the various tools are actually used in practice.

In the following, we therefore provide a working DiagMC implementation for a simple toy model. Starting from the diagrammatic (infinite series) expansion of the problem, we show how to rewrite it such that Eq. 2.35 applies and how Feynman diagrams can be used as visual aids. We describe a possible set of updates and measurements in detail and finally compare our numeric calculations to analytically known results.

Even though the example might seem artificial and trivial at first, the underlying DiagMC implementation incorporates all the previously mentioned concepts and serves as a perfect starting point for more complicated models. Furthermore, the series of the simple toy model has the same form as the diagrammatic expansion of the electron-hole two-particle Green’s function of an exciton model [83]. With few modifications, it would thus be possible to obtain various excitonic properties.

The model and many other ideas in this section are taken from Ref. [84].

Diagrammatic series

We are interested in calculating the following infinite series with DiagMC

$$Q(\tau) = \sum_{n=0}^{\infty} (-1)^n \int_0^{\tau} d\tau_n \cdots \int_0^{\tau_{i+1}} d\tau_i \cdots \int_0^{\tau_2} d\tau_1 e^{-(\varepsilon-\mu)\tau_1} V e^{-(\varepsilon-\mu)(\tau_2-\tau_1)} V \dots \\ \times V e^{-(\varepsilon-\mu)(\tau_{i+1}-\tau_i)} V \dots V e^{-(\varepsilon-\mu)(\tau-\tau_n)} , \quad (2.49)$$

for $\tau \geq 0$ and the model parameters $\varepsilon, \mu, V \in \mathbb{R}$. The 0th-order term is given by $\exp\{-(\varepsilon - \mu)\tau\}$ and the integration limits restrict the domain of each τ_i to $0 \leq \tau_1 \leq \tau_2 \leq \dots \leq \tau_n \leq \tau$. It is easy to show that the series simplifies to the analytic result

$$Q(\tau) = e^{-(\varepsilon-\mu)\tau} \sum_{n=0}^{\infty} (-1)^n V^n \int_0^{\tau} d\tau_n \cdots \int_0^{\tau_{i+1}} d\tau_i \cdots \int_0^{\tau_2} d\tau_1 \\ = e^{-(\varepsilon-\mu)\tau} \sum_{n=0}^{\infty} (-1)^n \frac{(V\tau)^n}{n!} = e^{-(\varepsilon-\mu+V)\tau} . \quad (2.50)$$

Our DiagMC implementation will work directly with Eq. 2.49. As indicated, we want to calculate Q as a function of τ . In this case, it is convenient to treat τ as another fixed parameter and introduce an additional integration variable τ' . Equation 2.49 can be rewritten as

$$\begin{aligned} Q(\tau) &= \int_0^{\tau_m} d\tau' \delta(\tau - \tau') Q(\tau') \\ &= \sum_{n=0}^{\infty} \int_0^{\tau_m} d\tau' \int_0^{\tau'} d\tau_n \cdots \int_0^{\tau_2} d\tau_1 \delta(\tau - \tau') (-1)^n V^n e^{-(\varepsilon-\mu)\tau'} \end{aligned} \quad (2.51)$$

where τ_m is chosen such that $0 \leq \tau < \tau_m$.

To make a connection to previous sections, let us first identify the configuration space

$$\mathcal{C} = \bigcup_{n=0}^{\infty} \mathcal{C}^n = \bigcup_{n=0}^{\infty} \{(\tau_1, \dots, \tau_n, \tau') : 0 \leq \tau_1 \leq \dots \leq \tau_n \leq \tau' < \tau_m\} \quad (2.52)$$

and the weight function

$$\mathcal{W}(C) = \mathcal{W}_n(\tau') = (-1)^n V^n e^{-(\varepsilon-\mu)\tau'}. \quad (2.53)$$

Note that the weights are only positive definite if $V \leq 0$. If $V > 0$, even terms in the series have a positive and odd terms a negative contribution leading to the sign problem. Since any $V \in \mathbb{R}$ should be allowed, we follow the discussion from Sec. 2.1.1 and rewrite Eq. 2.51 once more

$$\frac{Q(\tau)}{\mathcal{Z}} = \sum_{n=0}^{\infty} \int_0^{\tau_m} d\tau' \int_0^{\tau'} d\tau_n \cdots \int_0^{\tau_2} d\tau_1 \delta(\tau - \tau') \operatorname{sgn}\{\mathcal{W}_n(\tau')\} \frac{|\mathcal{W}_n(\tau')|}{\mathcal{Z}}, \quad (2.54)$$

where $|\mathcal{W}_n(\tau')| = |V|^n e^{-(\varepsilon-\mu)\tau'}$ and $\operatorname{sgn}\{\mathcal{W}_n(\tau')\} = \operatorname{sgn}(-V)^n$. Both sides have been divided by the normalization factor

$$\mathcal{Z} = \sum_C |\mathcal{W}_n(C)| = \sum_{n=0}^{\infty} \int_0^{\tau_m} d\tau' \int_0^{\tau'} d\tau_n \cdots \int_0^{\tau_2} d\tau_1 |\mathcal{W}_n(\tau')|, \quad (2.55)$$

which allows us to identify the probability density

$$p(C) = p_n(\tau') = \frac{|\mathcal{W}_n(\tau')|}{\mathcal{Z}} \quad (2.56)$$

and the quantity to be measured

$$q(C) = q_n(\tau') = \delta(\tau - \tau') \operatorname{sgn} \{ \mathcal{W}_n(\tau') \} . \quad (2.57)$$

Measurements

The right-hand side of Eq. 2.54 has now the same form as Eq. 2.35 and can therefore be calculated with a proper DiagMC implementation. The main idea is to generate configurations C_i according to $p(C) = p_n(\tau')$ and approximate the left hand side with its sample mean, i.e.

$$\frac{Q(\tau)}{\mathcal{Z}} \approx \frac{1}{M} \sum_{i=1}^M q(C_i) = \frac{1}{M} \sum_{i=1}^M q_n(\tau'_i) . \quad (2.58)$$

There are still two open problems with this approach: (i) the probability of generating a configuration C_i with $\tau = \tau'_i$, such that $q_n(\tau'_i)$ is non-zero, is infinitely small for a continuous variable τ' and (ii) the normalization $\mathcal{Z}$ is not known.

One possible solution to the first problem is to use the *histogram* approach. Instead of focusing on an isolated point τ , let us consider an interval $\mathcal{I} = [\tau_l, \tau_r] \in [0, \tau_m]$ of finite length $|\mathcal{I}| = \tau_r - \tau_l$ and the average $\bar{Q}(\mathcal{I})$ of $Q(\tau)$ over $\mathcal{I}$:

$$\bar{Q}(\mathcal{I}) = \frac{1}{|\mathcal{I}|} \int_{\tau_l}^{\tau_r} d\tau' Q(\tau') = \frac{1}{|\mathcal{I}|} \int_0^{\tau_m} d\tau' Q(\tau') \chi_{\mathcal{I}}(\tau') , \quad (2.59)$$

where

$$\chi_{\mathcal{I}}(\tau') = \begin{cases} 1 & \text{if } \tau' \in \mathcal{I} \\ 0 & \text{otherwise} \end{cases} \quad (2.60)$$

is the characteristic function for the interval $\mathcal{I}$. Repeating the same steps which led us to Eq. 2.54, we can derive the following estimator

$$\bar{q}(C) = \bar{q}_n(\tau') = \frac{\chi_{\mathcal{I}}(\tau')}{|\mathcal{I}|} \operatorname{sgn} \{ \mathcal{W}_n(\tau') \} \quad (2.61)$$

and use it to approximate $\bar{Q}(\mathcal{I})$ with its sample mean $\overline{\bar{Q}}(\mathcal{I})$:

$$\frac{\bar{Q}(\mathcal{I})}{\mathcal{Z}} \approx \frac{1}{M} \sum_{i=1}^M \bar{q}(C_i) = \frac{1}{M} \sum_{i=1}^M \bar{q}_n(\tau'_i) = \frac{\overline{\bar{Q}}(\mathcal{I})}{\mathcal{Z}} . \quad (2.62)$$

The mean value theorem for definite integrals tells us that there is some point $\tau \in \mathcal{I}$ such that $Q(\tau) = \bar{Q}(\mathcal{I})$. Since τ is usually not known, it is common practice to assign the value of $\bar{Q}(\mathcal{I})$ to the center, $\tau_c = (\tau_r + \tau_l)/2$, of the interval,

i.e. $Q(\tau_c) \approx \bar{Q}(\mathcal{I})$. For non-linear functions, $\bar{Q}(\mathcal{I})$ will generally not converge to the exact $Q(\tau_c)$, which represents a systematic error typical for histograms. In Chapter 3, we provide an exact estimator for $Q(\tau)$ without any associated bias.

There are several options on how to deal with the unknown normalization $\mathcal{Z}$. An obvious solution for our simple toy model would be to calculate it analytically from Eq. 2.55:

$$\mathcal{Z} = \sum_{n=0}^{\infty} \int_0^{\tau_m} d\tau' \int_0^{\tau'} d\tau_n \cdots \int_0^{\tau_2} d\tau_1 |V|^n e^{-(\varepsilon-\mu)\tau'} = \frac{1 - e^{-(\varepsilon-\mu-|V|)\tau_m}}{\varepsilon - \mu - |V|}. \quad (2.63)$$

A more universally valid approach is to use some known integral I_0 , which can either be part of the original series or added artificially. For example, it is often possible to integrate the 0th-order term analytically. In our case, this means

$$I_0 = \int_0^{\tau_m} d\tau' |\mathcal{W}_0(\tau')| = \int_0^{\tau_m} d\tau' e^{-(\varepsilon-\mu)\tau'} = \frac{1 - e^{-(\varepsilon-\mu)\tau_m}}{\varepsilon - \mu}. \quad (2.64)$$

Furthermore, we can also calculate $I_0/\mathcal{Z}$ with DiagMC:

$$\begin{aligned} \frac{I_0}{\mathcal{Z}} &= \int_0^{\tau_m} d\tau' \frac{|\mathcal{W}_0(\tau')|}{\mathcal{Z}} = \sum_{n=0}^{\infty} \int_0^{\tau_m} d\tau' \int_0^{\tau'} d\tau_n \cdots \int_0^{\tau_2} d\tau_1 \delta_{n,0} \frac{|\mathcal{W}_n(\tau')|}{\mathcal{Z}} \\ &\approx \frac{1}{M} \sum_{i=1}^M I(C_i) = \frac{N_0}{M} = \bar{I}_0, \end{aligned} \quad (2.65)$$

where

$$I(C) = \begin{cases} 1 & \text{if } C \in \mathcal{C}^0 \\ 0 & \text{otherwise} \end{cases} \quad (2.66)$$

and N_0 is simply the number of times the 0th-order term is generated during the DiagMC simulation. Since I_0 is known analytically, the normalization factor can be estimated with

$$\mathcal{Z} \approx \frac{I_0}{\bar{I}_0} = \frac{I_0 M}{N_0}. \quad (2.67)$$

Multiplying Eq. 2.62 with Eq. 2.67, gives us the final DiagMC approximation to $Q(\tau_c)$:

$$Q(\tau_c) \approx \bar{Q}(\mathcal{I}) = \frac{I_0}{|\mathcal{I}| N_0} \sum_{i=1}^M \chi_{\mathcal{I}}(\tau'_i) \text{sgn}(-V)^n. \quad (2.68)$$

In practice, the general strategy is to discretize the interval $[0, \tau_m]$ into N subintervals or bins $\mathcal{I}_i$ of size $|\mathcal{I}_i|$ and approximate the value of $Q(\tau)$ at the center of each

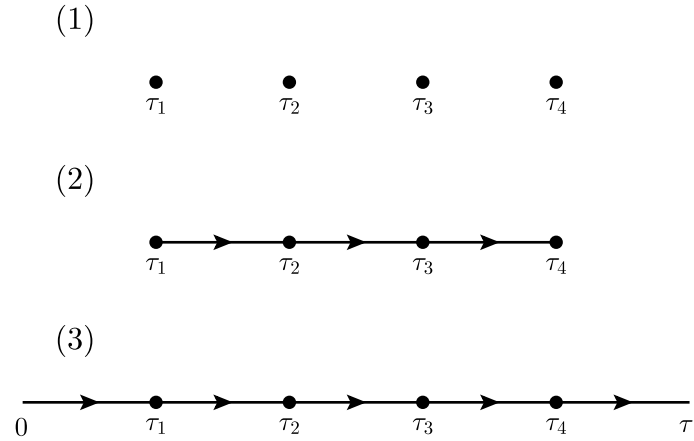


FIGURE 2.3: Recipe for drawing a 4th-order Feynman diagram for the simple toy model.

bin with Eq. 2.68.

Updates

When discussing the implementation of updates, it is usually much easier to think in terms of Feynman diagrams rather than points in a configuration space or algebraic expressions. Let us therefore introduce a possible diagrammatic representation for our toy model. For the time being, diagrams are just used as visual aids and have no particular physical meaning.

The goal is to create a one-to-one mapping between any $C \in \mathcal{C}$ and its graphical representation as a Feynman diagram. Suppose we are given a configuration $C = (\tau_1, \dots, \tau_n, \tau') \in \mathcal{C}^n$. We use the following steps to turn it into a Feynman diagram of order n :

1. Draw n vertices (dots) on a horizontal line and label them from left to right with τ_1 , τ_2 , and so on until τ_n .
2. Connect the vertices with directed straight lines.
3. Add two more directed straight lines, one going into vertex τ_1 and one going out of vertex τ_n and label the left end of the diagram with 0 and the right end with τ' .

Figure 2.3 shows the individual steps for a 4th-order diagram.

The numerical value of a diagram is the weight $\mathcal{W}(C)$ of the corresponding configuration C . We can use the dictionary in Fig. 2.4 to translate between a given diagram and its algebraic expression. For example, the value of the diagram in

$$\overrightarrow{\tau_i} \quad \overrightarrow{\tau_j} = e^{-(\varepsilon-\mu)(\tau_j-\tau_i)} \quad \overrightarrow{\tau_i} \bullet \overrightarrow{\tau_i} = -V$$

FIGURE 2.4: Feynman dictionary for the simple toy model.

Fig. 2.3 (3) is given by

$$\begin{aligned} \mathcal{W}(\tau_1, \tau_2, \tau_3, \tau_4, \tau') &= e^{-(\varepsilon-\mu)\tau_1} (-V) e^{-(\varepsilon-\mu)(\tau_2-\tau_1)} (-V) e^{-(\varepsilon-\mu)(\tau_3-\tau_2)} (-V) \\ &\quad \times e^{-(\varepsilon-\mu)(\tau_4-\tau_3)} (-V) e^{-(\varepsilon-\mu)(\tau'-\tau_4)} = V^4 e^{-(\varepsilon-\mu)\tau'} = \mathcal{W}_4(\tau'), \end{aligned} \quad (2.69)$$

which is just its weight from Eq. 2.53.

When designing a set of appropriate updates, we will follow the general advise from Refs. [81, 84] and try to keep the updates local. That means an update should only change a small part of the diagram, while leaving the rest unchanged. Local updates have the advantage of being computationally less expensive, they are less error-prone and their acceptance-rejection ratios are easier to control.

For our DiagMC simulation of the simple toy model, we use three updates:

- *Add-vertex* and *Remove-vertex*: Those are type-II updates which either increase (add-vertex) or decrease (remove-vertex) the order n by 1. Figure 2.5 (a) shows an example of an add-vertex (from left to right) and of a remove-vertex (from right to left) update.

Our implementation works as follows: Suppose the left diagram corresponds to the configuration $C = (\tau_1, \dots, \tau_n, \tau') \in \mathcal{C}^n$, while the right diagram corresponds to $C' = (\tau_1, \dots, \tau, \dots, \tau_{n+1}, \tau') \in \mathcal{C}^{n+1}$. The ratio of the moduli of their weights is

$$\frac{|\mathcal{W}(C')|}{|\mathcal{W}(C)|} = |V|. \quad (2.70)$$

To add a new vertex, we first choose a random line segment with probability $u(C'|C) = 1/(n+1)$. Let τ_l and τ_r be its left and right end, respectively. Then we propose a position τ of the new vertex uniformly on the line segment, i.e. with probability $T(\tau|C) = 1/(\tau_r - \tau_l)$. On the other hand, to remove a vertex we choose it randomly with probability $u(C|C') = 1/(n+1)$ (remember that C' has $n+1$ vertices). Finally, we can plug everything into Eq. 2.45 to calculate the acceptance probability for the add-vertex update

$$A(C'|C) = \min \{1, |V|(\tau_r - \tau_l)\} , \quad (2.71)$$

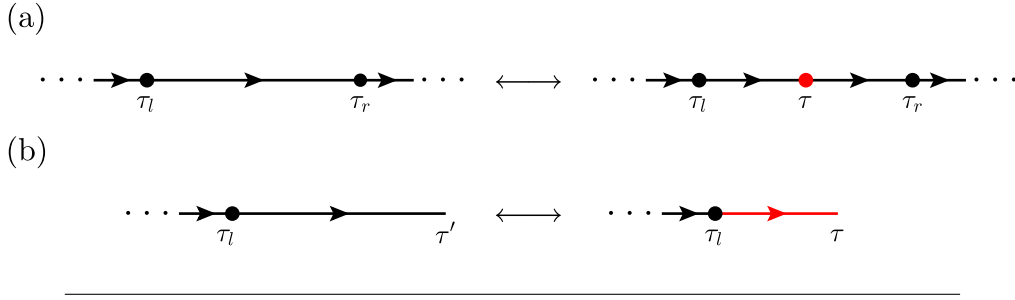


FIGURE 2.5: Updates for the simple toy model. In red are the parts of the diagrams which are subject to changes. (a) The add-vertex update is depicted from left to right and the remove-vertex update from right to left. (b) Change-length update.

as well as for the remove-vertex update

$$A(C|C') = \min \left\{ 1, \frac{1}{A(C'|C)} \right\} = \min \left\{ 1, \frac{1}{|V|(\tau_r - \tau_l)} \right\}. \quad (2.72)$$

Note that the above is just one of many possible implementations. For example, one could add and remove vertices only on the last line segment or one could choose to propose the position of the new vertex from the distribution $T(\tau|C) = 1/\tau'$. In the last case, $u(C'|C)$ would be unity!

- *Change-length*: A type-I update which changes the length τ' of a diagram. Figure 2.5 (b) shows an example of a change-length update.

Our implementation works as follows: Suppose the left (current) diagram corresponds to the configuration $C = (\tau_1, \dots, \tau_n, \tau') \in \mathcal{C}^n$, while the right (proposed) diagram corresponds to $C' = (\tau_1, \dots, \tau_n, \tau) \in \mathcal{C}^n$. The ratio of the moduli of their weights is

$$\frac{|\mathcal{W}(C')|}{|\mathcal{W}(C)|} = \frac{e^{-(\varepsilon-\mu)\tau'}}{e^{-(\varepsilon-\mu)\tau}}. \quad (2.73)$$

Only the last line segment is changed. Set $\tau_l = \tau_n$ if $n > 0$ and $\tau_l = 0$ if $n = 0$. We could propose a new length τ uniformly between τ_l and τ_m , i.e. from the distribution $T(\tau|C) = 1/(\tau_m - \tau_l)$. However, looking at Eq. 2.41, a more effective approach is to use $T(\tau|C) \propto e^{-(\varepsilon-\mu)\tau}$ normalized on the interval $[\tau_l, \tau_m]$, i.e.

$$T(\tau|C) = \frac{\varepsilon - \mu}{e^{-(\varepsilon-\mu)\tau_l} - e^{-(\varepsilon-\mu)\tau_m}} e^{-(\varepsilon-\mu)\tau}. \quad (2.74)$$

This way the acceptance probability will be unity: $A(C'|C) = 1$. Reference [69] explains in detail how to draw random samples from an exponential

distribution.

Before discussing the results, let us make some final remarks about our DiagMC implementation.

The reader can convince himself that the above forms an ergodic set of updates. It is not unique and one could think of other updates which might increase the convergence of the simulation, e.g. shifting a vertex on the line segment between its neighbors or scaling (stretching or squeezing) the diagram as a whole. For the current problem, performance and convergence are not crucial and the three updates are sufficient.

At every Markov step, we choose one of the three updates randomly with equal probability. This is not required and one could assign different weights to each update. In such a case, the detailed balance equations 2.40 and 2.44 should be modified to account for the change in probabilities.

It is possible for updates to propose invalid diagrams outside of the configuration space. We treat such cases as if the weight of the diagram is zero, i.e. we reject the update but still take measurements. For example, a frequently encountered situation is when the remove-vertex update is applied to a 0th-order diagram. In principle, one could work around the issue by never choosing the remove-vertex update if the current diagram order is 0. However, this would again complicate the detailed balance equations and it is much easier to simply take the approach suggested above.

Since computer storage is limited in size and we somehow have to store the current diagram in memory, DiagMC simulations are in practice limited to some maximum diagram order N_m . On modern hardware, N_m can easily be $\geq 10^5$ without running out of memory. If the simulation actually reaches such diagram orders, it would most likely have problems to converge in a reasonable amount of time anyway and DiagMC might not be the right tool to use. For all calculations done in the current thesis, N_m can always be chosen much larger than the highest diagram order generated during a simulation.

Results

All results presented in the current section were obtained with a standard laptop. Due to the locality of the updates and the simplicity of the performed measurements, the implementation, without special attention given to performance, can do $\approx 15 \times 10^6$ updates/sec. Note that this number might drop significantly for more complicated problems.

Figure 2.6 compares results for $Q(\tau)$ obtained with DiagMC (colored shapes) to the analytically known expression $Q(\tau) = \exp\{-(\varepsilon - \mu + V)\tau\}$ or $\log[Q(\tau)] =$

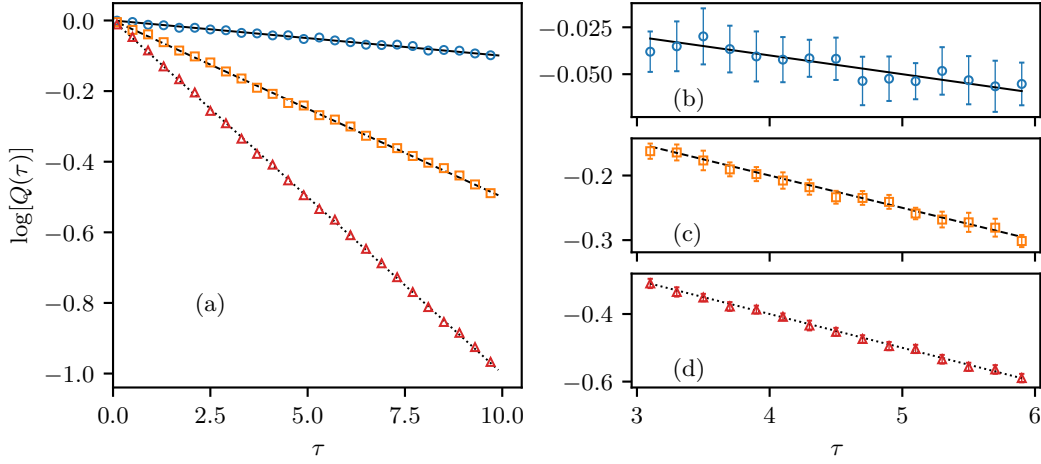


FIGURE 2.6: (a)-(d) DiagMC (colored shapes) in comparison with analytic results (black straight lines). $\varepsilon = 0$, $V = -0.1$ and $\tau_m = 10$ for all simulations. Blue circles (continuous lines) correspond to $\mu = -0.11$, orange squares (dashed lines) to $\mu = -0.15$ and red triangles (dotted lines) to $\mu = -0.2$. (b)-(d) Close ups including error bars.

$-(\varepsilon - \mu + V)\tau$ (black straight lines). For all three simulations, $\varepsilon = 0$, $V = -0.1$ and $\tau_m = 10$. Blue circles (continuous lines) correspond to $\mu = -0.11$, orange squares (dashed lines) to $\mu = -0.15$ and red triangles (dotted lines) to $\mu = -0.2$. The interval $[0, \tau_m]$ was divided into 50 bins of equal length to evaluate the histogram. The run time of each simulation was ≈ 1.3 seconds or equivalently 20×10^6 MC steps and measurements were performed after every 5 updates to reduce the correlation between samples, which means a total of 4×10^6 measurements.

It is clear from the left plot in Fig. 2.6 that DiagMC reproduces the overall analytic results very well for this simple problem. The right column features close up plots of the three simulations for the interval $[3, 6]$ including their error bars, which correspond to three times the standard deviation of the sample mean, i.e. $3\sigma_{\overline{Q}}$. For all points displayed, the analytic value lies within the error bars of the DiagMC result. Note that the size of the error bars are actually comparable for all three simulations, it is just the scaling of the y-axis which makes it appear to be shrinking with decreasing μ .

Since the simulations in Fig. 2.6 were performed for negative V , the weights of the diagrams were all positive such that their average sign $\langle \text{sgn}(\mathcal{W}) \rangle$ was equal 1.0. To demonstrate the effect of the sign problem on DiagMC results, Figs. 2.7–2.9 show the convergence of three DiagMC simulations with different $\langle \text{sgn}(\mathcal{W}) \rangle$. All calculations were done for $\varepsilon = 0$ and $\tau_m = 10$ and histograms were collected on the interval $[0, \tau_m]$ subdivided into 100 bins. M corresponds to the number of measurements.

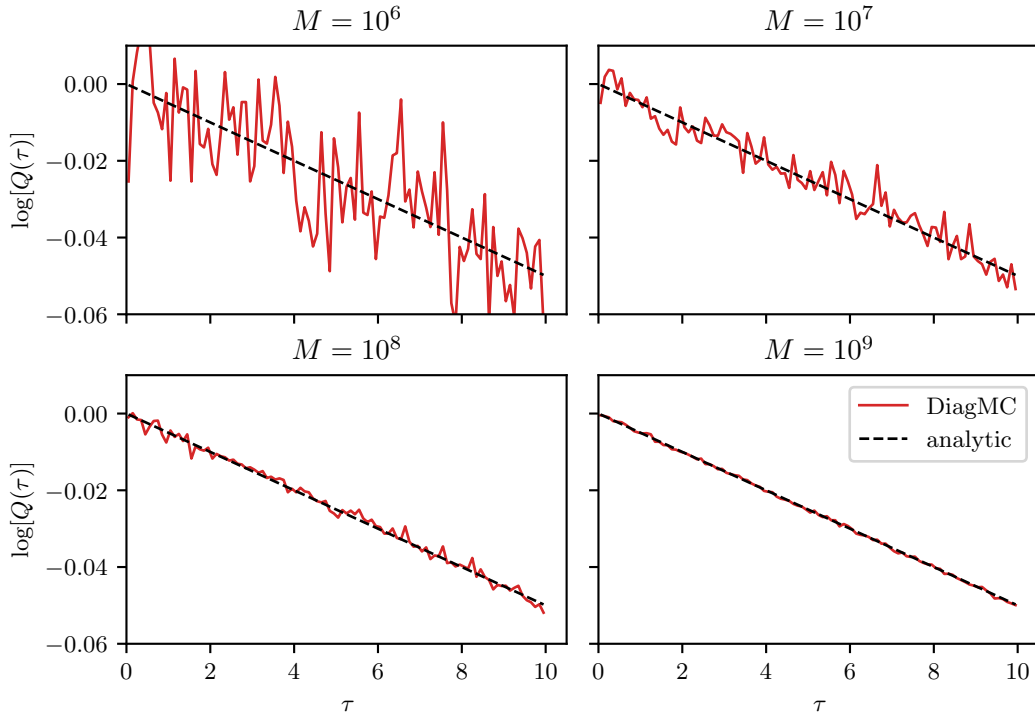


FIGURE 2.7: Convergence of a DiagMC simulation with an average sign of 1.0. Red lines show the DiagMC results, black dashed lines the analytic expression.

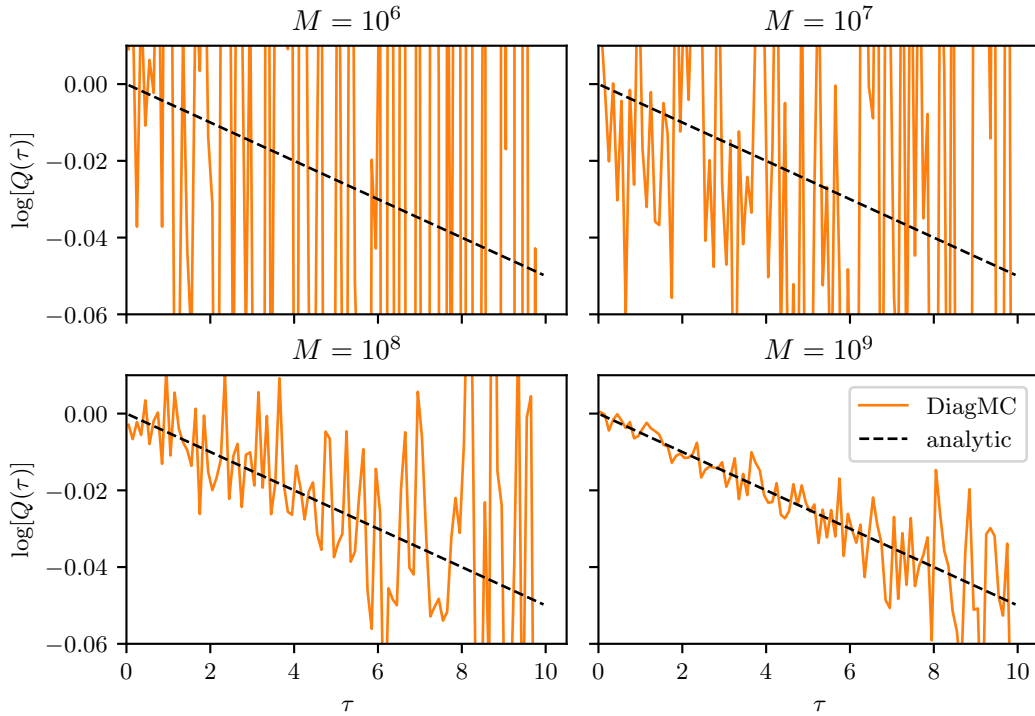


FIGURE 2.8: Convergence of a DiagMC simulation with an average sign of $\approx 3.4 \times 10^{-2}$. Orange lines show the DiagMC results, black dashed lines the analytic expression.

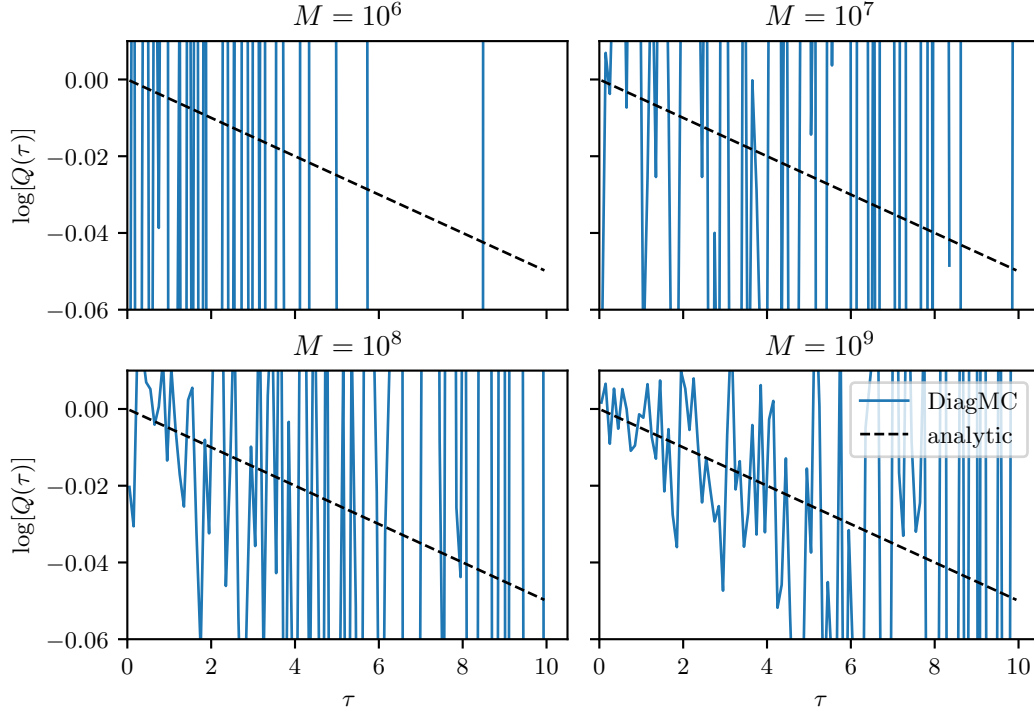


FIGURE 2.9: Convergence of a DiagMC simulation with an average sign of $\approx 2.7 \times 10^{-3}$. Blue lines show the DiagMC results, black dashed lines the analytic expression.

Figure 2.7 shows results for $V = -0.25$, $\mu = -0.255$ and $\langle \text{sgn}(\mathcal{W}) \rangle = 1.0$, Fig. 2.8 for $V = 0.25$, $\mu = 0.245$ and $\langle \text{sgn}(\mathcal{W}) \rangle \approx 0.03444$ and Fig. 2.9 for $V = 0.4$, $\mu = 0.395$ and $\langle \text{sgn}(\mathcal{W}) \rangle \approx 0.00274$. The analytic expression for the average sign is

$$\begin{aligned} \langle \text{sgn}(\mathcal{W}) \rangle &= \sum_{n=0}^{\infty} \int_0^{\tau_m} d\tau' \int_0^{\tau'} d\tau_n \cdots \int_0^{\tau_2} d\tau_1 \text{sgn} \{ \mathcal{W}_n(\tau') \} \frac{|\mathcal{W}_n(\tau')|}{\mathcal{Z}} \\ &= \frac{(\varepsilon - \mu - |V|) (1 - e^{-(\varepsilon - \mu + V)\tau_m})}{(\varepsilon - \mu + V) (1 - e^{-(\varepsilon - \mu - |V|)\tau_m})}. \end{aligned} \quad (2.75)$$

The overall effect of the sign problem is quite obvious from the three figures. The closer the average sign is to zero, the longer it will take the simulation to converge. However, the calculations in Figs. 2.8 and 2.9 also indicate that for sign problems which are not too severe, it is still possible for DiagMC to produce reliable results in a reasonable amount of time. For example in the case of our simple model, one can expect to reach convergence for average signs $\geq 10^{-3}$.

It is important to note that the sign problem is an artifact of the series expansion and of the DiagMC algorithm to interpret the weights as probabilities. The

analytic expression of $Q(\tau)$ from Eq. 2.50 is well defined for any V . Therefore, in some situations one might be able to avoid the sign problem by using a different expansion.

2.3 Numerical analytic continuation

DiagMC and other quantum Monte Carlo methods belong to the most successful and versatile tools for studying quantum many-body systems. Due to practical reasons, they are usually formulated in the imaginary time or Matsubara frequency representation and produce correlation functions $G(\xi)$ defined on the imaginary axis $\xi = \tau$ or $\xi = i\omega_n$, respectively. Here, we adopt the standard notation, where $\tau = it$ denotes imaginary time and

$$i\omega_n = \begin{cases} \frac{i2n\pi}{\hbar\beta} & \text{for bosons} \\ \frac{i(2n+1)\pi}{\hbar\beta} & \text{for fermions} \end{cases} \quad (2.76)$$

are Matsubara (imaginary) frequencies (see e.g. Ref. [85]). Associated with correlation functions are real frequency spectral densities $A(\omega)$, which are connected to experimentally measurable quantities through linear response theory [17, 85, 86]. It is therefore crucial to be able to perform analytic continuation of QMC data from the imaginary back to the real axis.

The relationship between $G(\xi)$ and $A(\omega)$ is given by a Fredholm integral equation of the first kind:

$$G(\xi) = \int_{-\infty}^{\infty} d\omega K(\xi, \omega) A(\omega) , \quad (2.77)$$

where the explicit form of the kernel $K(\xi, \omega)$ is determined by the type of correlation function G and its representation ξ [87, 88]. Depending on the analytic properties of $K(\xi, \omega)$, Equation 2.77 is generally *ill-posed*, i.e. its solution $A(\omega)$ might not exist, it might not be unique or it might be unstable with respect to the input $G(\xi)$ [89]. To make things worse, the left hand side in Eq. 2.77 is usually only known for a finite set of points $\{\xi_n : n = 1, \dots, N\}$ and with finite precision. The problem of inverting Eq. 2.77 and thereby restoring $A(\omega)$ from some numerical input data $\{\overline{G}(\xi_n)\}$ with associated error bars $\{\sigma_{\overline{G}(\xi_n)}\}$ is called *numerical analytic continuation*.

In the current thesis, we will show how DiagMC can be used to calculate (i) the imaginary time single-particle Green's function, $G(\tau)$, and (ii) the imaginary time current-current correlation function, $\Pi(\tau)$, for various polaron problems. At zero temperature, the former is related to the single-particle Lehmann spectral function,

$A(\omega)$, via

$$G(\tau) = \int_0^\infty d\omega e^{-\tau\omega} A(\omega) , \quad (2.78)$$

while the latter is connected to the optical conductivity, $\sigma(\omega)$, through

$$\Pi(\tau) = \int_0^\infty d\omega \frac{\omega}{\pi} e^{-\tau\omega} \sigma(\omega) . \quad (2.79)$$

Comparing Eqs. 2.78 and 2.79 with Eq. 2.77, we can identify the kernels

$$K(\tau, \omega) = \Theta(\omega) e^{-\tau\omega} \quad \text{and} \quad K(\tau, \omega) = \frac{\omega}{\pi} \Theta(\omega) e^{-\tau\omega} , \quad (2.80)$$

respectively. $\Theta(\omega)$ is the step function defined as

$$\Theta(\omega) = \begin{cases} 1 & \text{for } \omega \geq 0 \\ 0 & \text{for } \omega < 0 \end{cases} . \quad (2.81)$$

Both functions, $A(\omega)$ and $\sigma(\omega)$, are experimentally observable quantities. Lehmann spectral functions can be measured with angle-resolved photoemission spectroscopy (ARPES) [90] and optical conductivities with optical measurements [91].

The rest of this section gives a short summary of the main difficulties inherent to NAC problems and available strategies how to deal with them (Sec. 2.3.1), before focusing on the stochastic optimization with consistent constraints method (Sec. 2.3.2).

2.3.1 General remarks about NAC

Numerical analytic continuation is concerned with extracting real frequency, dynamical information from correlation functions defined on the imaginary time or frequency axis [86]. For this purpose, it tries to reconstruct a function $A(\omega)$ from a finite set of integrals [92]:

$$\overline{G}(\xi_n) \approx G[A](\xi_n) = \int_{-\infty}^{\infty} d\omega K(\xi_n, \omega) A(\omega) , \quad n = 1, \dots, N . \quad (2.82)$$

Here, $K(\xi_n, \omega)$ is a given integral kernel and the provided input, $\overline{G}(\xi_n)$, is only known for some selected ξ_n and with uncertainty $\sigma_{\overline{G}(\xi_n)}$. $G[A]$ denotes a functional of A defined by the integral on the right-hand side.

The goal is to find a function $A(\omega)$, which satisfies the system of equations in Eq. 2.82 without violating the error bars $\sigma_{\overline{G}(\xi_n)}$. More precisely, $A(\omega)$ should be chosen such that

$$G[A](\xi_n) \in [\overline{G}(\xi_n) - \sigma_{\overline{G}(\xi_n)}, \overline{G}(\xi_n) + \sigma_{\overline{G}(\xi_n)}] \quad \forall n = 1, \dots, N. \quad (2.83)$$

The main difficulty in NAC problems comes from the non-uniqueness of $A(\omega)$. In fact, there usually will be an infinite number of solutions satisfying Eq. 2.83 and one can only hope to find the best $A(\omega)$ with respect to some additional criteria [93].

The simplest approach looks for a least squares solution, $A_{\text{LS}}(\omega)$, by minimizing the deviation measure $D_{\text{LS}}[A]$, i.e.

$$A_{\text{LS}}(\omega) = \min_A D_{\text{LS}}[A] = \min_A \sum_{n=1}^N \{G[A](\xi_n) - \overline{G}(\xi_n)\}^2 = \min_A \|\mathbf{G}[A] - \overline{\mathbf{G}}\|^2. \quad (2.84)$$

Here, we have introduced two N -dimensional vectors, $\overline{\mathbf{G}} = (\overline{G}(\xi_1), \dots, \overline{G}(\xi_N))$ and $\mathbf{G}[A] = (G[A](\xi_1), \dots, G[A](\xi_N))$, and defined the deviation measure as their squared Euclidean distance. Due to the statistical errors in $\overline{\mathbf{G}}$, the least squares solution will suffer from so-called *sawtooth* instabilities. Those are fast oscillations appearing in $A_{\text{LS}}(\omega)$, constantly over- and undershooting the actual spectrum, but without compromising Eq. 2.83. For visual examples, we refer the reader to Ref. [93].

Techniques that try to suppress such spurious noise in the least squares solution are generally termed *regularization methods*. They use a modified deviation measure, which penalizes large fluctuations, to produce a smoother $A(\omega)$. It is also possible to incorporate other prior knowledge into the regularization procedure. This allows one to obtain solutions with a certain expected behavior. However, too much additional information and constraints can bias the result in an unwanted way. In the worst case, this could lead to unphysical features in the spectrum, which could be falsely attributed to real physical processes.

Depending on the regularization scheme and on what prior knowledge is used to restrict the possible solutions, one can distinguish between various NAC techniques, including the (probably most) popular maximum entropy method [69, 86, 94], averaging Padé approximants [95], stochastic continuation methods [96, 97] or the historically important Tikhonov-Phillips regularization [98–100].

The present work makes use of the stochastic optimization with consistent constraints method, which was first introduced by Goulko *et al.* in 2016 to study spectral functions of the Fermi polaron [101]. A more detailed description of the algorithm can be found in Ref. [92], while Refs. [87, 88] provide an open source

implementation based on the TRIQS library.

2.3.2 Stochastic optimization with consistent constraints

SOCC is a rather sophisticated NAC scheme, which combines the *stochastic optimization method* (SOM) [50] with the *method of consistent constraints* (MCC) [102]. In the following, we will only give a short overview of the algorithm and highlight some of its particular features. For implementation details, we refer the interested reader to Refs. [87, 92, 93].

The main idea of SOCC is to generate a large set of independent, *basic solutions* $\{A_l : l = 1, \dots, L\}$. They are found by minimizing the deviation measure

$$D[A] = \frac{1}{N} \sum_{n=1}^N \left\{ \frac{G[A](\xi_n) - \overline{G}(\xi_n)}{\sigma_{\overline{G}(\xi_n)}} \right\}^2, \quad (2.85)$$

with the additional constraints that $A(\omega) \geq 0$ and

$$\int_{-\infty}^{\infty} d\omega A(\omega) = \mathcal{N}. \quad (2.86)$$

Here, $\mathcal{N}$ is a known normalization and it is assumed that there are no correlations between the components of the input vector $\overline{\mathbf{G}}$ (otherwise one can work in the eigenbasis of the covariance matrix as described in Ref. [92]). Dividing the deviation $G[A](\xi_n) - \overline{G}(\xi_n)$ by $\sigma_{\overline{G}(\xi_n)}$ prioritizes points ξ_n with smaller error bars. Note that the basic solutions are not biased to be smooth but are expected to fully display sawtooth fluctuations.

In contrast to many other NAC methods, SOCC does not use a predetermined ω -grid. Instead, it parametrizes the spectra as a superposition of positive-definite rectangles $\{P_k\} = \{c_k, w_k, h_k\}$ restricted to some domain $[\omega_{\min}, \omega_{\max}]$:

$$A(\omega) = \sum_{k=1}^K \eta_{\{P_k\}}(\omega). \quad (2.87)$$

Here, $w_k > 0$ is the width, $h_k > 0$ the height and c_k the center of the k^{th} -rectangle and

$$\eta_{\{P_k\}}(\omega) = \begin{cases} h_k & \text{if } \omega \in [c_k - w_k/2, c_k + w_k/2] \\ 0 & \text{otherwise} \end{cases}. \quad (2.88)$$

The number of rectangles K as well as their heights, widths and positions of their centers are allowed to vary. A spectrum is therefore fully characterized by a set of

rectangles,

$$C = \{\{P_k\} : k = 1, \dots, K\} , \quad (2.89)$$

which we call its *configuration*. If one works with non-overlapping rectangles, a configuration always obeys

$$\sum_{k=1}^K h_k w_k = \mathcal{N} , \quad (2.90)$$

in accordance with Eq. 2.86 and the integrals in Eq. 2.82 can be evaluated as

$$G[A](\xi_n) = \sum_{k=1}^K h_k \int_{c_k - w_k/2}^{c_k + w_k/2} d\omega K(\xi_n, \omega) . \quad (2.91)$$

The minimization of Eq. 2.85 to obtain a single basic solution $A_l(\omega)$ proceeds in the following way. First, a random initial configuration $C^{(0)}$ with $0 < K^{(0)} < K_{max}$ rectangles is generated. Then, a total of N_G *global updates* are performed to produce a sequence of configurations $C^{(i)}$ with corresponding spectra $A^{(i)}$:

$$C^{(0)} \rightarrow \dots \rightarrow C^{(i)} \rightarrow \dots \rightarrow C^{(N_G)} . \quad (2.92)$$

Each global update consists of N_E *elementary updates*, which propose a new configuration by making local changes to the current spectrum, for example by adding or removing a rectangle, shifting the center of a rectangle or by changing the height or width of a rectangle. Since $D[A]$ is in general a complicated functional with many local minima, it would be ineffective to only accept proposed configurations with a lower deviation measure. SOCC therefore splits the N_E elementary updates into two stages:

1. The first stage, consisting of $N_{E_1} < N_E$ updates, accepts configurations with larger deviation measures with a higher probability. This allows the algorithm to escape local minima and explore the configuration space more effectively. During this stage, SOCC also makes use of a *consistent constraint* (CC) update, which is performed periodically after a certain number of elementary updates. It changes a configuration more radically and can speed up the search for a basic solution considerably. The details of the CC update are of technical nature and can be found in Refs. [92, 102].
2. The second stage, consisting of $N_{E_2} = N_E - N_{E_1}$ updates, strongly suppresses configurations with larger $D[A]$ in order to reach a local minimum.

The result of a global update is the configuration C' with the lowest deviation measure that was generated in the course of the two stages. It is only accepted as

the next configuration $C^{(i+1)}$ in Eq. 2.92, if its deviation measure is smaller than that of the current spectrum $C^{(i)}$, otherwise it is rejected, i.e.

$$C^{(i)} \rightarrow \begin{cases} C^{(i+1)} = C' & \text{if } D[A'] < D[A^{(i)}] \\ C^{(i+1)} = C^{(i)} & \text{otherwise} \end{cases} . \quad (2.93)$$

After N_G global updates, if the last configuration, $C^{(N_G)}$, fulfills $D[A^{(N_G)}] < D_{\max}$, where $D_{\max}$ is some maximal tolerance, it is stored as a basic solution for further processing.

Once a set of L basic solutions is found, they can be combined to form the final spectrum

$$A_f(\omega) = \sum_{l=1}^L c_l A_l(\omega) . \quad (2.94)$$

Here, c_l are coefficients which should be normalized to unity, $\sum_l c_l = 1$.

In the original SOM formulation [50], the coefficients are simply chosen to be $c_l = 1/L$ such that Eq. 2.94 represents the mean of all basic solutions. Although each $A_l(\omega)$ on its own possesses sawtooth instabilities, those fluctuations can be expected to average out in the final solution due to the stochastic nature of how they are generated. Including more basic solutions in the averaging procedure, i.e. increasing L , should therefore result in a smoother $A_f(\omega)$.

SOCC employs a more flexible strategy, where the optimal c_l are determined via a self-consistent optimization procedure based on the method of consistent constraints. Besides calculating the coefficients that produce the smoothest possible solution, one can also incorporate other constraints or prior knowledge about the problem to enforce some expected behavior. The main idea is to minimize some objective function, $O(\mathbf{c}) = \sum_i o_i(\mathbf{c})$, where $o_i(\mathbf{c})$ is a quadratic positive-definite form of the coefficient vector $\mathbf{c} = (c_1, \dots, c_L)$. The terms $o_i(\mathbf{c})$ can be chosen, for example, to penalize non-smooth behavior in the final solution or deviation from some default model. For readers, who are interested in the technicalities and various default parameters, we suggest Ref. [92] and the online documentation of Ref. [87].

Note that the computationally most expensive part of SOCC is the accumulation of basic solutions. However, it is trivial to generate them in parallel on multiple cores, since they are independent of each other.

Chapter 3

Diagrammatic Monte Carlo for Polarons

One of the early successes of DiagMC was its application to the Fröhlich polaron problem. In 1998, Prokof'ev and Svistunov demonstrated how DiagMC can be used to calculate imaginary time single-electron Green's functions, $G(\mathbf{k}, \tau)$, for the three-dimensional (3D) Fröhlich polaron at zero temperature [49]. Using the asymptotic behavior of $G(\mathbf{k}, \tau)$, they were able to extract the GS energy and quasiparticle weight as a function of the polaron wave vector $\mathbf{k}$ as well as the electron-phonon coupling strength α .

In a follow-up paper [50], Mishchenko *et al.* improved the DiagMC approach to the 3D Fröhlich polaron problem by introducing direct MC estimators for various GS properties: energy, quasiparticle weight, effective mass and group velocity. To get more information on the phonon cloud surrounding the electron, such as the average number of phonons or their distribution, they extended the DiagMC simulation to single-electron- N -phonon Green's functions, $G_{N_{\text{ph}}}(\mathbf{k}, \mathbf{q}_1, \dots, \mathbf{q}_{N_{\text{ph}}}, \tau) = G_{N_{\text{ph}}}(\mathbf{k}, \underline{\mathbf{q}}, \tau)$. Additionally, an estimator for $G(\mathbf{k}, \tau)$ was derived, which does not suffer from any systematic errors usually inherent to histograms. The numerically more exact data for $G(\mathbf{k}, \tau)$ enabled the authors to perform NAC and thus study excited states via the real frequency spectral function, $A(\mathbf{k}, \omega)$.

Subsequently, Mishchenko *et al.* further developed their approach to obtain the imaginary time current-current correlation function, $\Pi(\tau)$, and the corresponding optical conductivity, $\sigma(\omega)$, for the Fröhlich Hamiltonian [51].

Since then, the same combination of DiagMC and NAC has been applied to numerous other electron-phonon systems. For example, it was used to study GS properties and OC of the Holstein polaron [54, 55], self-trapping behavior in the Rashba-Pekar model [57], GS properties of the SSH [42, 64] and acoustic continuum polaron [63], GS properties, spectral functions and OC of the t - J model [58–60] and spectral functions of the $tt't''$ - J model [61, 62].

All these calculations have in common that they work with some specialized form of the general polaron Hamiltonian from Eq. 1.29. For the sake of convenience, let us reproduce it here once more:

$$\hat{H}_{\text{pol}} = \hat{H}_{\text{el}} + \hat{H}_{\text{ph}} + \hat{H}_{\text{el-ph}} , \quad (3.1)$$

$$\hat{H}_{\text{el}} = \sum_{n\mathbf{k}} \varepsilon_{n\mathbf{k}} \hat{c}_{n\mathbf{k}}^\dagger \hat{c}_{n\mathbf{k}} , \quad (3.2)$$

$$\hat{H}_{\text{ph}} = \sum_{\mathbf{q}\nu} \hbar\omega_{\mathbf{q}\nu} \hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu} , \quad (3.3)$$

$$\hat{H}_{\text{el-ph}} = \frac{1}{\sqrt{N}} \sum_{\substack{\mathbf{k}\mathbf{q} \\ mn\nu}} g_{mn\nu}(\mathbf{k}, \mathbf{q}) \hat{c}_{m\mathbf{k}+\mathbf{q}}^\dagger \hat{c}_{n\mathbf{k}} \left(\hat{a}_{\mathbf{q}\nu} + \hat{a}_{-\mathbf{q}\nu}^\dagger \right) . \quad (3.4)$$

From a numerical point of view, the various models only differ in their crystal structure, dimensionality, number of electron bands and phonon branches and in their analytic expressions for the electron band structure $\varepsilon_{n\mathbf{k}}$, phonon frequencies $\omega_{\mathbf{q}\nu}$ and electron-phonon matrix elements $g_{mn\nu}(\mathbf{k}, \mathbf{q})$. In particular, this means that their diagrammatic expansions of many-body Green's functions and other correlation functions contain exactly the same Feynman diagrams. It should therefore be possible to develop and implement a generic DiagMC algorithm, which can be used for any effective polaron model given in the form of Eqs. 3.1–3.4.

This chapter builds on the basic introduction given in Sec. 2.2 and discusses the most important aspects of a DiagMC algorithm for polaron problems. Detailed derivations of MC estimators, instructions on update procedures and various other implementation specifics can readily be found in some of the studies cited above, e.g. Refs. [49, 50, 103], as well as publicly available dissertations [70, 104] and lecture notes [81, 84, 105]. We will therefore refrain from repeating all the technical details here and instead focus on the bigger picture, how the algorithm for polarons relates to the algorithm for the simple toy model described in Sec. 2.2.3 and some of the intricacies that DiagMC users should be aware of.

Section 3.1 starts with a summary of several polaron properties that we are interested in and that can be calculated with DiagMC. In Section 3.2, we review some essential theory of many-body Green's functions and other correlation functions and how they relate to measurable quantities. Section 3.3 introduces polaron specific diagrammatic expansions and corresponding Feynman diagrams for the single-electron Green's function $G(m\mathbf{k}, \tau)$, the single-electron-N-phonon Green's function $G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n}_{\mathbf{q}\nu}, \tau)$ and the current-current correlation function $\Pi(\tau)$. Finally, DiagMC specific implementation details, especially possible updates and measurements, are provided in Sec. 3.4.

As already mentioned in Sec. 1.1, we will only consider the single polaron limit

at zero temperature. However, DiagMC can also be used for finite temperature [52, 56] and finite electron density calculations [106, 107]. While the differences between the zero and finite temperature DiagMC algorithm for a single polaron are small (we will discuss some of them in the following sections), finite density simulations need to be done with the bold diagrammatic MC technique due to the fermionic sign problem [108]. The details for the bold line extensions are beyond the scope of this thesis. Instead, we refer the interested reader to Refs. [70, 81, 105] for an overview.

3.1 Polaron properties

Our goal in studying polaron Hamiltonians is to learn how the properties of an electron change with varying electron-phonon coupling strengths and different interaction mechanisms. Before introducing various quantities of interest, let us state some general facts about $\hat{H}_{\text{pol}}$.

The polaron Hamiltonian, $\hat{H}_{\text{pol}} = \hat{H}_0 + \hat{H}_1$, can be split into an exactly solvable part consisting of the free electron and phonon subsystems

$$\hat{H}_0 = \hat{H}_{\text{el}} + \hat{H}_{\text{ph}} = \sum_{n\mathbf{k}} \varepsilon_{n\mathbf{k}} \hat{c}_{n\mathbf{k}}^\dagger \hat{c}_{n\mathbf{k}} + \sum_{\mathbf{q}\nu} \hbar\omega_{\mathbf{q}\nu} \hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu} , \quad (3.5)$$

and the remaining part describing their interactions

$$\hat{H}_1 = \hat{H}_{\text{el-ph}} = \frac{1}{\sqrt{N}} \sum_{\substack{\mathbf{k}\mathbf{q} \\ m\nu}} g_{m\nu}(\mathbf{k}, \mathbf{q}) \hat{c}_{m\mathbf{k}+\mathbf{q}}^\dagger \hat{c}_{m\mathbf{k}} \left(\hat{a}_{\mathbf{q}\nu} + \hat{a}_{-\mathbf{q}\nu}^\dagger \right) . \quad (3.6)$$

The eigenstates and eigenvalues of $\hat{H}_0$ are known. Considering only the subspace spanned by single-electron Bloch states $|m\mathbf{k}_{\text{el}}\rangle$, we write them as

$$\begin{aligned} \hat{H}_0 |m\mathbf{k}_{\text{el}}, n_{\mathbf{q}_1\nu_1}, \dots, n_{\mathbf{q}_N\nu_r}\rangle &= \left(\varepsilon_{m\mathbf{k}_{\text{el}}} + \sum_{\mathbf{q}\nu} \hbar\omega_{\mathbf{q}\nu} n_{\mathbf{q}\nu} \right) |m\mathbf{k}_{\text{el}}, n_{\mathbf{q}_1\nu_1}, \dots, n_{\mathbf{q}_N\nu_r}\rangle \\ &= \left(\varepsilon_{m\mathbf{k}_{\text{el}}} + \sum_{\mathbf{q}\nu} \hbar\omega_{\mathbf{q}\nu} n_{\mathbf{q}\nu} \right) |m\mathbf{k}_{\text{el}}, \underline{n_{\mathbf{q}\nu}}\rangle , \end{aligned} \quad (3.7)$$

where N is the number of unit cells in the BvK supercell, r is the number of phonon branches, $n_{\mathbf{q}\nu}$ denotes the number of phonons in the state $|\mathbf{q}\nu\rangle$ and $\underline{n_{\mathbf{q}\nu}} = (n_{\mathbf{q}_1\nu_1}, \dots, n_{\mathbf{q}_N\nu_r})$ is a vector notation for a specific phonon occupation. The expected number of phonons in a given state is then

$$N_{\text{ph}}(\underline{n_{\mathbf{q}\nu}}) = \left\langle m\mathbf{k}_{\text{el}}, \underline{n_{\mathbf{q}\nu}} \left| \sum_{\mathbf{q}\nu} \hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu} \right| m\mathbf{k}_{\text{el}}, \underline{n_{\mathbf{q}\nu}} \right\rangle = \sum_{\mathbf{q}\nu} n_{\mathbf{q}\nu} . \quad (3.8)$$

The total wave vector of the combined electron-phonon system, the polaron wave vector, is represented by the operator

$$\hat{\mathbf{k}} = \sum_{n\mathbf{k}'} \mathbf{k}' \hat{c}_{n\mathbf{k}'}^\dagger \hat{c}_{n\mathbf{k}'} + \sum_{\mathbf{q}\nu} \mathbf{q} \hat{a}_{\mathbf{q}\nu}^\dagger \hat{a}_{\mathbf{q}\nu} . \quad (3.9)$$

Since the eigenstates of $\hat{H}_0$ are simultaneous eigenstates of $\hat{\mathbf{k}}$, i.e.

$$\hat{\mathbf{k}} \left| m\mathbf{k}_{\text{el}}, \underline{n_{\mathbf{q}\nu}} \right\rangle = \left(\mathbf{k}_{\text{el}} + \sum_{\mathbf{q}\nu} \mathbf{q} n_{\mathbf{q}\nu} \right) \left| m\mathbf{k}_{\text{el}}, \underline{n_{\mathbf{q}\nu}} \right\rangle = \mathbf{k} \left| m\mathbf{k}_{\text{el}}, \underline{n_{\mathbf{q}\nu}} \right\rangle , \quad (3.10)$$

$\hat{H}_0$ commutes with $\hat{\mathbf{k}}$ and therefore conserves the total wave vector $\mathbf{k}$ [109]. If we ignored the so-called Umklapp processes in $\hat{H}_1$, i.e. terms for which $\mathbf{G}_{\mathbf{m}} \neq 0$ (see Eq. 1.27), then $[\hat{\mathbf{k}}, \hat{H}_1] = 0$ and $\mathbf{k}$ would also be a constant of motion for $\hat{H}_{\text{pol}}$. This is not true anymore for the general case, since states with total wave vector $\mathbf{k}$ can mix with states with total wave vector $\mathbf{k} + \mathbf{G}_{\mathbf{m}}$ for some reciprocal lattice vector. Nevertheless, it is still possible to use $\mathbf{k}$ as a good quantum number for the polaron Hamiltonian by restricting it to the first BZ.

The usual starting point when studying any quantum system is the time-independent Schrödinger equation

$$\hat{H}_{\text{pol}} |\eta, \mathbf{k}\rangle = E_\eta(\mathbf{k}) |\eta, \mathbf{k}\rangle , \quad (3.11)$$

which provides the polaron energies $E_\eta(\mathbf{k})$ and polaron states $|\eta, \mathbf{k}\rangle$. Here, η indexes different eigenstates with the same polaron wave vector $\mathbf{k}$. The GS and corresponding energy will be denoted by $|0, \mathbf{k}\rangle$ and $E_0(\mathbf{k})$, respectively.

A property closely related to the polaron energy dispersion, $E_\eta(\mathbf{k})$, is its effective mass. The $\mathbf{k}$ -dependent effective polaron mass tensor, $m_{ij}^*(\mathbf{k})$, is defined in the usual way

$$\frac{1}{m_{ij}^*(\mathbf{k})} = \frac{1}{\hbar^2} \frac{\partial E_0(\mathbf{k})}{\partial k_i \partial k_j} = \frac{1}{\hbar^2} [\mathcal{H}_{E_0}(\mathbf{k})]_{ij} , \quad (3.12)$$

where i and j are Cartesian directions and $\mathcal{H}_{E_0}(\mathbf{k})$ is the Hessian matrix of E_0 evaluated at $\mathbf{k}$. In this thesis, we are only interested in the effective mass at the bottom of the polaron band, which for all our models is located at the Γ -point, i.e. at $\mathbf{k} = 0$. Moreover, the diagonal entries of $m_{ij}^*(\mathbf{k} = 0)$ turn out to be equal due to symmetry considerations, e.g. spherical symmetry in the Fröhlich model or cubic symmetry in the acoustic lattice model. We therefore simply use the notation $m^* = m_{ii}^*(\mathbf{k} = 0)$ for the effective mass of the polaron.

In general, any polaron eigenstate $|\eta, \mathbf{k}\rangle$ can be written as a linear combination of non-interacting electron and phonon states:

$$\begin{aligned}
 |\eta, \mathbf{k}\rangle &= \sum_m \sum_{n_{\mathbf{q}_1 \nu_1}} \cdots \sum_{n_{\mathbf{q}_N \nu_r}} \Theta_{m, n_{\mathbf{q}_1 \nu_1} \dots n_{\mathbf{q}_N \nu_r}}^{(\eta, \mathbf{k})} |m \mathbf{k}_{\text{el}}, n_{\mathbf{q}_1 \nu_1}, \dots, n_{\mathbf{q}_N \nu_r}\rangle \\
 &= \sum_m \sum_{n_{\mathbf{q}_1 \nu_1}} \cdots \sum_{n_{\mathbf{q}_N \nu_r}} \Theta_{m, n_{\mathbf{q}_1 \nu_1} \dots n_{\mathbf{q}_N \nu_r}}^{(\eta, \mathbf{k})} \hat{c}_{m \mathbf{k}_{\text{el}}}^\dagger \frac{(\hat{a}_{\mathbf{q}_1 \nu_1}^\dagger)^{n_{\mathbf{q}_1 \nu_1}}}{\sqrt{n_{\mathbf{q}_1 \nu_1}!}} \cdots \frac{(\hat{a}_{\mathbf{q}_N \nu_r}^\dagger)^{n_{\mathbf{q}_N \nu_r}}}{\sqrt{n_{\mathbf{q}_N \nu_r}!}} |\emptyset\rangle \\
 &= \sum_m \sum_{\underline{n}_{\mathbf{q}\nu}} \Theta_{m, \underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})} |m \mathbf{k}_{\text{el}}, \underline{n}_{\mathbf{q}\nu}\rangle,
 \end{aligned} \tag{3.13}$$

where $\Theta_{m, \underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})}$ are expansion coefficients, $|\emptyset\rangle$ is the electron-phonon vacuum state and summations run over all electron bands m and over all possible phonon occupations. The electron wave vector is fixed by the condition

$$\mathbf{k}_{\text{el}} = \mathbf{k} - \sum_{\mathbf{q}\nu} \mathbf{q} n_{\mathbf{q}\nu} + \mathbf{G}_{\mathbf{m}} \quad \wedge \quad \mathbf{k}_{\text{el}}, \mathbf{k}, \mathbf{q} \in 1.\text{BZ}, \tag{3.14}$$

for some $\mathbf{G}_{\mathbf{m}}$.

Assuming that $|\eta, \mathbf{k}\rangle$ is normalized, the absolute squared value of an expansion coefficient can be interpreted as the probability that the polaron state contains the electron in band m , $n_{\mathbf{q}_1 \nu_1}$ phonons with wave vector $\mathbf{q}_1$ in branch ν_1 , $n_{\mathbf{q}_1 \nu_2}$ phonons with wave vector $\mathbf{q}_1$ in branch ν_2 , and so on:

$$Z_{m, \underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})} = \left| \Theta_{m, \underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})} \right|^2 = \left| \langle \eta, \mathbf{k} | m \mathbf{k}_{\text{el}}, \underline{n}_{\mathbf{q}\nu} \rangle \right|^2. \tag{3.15}$$

A special name is given to the squared overlap of the polaron state with the free electron state, the so-called quasiparticle weight:

$$Z_m^{(\eta, \mathbf{k})} = Z_{m, \underline{n}_{\mathbf{q}\nu}=0}^{(\eta, \mathbf{k})} = |\langle \eta, \mathbf{k} | m \mathbf{k} \rangle|^2 = \left| \langle \eta, \mathbf{k} | \hat{c}_{m \mathbf{k}}^\dagger | \emptyset \rangle \right|^2. \tag{3.16}$$

In the following, we derive more general probabilities based on $Z_{m, \underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})}$. It shall be noted that one can come up with several other ways to combine the individual $Z_{m, \underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})}$ and so obtain different information on the phonon cloud of the polaron.

We start by summing $Z_{m, \underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})}$ over all bands m . This gives us the probability of finding the specific phonon occupation $\underline{n}_{\mathbf{q}\nu}$ in the state $|\eta, \mathbf{k}\rangle$ irrespective of the electron band:

$$Z_{\underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})} = \sum_m Z_{m, \underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})}. \tag{3.17}$$

Furthermore, we introduce the phonon distribution function, $Z_{N_{\text{ph}}}^{(\eta, \mathbf{k})}$. It is defined

as the probability that a polaron state contains exactly N_{ph} phonons. To get $Z_{N_{\text{ph}}}^{(\eta, \mathbf{k})}$, $Z_{\underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})}$ has to be summed over all possible phonon occupations with the restriction that the total number of phonons is equal to N_{ph} , i.e.

$$Z_{N_{\text{ph}}}^{(\eta, \mathbf{k})} = \sum_{n_{\mathbf{q}_1\nu_1}}^{\sum_{\mathbf{q}\nu} n_{\mathbf{q}\nu}=N_{\text{ph}}} \cdots \sum_{n_{\mathbf{q}_N\nu_r}} Z_{\underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})} = \sum_{\underline{n}_{\mathbf{q}\nu}}^{N_{\text{ph}}} Z_{\underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})}. \quad (3.18)$$

The phonon number distribution has the simple normalization condition

$$\sum_{N_{\text{ph}}=0}^{\infty} Z_{N_{\text{ph}}}^{(\eta, \mathbf{k})} = 1. \quad (3.19)$$

Closely related to the phonon number distribution is the average number of phonons in the polaron state. Using the probability interpretation of $Z_{N_{\text{ph}}}^{(\eta, \mathbf{k})}$ and Eq. 3.19, it is simply given as

$$\langle N_{\text{ph}} \rangle^{(\eta, \mathbf{k})} = \sum_{N_{\text{ph}}=0}^{\infty} N_{\text{ph}} Z_{N_{\text{ph}}}^{(\eta, \mathbf{k})}. \quad (3.20)$$

In Chapter 5 on the acoustic lattice polaron, we calculate two more probabilities related to the phonon cloud. For this purpose, let us first introduce so-called LME and HME phonons. An LME phonon has a wave vector close to the Γ -point and a lower energy, whereas an HME phonon lies in the vicinity of the BZ boundary with a higher energy (see inset of Fig. 5.3). More specifically, we divide the first BZ into two volumes: (i) a sphere centered around the Γ -point with volume $V_{\text{LME}} = V_{\text{BZ}}f$ and corresponding radius

$$q_f = \sqrt[3]{\frac{3V_{\text{BZ}}f}{4\pi}}, \quad (3.21)$$

and (ii) the rest of the BZ with volume $V_{\text{HME}} = V_{\text{BZ}}(1 - f)$, where $f \in [0, 1]$. A phonon with wave vector $\mathbf{q}$ is now classified as LME if $|\mathbf{q}| < q_f$, or equivalently if $\mathbf{q} \in \text{LME}$, and as HME otherwise. Similar to the phonon number distribution in Eq. 3.18, it is possible to define the quantity $Z_{N_{\text{LME}}}^{(\eta, \mathbf{k})}$ ($Z_{N_{\text{HME}}}^{(\eta, \mathbf{k})}$) as the probability of finding N_{LME} LME (N_{HME} HME) phonons in the polaron state $|\eta, \mathbf{k}\rangle$:

$$Z_{N_{\alpha}}^{(\eta, \mathbf{k})} = \sum_{n_{\mathbf{q}_1\nu_1}}^{\sum_{\mathbf{q}\nu} n_{\mathbf{q}\nu}=N_{\alpha}} \cdots \sum_{n_{\mathbf{q}_N\nu_r}} Z_{\underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})} = \sum_{\underline{n}_{\mathbf{q}\nu}}^{N_{\alpha}} Z_{\underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})}, \quad (3.22)$$

Here, the summation over all possible phonon occupations is restricted to states with exactly N_{α} α phonons, where α can be replaced with either LME or HME.

Note that the normalization from Eq. 3.19 is still satisfied:

$$\sum_{N_{\text{LME}}=0}^{\infty} Z_{N_{\text{LME}}}^{(\eta, \mathbf{k})} = 1, \quad \sum_{N_{\text{HME}}=0}^{\infty} Z_{N_{\text{HME}}}^{(\eta, \mathbf{k})} = 1. \quad (3.23)$$

The rest of this thesis is mostly concerned with phonon cloud properties of the polaron GS at the Γ -point. We therefore use the simplified notation $\langle N_{\text{ph}} \rangle = \langle N_{\text{ph}} \rangle^{(0, \mathbf{k}=0)}$ and $Z_{\beta} = Z_{\beta}^{(0, \mathbf{k}=0)}$, where β depends on the type of Z-factor.

Information on excited states is contained in the spectral function $A(m\mathbf{k}, \omega)$ and optical conductivity $\sigma_{ij}(\mathbf{k}, \omega)$ at zero temperature. $A(m\mathbf{k}, \omega)$ is closely related to the imaginary time single-electron Green's function, $G(m\mathbf{k}, \tau)$, whereas $\sigma_{ij}(\mathbf{k}, \omega)$ is calculated from the imaginary time current-current correlation function, $\Pi_{ij}(\mathbf{k}, \tau)$. They are discussed in more detail in Sec. 3.2.1 and Sec. 3.2.3, respectively. The connection of $A(m\mathbf{k}, \omega)$ and $\sigma_{ij}(\mathbf{k}, \omega)$ to the excited spectrum is easily seen from their Lehmann representations:

$$A(m\mathbf{k}, \omega) = \sum_{\eta} \left| \langle \eta, \mathbf{k} | \hat{c}_{m\mathbf{k}}^{\dagger} | \emptyset \rangle \right|^2 \delta(\omega - E_{\eta}(\mathbf{k})/\hbar), \quad (3.24)$$

$$\sigma_{ij}(\mathbf{k}, \omega) = \frac{\pi}{\omega} \sum_{\eta} \langle 0, \mathbf{k} | \hat{j}_i | \eta, \mathbf{k} \rangle \langle \eta, \mathbf{k} | \hat{j}_j | 0, \mathbf{k} \rangle \delta(\omega + [E_0(\mathbf{k}) - E_{\eta}(\mathbf{k})]/\hbar). \quad (3.25)$$

Here, $\hat{j}_i$ is the charge current operator for the Cartesian direction i . Its expression for the polaron Hamiltonian consists of two terms, one originating from $\hat{H}_{\text{el}}$ and the other from $\hat{H}_{\text{el-pol}}$, and its general form is rather complicated. We will only consider the electronic contribution and further assume that it is diagonal in the band indices. This is justified for the model systems in the current thesis. The current operator may then be written in terms of the band velocity of the electron [110]

$$\hat{j}_i = -\frac{e}{\hbar} \sum_{n\mathbf{k}} \frac{\partial \varepsilon_{n\mathbf{k}}}{\partial k_i} \hat{c}_{n\mathbf{k}}^{\dagger} \hat{c}_{n\mathbf{k}}, \quad (3.26)$$

where e is the elementary charge. A more detailed discussion on current operators for electron-phonon systems can be found in Ref. [103].

Similar to the other polaron properties, we will use a simplified notation for specific results: $A(\omega) = A(\mathbf{k} = 0, \omega)$ for spectral functions of single-band models at the Γ -point and $\Pi(\tau) = \Pi_{ii}(\mathbf{k} = 0, \tau)$ and $\sigma(\omega) = \sigma_{ii}(\mathbf{k} = 0, \omega)$ for the diagonal entries of current-current correlation functions and optical conductivities at the Γ -point, respectively.

The next section shows how various polaron properties can be calculated with the help of many-body Green's functions.

3.2 Many-body Green's functions and correlation functions

In quantum mechanics, physically measurable quantities often appear as some kind of averages, either as expectation values of operators, $\overline{A}(t) = \langle \hat{A}(t) \rangle$, or as correlation functions between them, $C_{AB}(t, t') = \langle \hat{A}(t) \hat{B}(t') \rangle$. The calculation of these averages requires the full knowledge of the eigenfunctions, $|\Psi_n\rangle$, and eigenvalues, E_n , of a given system, which have to be obtained as solutions to the corresponding Schrödinger equation, $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$. For interacting many-body systems, this quickly becomes an impossible task and it is necessary to resort to approximate schemes.

The method of Green's functions offers a direct way to calculate averages such as $\overline{A}(t)$ and $C_{AB}(t, t')$ without knowing $|\Psi_n\rangle$ and E_n in advance. For this purpose, it uses an infinite series expansion in terms of Feynman diagrams. Compared to ordinary perturbation theory, this allows for a more systematic approach to the problem since drawing all Feynman diagrams of a given order is much easier than writing down the complicated terms of a perturbation series. It also becomes possible to carry out perturbation theory up to infinite order by restricting the sum to a specific class of diagrams. Such partial summation techniques are crucial for systems that have divergent terms in the low-order perturbation expansion, e.g. the jellium model [17, 111]. Additionally, Feynman diagrams usually have a straightforward physical interpretation in which particles propagate and interact with each other.

Many-body Green's functions and correlation functions can appear in different forms: retarded, advanced, causal (time-ordered), greater, lesser, and so on [17]. They are usually closely interrelated but depending on the problem, one might be more useful than the others. In the following, we will not bother about the terminology and simply give the mathematical definition that will be used for our DiagMC algorithm.

Let us start by defining a general real time correlation function at some temperature $T = 1/(k_B\beta)$ as

$$C_{AB}(t, t') = \langle \hat{A}(t) \hat{B}(t') \rangle = Z^{-1} \text{Tr} \left[e^{-\hat{H}\beta} \hat{A}(t) \hat{B}(t') \right]. \quad (3.27)$$

Here, $\hat{H}$ is the Hamiltonian of the system, $\langle \dots \rangle$ represents an ensemble average, $Z = \text{Tr} \left[e^{-\hat{H}\beta} \right]$ is the partition function and $\hat{A}(t)$ and $\hat{B}(t')$ are arbitrary operators

in the Heisenberg picture, i.e.

$$\hat{A}(t) = e^{i\hat{H}t/\hbar} \hat{A} e^{-i\hat{H}t/\hbar}, \quad \hat{B}(t') = e^{i\hat{H}t'/\hbar} \hat{B} e^{-i\hat{H}t'/\hbar}. \quad (3.28)$$

At zero temperature, the ensemble average in Eq. 3.27 simplifies to an expectation value with respect to the ground state $|\Psi_0\rangle$:

$$C_{AB}(t, t') = \left\langle \Psi_0 \left| \hat{A}(t) \hat{B}(t') \right| \Psi_0 \right\rangle. \quad (3.29)$$

Note that the finite temperature correlation function contains two different kinds of exponential operators, one with a purely real $(-\hat{H}\beta)$ and others with purely imaginary $(\pm i\hat{H}t/\hbar)$ exponents. This would lead to various complications when we later want to perform the perturbation expansion. Mathematically, it is more convenient to work with imaginary times. Introducing the real quantity $\tau = it$, we can define the imaginary time (Matsubara) analog of Eq. 3.27 as

$$C_{AB}(\tau, \tau') = \left\langle \hat{A}(\tau) \hat{B}(\tau') \right\rangle = Z^{-1} \text{Tr} \left[e^{-\hat{H}\beta} \hat{A}(\tau) \hat{B}(\tau') \right], \quad (3.30)$$

with the modified Heisenberg operators

$$\hat{A}(\tau) = e^{\hat{H}\tau/\hbar} \hat{A} e^{-\hat{H}\tau/\hbar}, \quad \hat{B}(\tau') = e^{\hat{H}\tau'/\hbar} \hat{B} e^{-\hat{H}\tau'/\hbar}. \quad (3.31)$$

Although the imaginary time formalism is usually associated only with finite temperature calculations, it is also better suited for the DiagMC algorithm at zero temperature. The corresponding correlation function takes the form

$$C_{AB}(\tau, \tau') = \left\langle \Psi_0 \left| \hat{A}(\tau) \hat{B}(\tau') \right| \Psi_0 \right\rangle. \quad (3.32)$$

From now on, we will exclusively work with imaginary times unless otherwise noted.

Before introducing various specializations of Eq. 3.32, let us state a useful property of $C_{AB}(\tau, \tau')$: For time-independent Hamiltonians, $C_{AB}(\tau, \tau')$ only depends on the difference $\tau - \tau'$, allowing us to focus on $C_{AB}(\tau) = C_{AB}(\tau, 0)$ without loss of generality [111].

3.2.1 Single-electron Green's function

The main quantity of interest for our calculations is the zero temperature single-electron Green's function. It is defined as follows:

$$G(m\mathbf{k}, \tau) = \left\langle \emptyset \left| \hat{c}_{m\mathbf{k}}(\tau) \hat{c}_{m\mathbf{k}}^\dagger(0) \right| \emptyset \right\rangle. \quad (3.33)$$

Here, $\tau \geq 0$ and $|\emptyset\rangle$ is the electron and phonon vacuum state. The reason why we use $|\emptyset\rangle$ instead of the polaron GS, $|0, \mathbf{k} = 0\rangle$, is connected to the fact that we are only interested in the single polaron limit. Note that many textbooks have an extra factor of -1 on the right-hand side of Eq. 3.33. For our purposes, however, it is more convenient to omit this convention.

$G(m\mathbf{k}, \tau)$ gives the probability amplitude to add an electron in the Bloch state $|m\mathbf{k}\rangle$ to the system and to find it in the same state at a later time τ . This becomes obvious, when we plug the τ -dependence of the modified Heisenberg operators into Eq. 3.33 and use $e^{\hat{H}_{\text{pol}}\tau/\hbar}|0\rangle = |0\rangle$:

$$G(m\mathbf{k}, \tau) = \langle \emptyset | e^{\hat{H}_{\text{pol}}\tau/\hbar} \hat{c}_{m\mathbf{k}} e^{-\hat{H}_{\text{pol}}\tau/\hbar} \hat{c}_{m\mathbf{k}}^\dagger | \emptyset \rangle = \langle m\mathbf{k} | e^{-\hat{H}_{\text{pol}}\tau/\hbar} | m\mathbf{k} \rangle . \quad (3.34)$$

The operator, $\hat{U}(\tau) = \hat{U}(\tau, 0) = e^{-\hat{H}_{\text{pol}}\tau/\hbar}$, is just the imaginary time analog of the time-evolution operator for a time-independent Hamiltonian in the Schrödinger picture and has the effect of evolving a state in imaginary time according to the Schrödinger equation:

$$-\hbar \frac{\partial |\psi(\tau)\rangle}{\partial \tau} = \hat{H}_{\text{pol}} |\psi(\tau)\rangle . \quad (3.35)$$

To see how certain polaron properties can be obtained from $G(m\mathbf{k}, \tau)$, let us insert a complete set of polaron eigenstates into Eq. 3.33:

$$\begin{aligned} G(m\mathbf{k}, \tau) &= \sum_{\eta} \langle \emptyset | \hat{c}_{m\mathbf{k}}(\tau) | \eta, \mathbf{k} \rangle \langle \eta, \mathbf{k} | \hat{c}_{m\mathbf{k}}^\dagger(0) | \emptyset \rangle \\ &= \sum_{\eta} e^{-E_{\eta}(\mathbf{k})\tau/\hbar} \langle \emptyset | \hat{c}_{m\mathbf{k}} | \eta, \mathbf{k} \rangle \langle \eta, \mathbf{k} | \hat{c}_{m\mathbf{k}}^\dagger | \emptyset \rangle \\ &= \sum_{\eta} e^{-E_{\eta}(\mathbf{k})\tau/\hbar} Z_m^{(\eta, \mathbf{k})} , \end{aligned} \quad (3.36)$$

where $E_{\eta}(\mathbf{k})$ is the polaron energy and $Z_m^{(\eta, \mathbf{k})}$ is the quasiparticle weight from Eq. 3.11 and 3.16, respectively. If we assume that $E_{\eta}(\mathbf{k})$ is positive and that there is a finite energy gap between the polaron GS and all excited states, the term with the lowest energy, i.e. $E_0(\mathbf{k})$, will dominate the behavior of $G(m\mathbf{k}, \tau)$ for large τ values. Taking the limit $\tau \rightarrow \infty$, we get

$$G(m\mathbf{k}, \tau \rightarrow \infty) \xrightarrow{\tau \rightarrow \infty} e^{-E_0(\mathbf{k})\tau/\hbar} Z_m^{(0, \mathbf{k})} , \quad (3.37)$$

which enables us to calculate the polaron energy dispersion $E_0(\mathbf{k})$, the corresponding quasiparticle weights $Z_m^{(0, \mathbf{k})}$ and other derived quantities, like the polaron effective mass (see Eq. 3.12).

Furthermore, $G(m\mathbf{k}, \tau)$ is also related to the real frequency spectral function, $A(m\mathbf{k}, \omega)$, via the integral equation

$$G(m\mathbf{k}, \tau) = \int_0^\infty d\omega e^{-\tau\omega} A(m\mathbf{k}, \omega) . \quad (3.38)$$

Together with Eq. 3.36, it is now clear that Eq. 3.24 is indeed the correct Lehmann representation of $A(m\mathbf{k}, \omega)$. The spectral function provides energies of various excited states of the polaron as well as their corresponding spectral weights, $Z_m^{(\eta, \mathbf{k})}$. As already discussed in Sec. 2.3, to retrieve $A(m\mathbf{k}, \omega)$ from a known $G(m\mathbf{k}, \tau)$, one has to perform numerical analytical continuation.

3.2.2 Single-electron-N-phonon Green's function

Another interesting quantity for the polaron problem is the zero temperature single-electron-N-phonon Green's function. Its definition and interpretation are similar to $G(m\mathbf{k}, \tau)$, except that additional N_{ph} phonons are added to the vacuum state:

$$\begin{aligned} G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n}_{\mathbf{q}\nu}, \tau) &= \left\langle \emptyset \left| \prod_{\mathbf{q}\nu} \frac{(\hat{a}_{\mathbf{q}\nu}(\tau))^{n_{\mathbf{q}\nu}}}{\sqrt{n_{\mathbf{q}\nu}!}} \hat{c}_{m\mathbf{k}_{\text{el}}}(\tau) \hat{c}_{m\mathbf{k}_{\text{el}}}^\dagger(0) \prod_{\mathbf{q}\nu} \frac{(\hat{a}_{\mathbf{q}\nu}^\dagger(0))^{n_{\mathbf{q}\nu}}}{\sqrt{n_{\mathbf{q}\nu}!}} \right| \emptyset \right\rangle \\ &= \left\langle m\mathbf{k}_{\text{el}}, \underline{n}_{\mathbf{q}\nu} \left| e^{-\hat{H}_{\text{pol}}\tau/\hbar} \right| m\mathbf{k}_{\text{el}}, \underline{n}_{\mathbf{q}\nu} \right\rangle \\ &= \sum_{\eta} e^{-E_{\eta}(\mathbf{k})\tau/\hbar} Z_{m, \underline{n}_{\mathbf{q}\nu}}^{(\eta, \mathbf{k})} . \end{aligned} \quad (3.39)$$

Here, the electron wave vector, $\mathbf{k}_{\text{el}}$, is given in Eq. 3.14 and $\underline{n}_{\mathbf{q}\nu}$ is some specific phonon occupation with a total of N_{ph} phonons. $G(m\mathbf{k}, \tau)$ is obviously a special case of $G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n}_{\mathbf{q}\nu}, \tau)$ with $N_{\text{ph}} = 0$.

Using the same reasoning as before, the large τ limit takes the form

$$G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n}_{\mathbf{q}\nu}, \tau) \xrightarrow{\tau \rightarrow \infty} e^{-E_0(\mathbf{k})\tau/\hbar} Z_{m, \underline{n}_{\mathbf{q}\nu}}^{(0, \mathbf{k})} , \quad (3.40)$$

and provides us with $E_0(\mathbf{k})$ and the probabilities $Z_{m, \underline{n}_{\mathbf{q}\nu}}^{(0, \mathbf{k})}$ defined in Eq. 3.15.

For the DiagMC algorithm, it will be convenient to also introduce the sum of $G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n}_{\mathbf{q}\nu}, \tau)$ over all phonon occupations:

$$\begin{aligned} P(m\mathbf{k}, \tau) &= \sum_{\underline{n}_{\mathbf{q}\nu}} G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n}_{\mathbf{q}\nu}, \tau) = \sum_{N_{\text{ph}}=0}^{\infty} \sum_{\underline{n}_{\mathbf{q}\nu}}^{N_{\text{ph}}} G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n}_{\mathbf{q}\nu}, \tau) \\ &= \sum_{n_{\mathbf{q}_1\nu_1}} \cdots \sum_{n_{\mathbf{q}_N\nu_r}} G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n}_{\mathbf{q}\nu}, \tau) . \end{aligned} \quad (3.41)$$

Because of Eqs. 3.37, 3.40 and 3.19, $P(m\mathbf{k}, \tau)$ has the limiting behavior

$$P(m\mathbf{k}, \tau) \xrightarrow{\tau \rightarrow \infty} e^{-E_0(\mathbf{k})\tau/\hbar} . \quad (3.42)$$

3.2.3 Current-current correlation function

The zero temperature current-current correlation function is defined as

$$\begin{aligned} \Pi_{ij}(\mathbf{k}, \tau) &= \langle 0, \mathbf{k} | \hat{j}_i(\tau) \hat{j}_j(0) | 0, \mathbf{k} \rangle \\ &= \sum_{\eta} e^{-[E_{\eta}(\mathbf{k}) - E_0(\mathbf{k})]\tau/\hbar} \langle 0, \mathbf{k} | \hat{j}_i | \eta, \mathbf{k} \rangle \langle \eta, \mathbf{k} | \hat{j}_j | 0, \mathbf{k} \rangle , \end{aligned} \quad (3.43)$$

with $\tau \geq 0$ and the current operator $\hat{j}_i$ specified in Eq. 3.26. Note that $|0, \mathbf{k}\rangle$ is the polaron GS, i.e. an eigenstate of $\hat{H}_{\text{pol}}$, and not of $\hat{H}_0$.

The current-current correlation function is a key quantity, as it directly links microscopic dynamics to measurable transport properties; in particular, the optical conductivity $\sigma_{ij}(\mathbf{k}, \omega)$ is obtained from $\Pi_{ij}(\mathbf{k}, \tau)$ via numerical analytic continuation by solving the equation

$$\Pi_{ij}(\mathbf{k}, \tau) = \int_0^{\infty} d\omega \frac{\omega}{\pi} e^{-\tau\omega} \sigma_{ij}(\mathbf{k}, \omega) . \quad (3.44)$$

We can again check the Lehmann representation of $\sigma_{ij}(\mathbf{k}, \omega)$ by plugging Eq. 3.25 into Eq. 3.44 and comparing with Eq. 3.43. Similar to the spectral function, the optical conductivity gives us information on the excited polaron spectrum but with different symmetry selection rules [112].

3.3 Diagrammatic expansions and Feynman diagrams

The previous section has introduced the concept of many-body Green's functions and has shown how they relate to the various polaron properties from Sec. 3.1. However, Eqs. 3.36, 3.39 and 3.43 make it clear that a direct calculation of $G(m\mathbf{k}, \tau)$, $G_{N_{\text{ph}}}(m\mathbf{k}, n_{\text{qu}}, \tau)$ and $\Pi_{ij}(\mathbf{k}, \tau)$ requires the complete polaron spectrum, $E_{\eta}(\mathbf{k})$, and eigenstates, $|\eta, \mathbf{k}\rangle$. To work around this issue, a perturbation expansion of the time-evolution operator, $e^{-\hat{H}_{\text{pol}}\tau/\hbar}$, or the density matrix, $e^{-\beta\hat{H}_{\text{pol}}}$, in the interaction picture can be used. Then, by mapping individual terms of the resulting series to Feynman diagrams, we will immediately be able to write down all contributions

for a given perturbation order and even assign them an intuitive physical interpretation. The diagrammatic series may then be evaluated (approximately) by either focusing on a few dominant terms, by partially summing a specific class of diagrams up to infinite order or by using more sophisticated techniques like DiagMC as discussed in Sec. 3.4.

In the following, we will abstain from deriving the diagrammatic expansions in all its details, something that can be found in many textbooks [17, 85, 111, 113] and other references [70, 103]. Instead, we will only summarize some important steps and put our focus on the mathematical structure of the infinite series, the topology of the Feynman diagrams and the connection to Sec. 2.2 from the last chapter.

3.3.1 Perturbation expansion of the time-evolution operator

As already mentioned above, the derivation of Feynman diagrams is based on an expansion of the imaginary time-evolution operator

$$\hat{U}(\tau) = e^{-\hat{H}_{\text{pol}}\tau/\hbar} = e^{-(\hat{H}_0 + \hat{H}_1)\tau/\hbar}, \quad (3.45)$$

where $\hat{H}_0$ is the non-interacting part of the Hamiltonian given in Eq. 3.5 and $\hat{H}_1$ is the electron-phonon interaction given in Eq. 3.6.

Introducing the modified time-evolution operator

$$\hat{U}^{(I)}(\tau) = e^{\hat{H}_0\tau/\hbar} \hat{U}(\tau). \quad (3.46)$$

and differentiating with respect to τ , leads to a Schrödinger-like differential equation for $\hat{U}^{(I)}(\tau)$:

$$\begin{aligned} \frac{d}{d\tau} \hat{U}^{(I)}(\tau) &= \frac{d}{d\tau} \left(e^{\hat{H}_0\tau/\hbar} e^{-(\hat{H}_0 + \hat{H}_1)\tau/\hbar} \right) \\ &= \frac{1}{\hbar} \hat{H}_0 e^{\hat{H}_0\tau/\hbar} e^{-(\hat{H}_0 + \hat{H}_1)\tau/\hbar} - \frac{1}{\hbar} e^{\hat{H}_0\tau/\hbar} (\hat{H}_0 + \hat{H}_1) e^{-(\hat{H}_0 + \hat{H}_1)\tau/\hbar} \\ &= -\frac{1}{\hbar} e^{\hat{H}_0\tau/\hbar} \hat{H}_1 e^{-(\hat{H}_0 + \hat{H}_1)\tau/\hbar} = -\frac{1}{\hbar} \hat{H}_1^{(I)}(\tau) \hat{U}^{(I)}(\tau), \end{aligned} \quad (3.47)$$

where we have defined the interaction-picture operator

$$\hat{H}_1^{(I)}(\tau) = e^{\hat{H}_0\tau/\hbar} \hat{H}_1 e^{-\hat{H}_0\tau/\hbar}. \quad (3.48)$$

We can integrate Eq. 3.47 from 0 to τ to give

$$\hat{U}^{(I)}(\tau) = \hat{U}^{(I)}(0) - \frac{1}{\hbar} \int_0^\tau d\tau_1 \hat{H}_1^{(I)}(\tau_1) \hat{U}^{(I)}(\tau_1). \quad (3.49)$$

The imaginary time-evolution operator appears again under the integral and so, by using the initial condition $\hat{U}^{(I)}(0) = 1$ and iterating, one obtains an expansion of $\hat{U}^{(I)}(\tau)$ in terms of an infinite series of integrals:

$$\begin{aligned}\hat{U}^{(I)}(\tau) &= 1 - \frac{1}{\hbar} \int_0^\tau d\tau_1 \hat{H}_1^{(I)}(\tau_1) + \left(-\frac{1}{\hbar}\right)^2 \int_0^\tau d\tau_2 \int_0^{\tau_2} d\tau_1 \hat{H}_1^{(I)}(\tau_2) \hat{H}_1^{(I)}(\tau_1) + \dots = \\ &= \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \int_0^\tau d\tau_n \dots \int_0^{\tau_2} d\tau_1 \hat{H}_1^{(I)}(\tau_n) \dots \hat{H}_1^{(I)}(\tau_1) .\end{aligned}\quad (3.50)$$

Textbooks often write this formally as

$$\hat{U}^{(I)}(\tau) = \mathcal{T}_\tau \exp\left(-\frac{1}{\hbar} \int_0^\tau d\tau' \hat{H}_1^{(I)}(\tau')\right) , \quad (3.51)$$

where $\mathcal{T}_\tau$ is the imaginary time-ordering operator [17, 85, 111, 113].

Equations 3.45, 3.46 and 3.50 can be combined into

$$\begin{aligned}e^{-\hat{H}_{\text{pol}}\tau/\hbar} &= e^{-(\hat{H}_0 + \hat{H}_1)\tau/\hbar} \\ &= e^{-\hat{H}_0\tau/\hbar} \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \int_0^\tau d\tau_n \dots \int_0^{\tau_2} d\tau_1 \hat{H}_1^{(I)}(\tau_n) \dots \hat{H}_1^{(I)}(\tau_1) ,\end{aligned}\quad (3.52)$$

which forms the basis for diagrammatic expansions of Green's functions, partition functions and other correlation functions.

3.3.2 Perturbation expansion of the single-electron Green's function

The standard way to derive Feynman diagrams perturbatively at zero temperature involves the following steps: (i) switch on interactions adiabatically, (ii) apply the Gell-Mann-Low theorem to turn expectation values with respect to the interacting GS into expectation values with respect to the non-interacting GS, (iii) replace time-evolution operators by their series expansion in Eq. 3.50, (iv) use Wick's theorem to evaluate expectation values of time-ordered products of operators and (v) identify Feynman rules to translate the resulting terms and its individual factors to diagrams and back.

This is a rather technical and lengthy procedure which is beyond the scope of this thesis. We refer interested readers to one of the excellent textbooks in Refs. [17, 85, 113]. Instead, we will rely on a more intuitive approach that makes use of some characteristic properties of the polaron problem which leads to various simplifications.

Let's start by plugging Eq. 3.52 into Eq. 3.34. This immediately gives us the single-electron Green's function for the polaron problem as an infinite series of integrals:

$$\begin{aligned}
 G(m\mathbf{k}, \tau) &= \left\langle m\mathbf{k} \left| e^{-\hat{H}_{\text{pol}}\tau/\hbar} \right| m\mathbf{k} \right\rangle \\
 &= \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar} \right)^n \int_0^{\tau} d\tau_n \cdots \int_0^{\tau_2} d\tau_1 \left\langle m\mathbf{k} \left| e^{-\hat{H}_0\tau/\hbar} \hat{H}_1^{(I)}(\tau_n) \cdots \hat{H}_1^{(I)}(\tau_1) \right| m\mathbf{k} \right\rangle \\
 &= \sum_{n=0}^{\infty} G^{(n)}(m\mathbf{k}, \tau) .
 \end{aligned} \tag{3.53}$$

Note that the integrands in Eq. 3.53 are expectation values with respect to the free electron state, $|m\mathbf{k}\rangle = \hat{c}_{m\mathbf{k}}^\dagger |\emptyset\rangle$, an eigenstate of $\hat{H}_0$ containing one electron and no phonons. This is a unique feature of the single polaron limit that we are interested in. For finite electron densities, the expectation value would be with respect to the true interacting ground state $|\Psi_0\rangle$ of the full Hamiltonian $\hat{H}$ which would require a more careful analysis centered around the Gell-Mann-Low theorem [114].

Another important observation is that odd expansion orders vanish. To see this, note that each term of $\hat{H}_1$ is proportional to $(\hat{a}_{\mathbf{q}\nu} + \hat{a}_{-\mathbf{q}\nu}^\dagger)$. Therefore acting with $\hat{H}_1$ on some eigenstate of $\hat{H}_0$, e.g. $|m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}\rangle$, produces a superposition of two different eigenstates of $\hat{H}_0$, one with an additional phonon in mode $(-\mathbf{q}, \nu)$ and one with a phonon in mode $(\mathbf{q}, \nu)$ removed. Since the initial and final state is given by $|m\mathbf{k}\rangle$, every phonon created by some $\hat{a}_{\mathbf{q}\nu}^\dagger$ at time τ_i has to be destroyed by a corresponding $\hat{a}_{\mathbf{q}\nu}$ at a later time τ_j . Hence, there must be an even number of $\hat{H}_1$ operators in the expectation value.

A direct consequence of this is that all exponential operators appearing in the expectation value, $e^{-\hat{H}_0\tau/\hbar}$ as well as $e^{\pm\hat{H}_0\tau_i/\hbar}$ coming from $\hat{H}_1^{(I)}(\tau_i)$, simply propagate whatever state they act on in imaginary time without modifying it, i.e.

$$e^{-\hat{H}_0\tau/\hbar} |m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}\rangle = \exp \left\{ -\left(\varepsilon_{m\mathbf{k}} + \sum_{\mathbf{q}\nu} \hbar\omega_{\mathbf{q}\nu} n_{\mathbf{q}\nu} \right) \tau / \hbar \right\} |m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}\rangle , \tag{3.54}$$

where we have used Eq. 3.7.

Equipped with this knowledge, let's take a closer look at the first non-zero contributions to the series in Eq. 3.53.

Using Eq. 3.54, the expectation value for the 0th-order term gives

$$F^{(0)} = \left\langle m\mathbf{k} \left| e^{-\hat{H}_0\tau/\hbar} \right| m\mathbf{k} \right\rangle = e^{-\varepsilon_{m\mathbf{k}}\tau/\hbar} . \tag{3.55}$$

Since there are no integrations at 0th-order, its full contribution to Eq. 3.53 is simply

$$G^{(0)}(m\mathbf{k}, \tau) = e^{-\varepsilon_{m\mathbf{k}}\tau/\hbar} . \quad (3.56)$$

In fact, as the notation already suggests, this is identical to the free electron Green's function of the non-interacting system.

The expectation value of the 2nd-order term looks as follows:

$$\begin{aligned} F^{(2)} &= \left\langle m\mathbf{k} \left| e^{-\hat{H}_0\tau/\hbar} \hat{H}_1^{(I)}(\tau_2) \hat{H}_1^{(I)}(\tau_1) \right| m\mathbf{k} \right\rangle \\ &= e^{-\varepsilon_{m\mathbf{k}}\tau/\hbar} \left\langle m\mathbf{k} \left| \hat{H}_1^{(I)}(\tau_2) \hat{H}_1^{(I)}(\tau_1) \right| m\mathbf{k} \right\rangle . \end{aligned} \quad (3.57)$$

From previous considerations, we already know that the only way to get a non-zero contribution is to have $\hat{H}_1^{(I)}(\tau_1)$ create a phonon and $\hat{H}_1^{(I)}(\tau_2)$ destroy the same phonon at a later time. Applying $\hat{H}_1^{(I)}(\tau_1)$ to $|m\mathbf{k}\rangle$ in Eq. 3.57 results in

$$\begin{aligned} F^{(2)} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{q}'m'\nu'} g_{m'm\nu'}(\mathbf{k}, \mathbf{q}') e^{-\varepsilon_{m\mathbf{k}}\tau/\hbar} e^{-\varepsilon_{m\mathbf{k}}\tau_1/\hbar} e^{(\varepsilon_{m'\mathbf{k}+\mathbf{q}'} + \hbar\omega_{-\mathbf{q}'\nu'})\tau_1/\hbar} \\ &\quad \times \left\langle m\mathbf{k} \left| \hat{H}_1^{(I)}(\tau_2) \right| m'\mathbf{k} + \mathbf{q}', n_{-\mathbf{q}'\nu'} = 1 \right\rangle . \end{aligned} \quad (3.58)$$

where we have used the fact that $\hat{c}_{n'\mathbf{k}'}$ from $\hat{H}_1^{(I)}(\tau_1)$ must annihilate the electron in the initial state $|m\mathbf{k}\rangle$, which leads to two Kronecker deltas, $\delta_{n'm}\delta_{\mathbf{k}'\mathbf{k}}$, and gets rid of the summations over n' and $\mathbf{k}'$.

Doing the same for $\hat{H}_1^{(I)}(\tau_2)$ and again summing over all constrained degrees of freedom gives

$$\begin{aligned} F^{(2)} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{q}'m'\nu'} g_{m'm\nu'}(\mathbf{k}, \mathbf{q}') e^{-\varepsilon_{m\mathbf{k}}\tau/\hbar} e^{-\varepsilon_{m\mathbf{k}}\tau_1/\hbar} e^{(\varepsilon_{m'\mathbf{k}+\mathbf{q}'} + \hbar\omega_{-\mathbf{q}'\nu'})\tau_1/\hbar} \\ &\quad \times \frac{1}{\sqrt{N}} g_{mm'\nu'}(\mathbf{k} + \mathbf{q}', -\mathbf{q}') e^{\varepsilon_{m\mathbf{k}}\tau_2/\hbar} e^{-(\varepsilon_{m'\mathbf{k}+\mathbf{q}'} + \hbar\omega_{-\mathbf{q}'\nu'})\tau_2/\hbar} . \end{aligned} \quad (3.59)$$

Eq. 3.56 allows us to replace certain exponential factors by free electron Green's functions $G^{(0)}(m\mathbf{k}, \tau)$. In the same spirit, we introduce corresponding free phonon Green's functions

$$D^{(0)}(\mathbf{q}\nu, \tau) = e^{-\omega_{\mathbf{q}\nu}\tau} . \quad (3.60)$$

Then, the full 2nd-order contribution to Eq. 3.53 can be written as

$$\begin{aligned} G^{(2)}(m\mathbf{k}, \tau) &= \frac{1}{\hbar^2 N} \sum_{\mathbf{q}n\nu} \int_0^\tau d\tau_2 \int_0^{\tau_2} d\tau_1 |g_{nm\nu}(\mathbf{k}, \mathbf{q})|^2 G^{(0)}(m\mathbf{k}, \tau - \tau_2) \\ &\quad \times G^{(0)}(n\mathbf{k} + \mathbf{q}, \tau_2 - \tau_1) D^{(0)}(-\mathbf{q}\nu, \tau_2 - \tau_1) G^{(0)}(m\mathbf{k}, \tau_1) , \end{aligned} \quad (3.61)$$

where we have renamed the summation indices in Eq. 3.59, $m' \rightarrow n$, $\nu' \rightarrow \nu$ and $\mathbf{q}' \rightarrow \mathbf{q}$, and used the identity

$$g_{mn\nu}(\mathbf{k} + \mathbf{q}, -\mathbf{q}) = [g_{nm\nu}(\mathbf{k}, \mathbf{q})]^* , \quad (3.62)$$

which follows from the hermiticity of $\hat{H}_1$.

Deriving higher order contributions follows the same procedure. However, due to the increasing number of terms and possibilities to pair phonon creation and annihilation operators, the algebra becomes more and more tedious. Writing down all 4th order contributions, for example, would require ≈ 10 lines of equations. It is much more intuitive and convenient to work with Feynman diagrams as we will see in the next section.

3.3.3 Feynman diagrams for the single-electron Green's function

Similar to Sec. 2.2.3, where we used diagrammatics for the simple toy model to help with the visualization of complicated terms of an infinite series, the current section introduces Feynman diagrams for the perturbation expansion of the single-electron Green's function given in Eq. 3.53.

It was shown above that the 0th- and 2nd-order contributions can be written in terms of free electron and phonon Green's functions, $G^{(0)}(m\mathbf{k}, \tau)$ and $D^{(0)}(\mathbf{q}\nu, \tau)$, as well as electron-phonon matrix elements, $g_{mn\nu}(\mathbf{k}, \mathbf{q})$. The same is actually true for all terms in the series. To make this plausible, consider that (i) every exponential operator in the expectation value simply propagates states of the form $|m\mathbf{k}, n_{\mathbf{q}\nu}\rangle$ in imaginary time resulting in one free electron Green's function (there is always exactly a single electron in the system) times zero or more free phonon Green's functions (depending on the state's phonon occupation $n_{\mathbf{q}\nu}$), and (ii) every interaction Hamiltonian $\hat{H}_1$ creates or destroys a phonon with amplitude $g_{mn\nu}(\mathbf{k}, \mathbf{q})$ while scattering the electron into a new state.

That means that these three quantities are the fundamental building blocks of our Feynman diagrams. Figure 3.1 shows the corresponding Feynman dictionary (cf. Fig. 2.4 for the toy model analog):

- Free electron Green's functions are represented by directed, straight lines from τ_i to τ_j and are associated with a factor $G^{(0)}(m\mathbf{k}, \tau_j - \tau_i)$.
- Free phonon Green's functions are represented by undirected, wavy lines from τ_i to τ_j and are associated with a factor $D^{(0)}(\mathbf{q}\nu, \tau_j - \tau_i)$.

FIGURE 3.1: Feynman dictionary for the polaron problem. (a) Free electron Green's function, $G^{(0)}(m\mathbf{k}, \tau)$, (b) free phonon Green's function, $D^{(0)}(\mathbf{q}\nu, \tau)$, and (c) electron-phonon interaction vertex, $g_{mn\nu}(\mathbf{k}, \mathbf{q})$.

- The dictionary can be used to turn any term of the series into a Feynman diagram and back. For example, the 0th- and 2nd-order contributions from Eqs. 3.56 and 3.61 are depicted in Fig. 3.2. Their interpretations are straightforward.

The 2nd-order diagram in Fig. 3.2(b) describes the process in which the electron first propagates freely in state $|m\mathbf{k}\rangle$ from 0 to τ_1 ($= G^{(0)}(m\mathbf{k}, \tau_1)$). At τ_1 , the electron scatters into state $|n\mathbf{k} + \mathbf{q}\rangle$ by emitting a phonon in mode $(-\mathbf{q}, \nu)$ ($= g_{nm\nu}(\mathbf{k}, \mathbf{q})$). Both, electron and phonon, propagate in their respective states until τ_2 ($= G^{(0)}(n\mathbf{k} + \mathbf{q}, \tau_2 - \tau_1) D^{(0)}(-\mathbf{q}\nu, \tau_2 - \tau_1)$), where the electron scatters back into the original state $|m\mathbf{k}\rangle$ by absorbing the same phonon ($= g_{mn\nu}(\mathbf{k} + \mathbf{q}, -\mathbf{q}) = [g_{nm\nu}(\mathbf{k}, \mathbf{q})]^*$) and finally propagates freely from τ_2 to τ ($= G^{(0)}(m\mathbf{k}, \tau - \tau_2)$).

1. Draw n interaction vertices (dots) on a horizontal line and label them from left to right with τ_1 , τ_2 , and so on until τ_n (Fig. 3.3(1)).

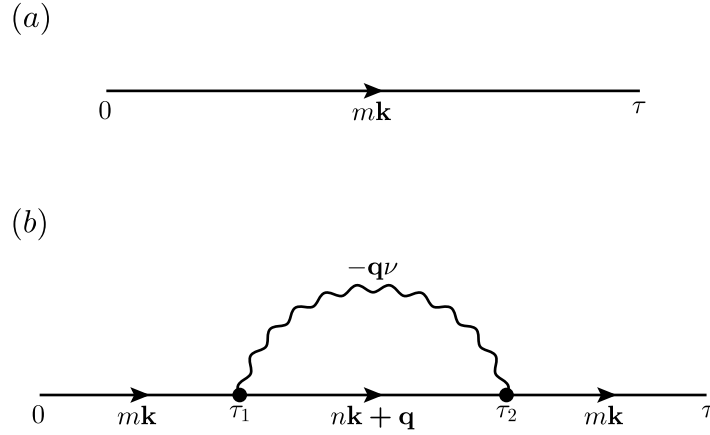


FIGURE 3.2: Feynman diagrams for the (a) 0th- and (b) 2nd-order contributions to the single-electron Green's function, $G(m\mathbf{k}, \tau)$.

2. Connect the vertices with directed, straight lines, i.e. with free electron Green's functions (Fig. 3.3(2)).
3. Add two more free electron Green's functions, one going into vertex τ_1 and one going out of vertex τ_n . Label the left end of the diagram with 0, the right end with τ and both Green's functions with $m\mathbf{k}$ (Fig. 3.3(3)).
4. Connect pairs of vertices with undirected, wavy lines, i.e. with free phonon Green's functions, such that each vertex is connected to exactly three propagators (one incoming electron line, one outgoing electron line and one phonon line). Fill in the missing labels for the propagators. Remember that phonon wave vectors and branches as well as electron band indices are summed or integrated over and are therefore free variables. Only the electron wave vectors are fixed by crystal momentum conservation at the vertices according to Eq. 3.14 (Fig. 3.3(4a)).
5. Repeat steps 1 - 4 for all possible ways the vertices can be connected by phonon propagators, i.e. for all possible diagram topologies ξ_n (Fig. 3.3(4b)-(4c)).

Figure 3.3 depicts the recipe step by step for the 4th-order contribution. Note that the number of diagrams belonging to the same order n but with a different topology grows as

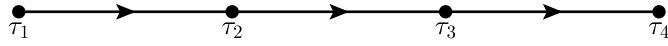
$$N_{\xi_n} = \frac{n!}{2^{n/2}(n/2)!} = (n-1)!! . \quad (3.63)$$

Table 3.1 lists the number of topologies for some diagram orders. It is obvious that any attempt to treat the series manually or deterministically is unrealistic for higher orders. This is where DiagMC, discussed in Sec. 3.4, comes into play.

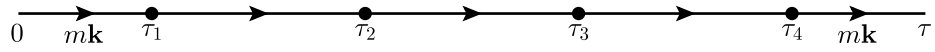
(1)



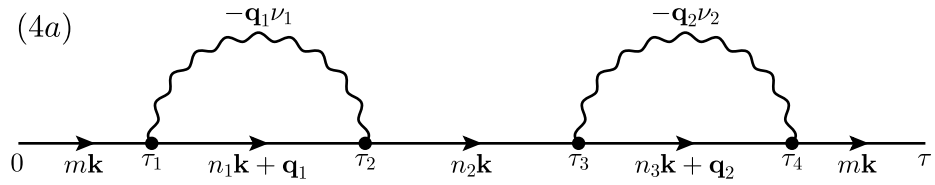
(2)



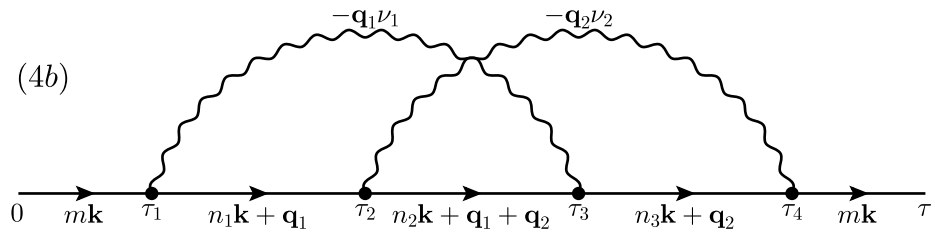
(3)



(4a)



(4b)



(4c)

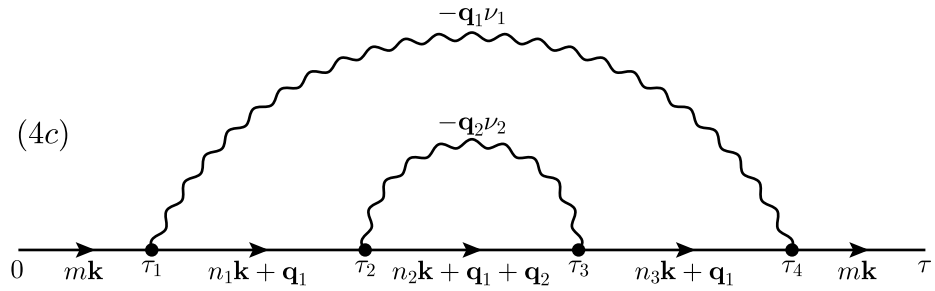


FIGURE 3.3: Recipe for drawing a 4th-order Feynman diagram for the single-electron Green's function. See text for detailed instructions.

TABLE 3.1: Number of diagram topologies, N_{ξ_n} , for the single-electron Green's function for various orders n .

n	N_{ξ_n}
0	1
2	1
4	3
6	15
10	945
20	654729075
100	$\approx 2.7 \times 10^{78}$

Before we move on to the diagrams for the single-electron-N-phonon Green's function and the current-current correlation function, let us rewrite the diagrammatic expansion of Eq. 3.53 in a form better suited for DiagMC:

$$G(m\mathbf{k}, \tau) = \sum_{n=0}^{\infty} \sum_{\xi_n=1}^{(n-1)!!} \int \cdots \int d\mathbf{x}_n \mathcal{D}_{n,\xi_n}(m\mathbf{k}, \tau; \mathbf{x}_n) . \quad (3.64)$$

Here, the sums are over all diagram orders n and topologies ξ_n and the integrals over $\mathbf{x}_n$ denote sums/integrals over all imaginary time points, phonon wave vectors, phonon branches and electron band indices, i.e.

$$\mathbf{x}_n = (\tau_1, \dots, \tau_n, \mathbf{q}_1, \nu_1, \dots, \mathbf{q}_{n/2}, \nu_{n/2}, n_1, \dots, n_{n-1}) . \quad (3.65)$$

Note that sometimes the letter n is used for both the diagram order and the electron band indices. However, it should be clear from the context which one is meant. For example, in Eq. 3.65, subscript n refers to the diagram order, while $n_1, \dots, n_{n-1}$ refer to the electron band indices.

The integrand $\mathcal{D}_{n,\xi_n}(m\mathbf{k}, \tau; \mathbf{x}_n)$ corresponds to the diagram weight or the numeric value of the diagram with order n and topology ξ_n . We assume that all missing factors like $(-1/\hbar)^n$ and $N^{-n/2}$ are included in $\mathcal{D}_{n,\xi_n}(m\mathbf{k}, \tau; \mathbf{x}_n)$, e.g. by incorporating them into the interaction vertices.

To make things clear, consider the numeric value of the 4th-order diagram in Fig. 3.3(4c):

$$\begin{aligned} \mathcal{D}_{4,3}(m\mathbf{k}, \tau; \mathbf{x}_n) = & \frac{1}{\hbar^4 N^2} g_{n_1 m \nu_1}(\mathbf{k}, \mathbf{q}_1) g_{n_2 n_1 \nu_2}(\mathbf{k} + \mathbf{q}_1, \mathbf{q}_2) g_{n_3 n_2 \nu_1}(\mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2, -\mathbf{q}_1) \\ & \times g_{m n_3 \nu_2}(\mathbf{k} + \mathbf{q}_2, -\mathbf{q}_2) G^{(0)}(m\mathbf{k}, \tau_1) G^{(0)}(n_1 \mathbf{k} + \mathbf{q}_1, \tau_2 - \tau_1) \\ & \times G^{(0)}(n_2 \mathbf{k} + \mathbf{q}_1 + \mathbf{q}_2, \tau_3 - \tau_2) G^{(0)}(n_3 \mathbf{k} + \mathbf{q}_2, \tau_4 - \tau_3) G^{(0)}(m\mathbf{k}, \tau - \tau_4) \\ & \times D^{(0)}(-\mathbf{q}_1 \nu_1, \tau_3 - \tau_1) D^{(0)}(-\mathbf{q}_2 \nu_2, \tau_4 - \tau_2) . \end{aligned} \quad (3.66)$$

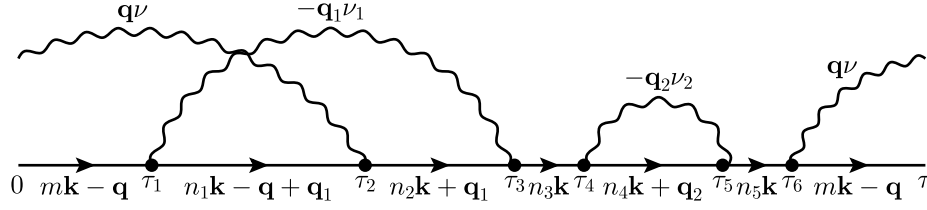


FIGURE 3.4: 6th-order Feynman diagram of the single-electron-1-phonon Green's function, $G_1(m\mathbf{k}, \mathbf{q}\nu, \tau)$.

3.3.4 Feynman diagrams for the single-electron-N-phonon Green's function

The starting point for deriving a diagrammatic expansion for the single-electron-N-phonon Green's function, $G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}, \tau)$, is Eq. 3.39. The procedure is exactly the same as for the single-electron Green's function, so we will not go into the details again.

Figure 3.4 shows a 6th-order Feynman diagram for the single-electron-1-phonon Green's function, $G_1(m\mathbf{k}, \mathbf{q}\nu, \tau)$. As you can see, diagrams for $G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}, \tau)$ have N_{ph} phonon propagators attached to the beginning and end of the diagram corresponding to the phonons present in the initial and final state, $|m\mathbf{k}_{\text{el}}, \underline{n_{\mathbf{q}\nu}}\rangle$. We refer to such phonon lines as external phonons. Their modes and wave vectors are fixed, as opposed to the internal phonon lines which are summed or integrated over. Also note that $\mathbf{k}$ is the polaron wave vector, while the initial and final electron wave vector, $\mathbf{k}_{\text{el}}$, is again given by Eq. 3.14.

The Feynman dictionary from Fig. 3.1 remains valid and can be used to translate between pictorial and algebraic representations of the diagrams. On the other hand, the recipe for drawing or enumerating all diagrams of a given order n in Fig. 3.3 needs a little bit more attention.

In principle, external phonon propagators do not need to interact with the electron at all. For example, the 0th-order diagram for $G_1(m\mathbf{k}, \mathbf{q}\nu, \tau)$ simply consists of a free electron and external phonon propagator from 0 to τ . However, as was shown in Ref. [50], such diagrams do not contribute to the asymptotic $\tau \rightarrow \infty$ behavior of the Green's function. Since we are only using $G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}, \tau)$ to extract GS properties of the polaron in the spirit of Eq. 3.40, we can subtract all terms with disconnected external phonon lines from the diagrammatic expansion and focus only on fully connected or irreducible diagrams. The same is true for diagrams with external phonons crossing each other, i.e. where the length of the resulting propagator is $> \tau$. Such diagrams can always be rewritten in terms of a connected diagram times disconnected phonon lines and thus can also be ignored.

From now on, we don't distinguish between $G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}, \tau)$ and its irreducible part and we keep the same notation for both. This should not cause any confusion.

With all that in mind, we can write down the diagrammatic expansion for $G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}, \tau)$, similar to Eq. 3.64:

$$G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}, \tau) = \sum_{n=2N_{\text{ph}}}^{\infty} \sum_{\xi_n} \int \cdots \int d\mathbf{x}_n \mathcal{D}_{n, \xi_n}^{N_{\text{ph}}}(m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}, \tau; \mathbf{x}_n). \quad (3.67)$$

Here, $\mathcal{D}_{n, \xi_n}^{N_{\text{ph}}}(m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}, \tau; \mathbf{x}_n)$ is again the diagram weight and $\mathbf{x}_n$ is the tuple of all internal integration or summation variables. Note that the sum over diagram orders starts at $2N_{\text{ph}}$, which is the lowest order for which fully connected diagrams with N_{ph} external phonons can be drawn.

Combining Eqs. 3.41 and 3.67 gives the diagrammatic expansion for $P(m\mathbf{k}, \tau)$ (or to be more precise, for its irreducible part):

$$\begin{aligned} P(m\mathbf{k}, \tau) &= \sum_{N_{\text{ph}}=0}^{\infty} \sum_{\underline{n_{\mathbf{q}\nu}}}^{N_{\text{ph}}} G_{N_{\text{ph}}}(m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}, \tau) \\ &= \sum_{N_{\text{ph}}=0}^{\infty} \sum_{\underline{n_{\mathbf{q}\nu}}}^{N_{\text{ph}}} \sum_{n=2N_{\text{ph}}}^{\infty} \sum_{\xi_n} \int \cdots \int d\mathbf{x}_n \mathcal{D}_{n, \xi_n}^{N_{\text{ph}}}(m\mathbf{k}, \underline{n_{\mathbf{q}\nu}}, \tau; \mathbf{x}_n). \end{aligned} \quad (3.68)$$

3.3.5 Feynman diagrams for the current-current correlation function

Although we are interested in the zero temperature, imaginary time current-current correlation function, $\Pi(\mathbf{k}, \tau)$, defined in Eq. 3.43, the diagrammatic series used to calculate it is based on an expansion of the partition function, $\mathcal{Z}(\beta)$, at finite temperature. The $T \rightarrow 0$ limit can then be recovered by performing simulations for $\beta \rightarrow \infty$ [51].

The partition function for the single polaron problem is given by

$$\begin{aligned} \mathcal{Z}(\beta) &= \text{Tr} \left[e^{-\beta \hat{H}_{\text{pol}}} \right] \\ &= \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar} \right)^n \int_0^{\hbar\beta} d\tau_n \cdots \int_0^{\tau_2} d\tau_1 \text{Tr} \left[e^{-\hat{H}_0\beta} \hat{H}_1^{(I)}(\tau_n) \cdots \hat{H}_1^{(I)}(\tau_1) \right], \end{aligned} \quad (3.69)$$

where we have used Eq. 3.52.

Evaluating and simplifying the trace is not very complicated but rather technical. We refer the interested reader to the detailed derivation in Ref. [103] and simply focus on the result here.

The diagrammatic expansion of $\mathcal{Z}(\beta)$ turns out to be very similar to that of $G(m\mathbf{k}, \tau)$. The relevant differences are that (i) the phonon propagator from Eq. 3.60 has to be replaced by its thermal counterpart

$$\begin{aligned} D^{(0)}(\mathbf{q}\nu, \tau) &= \frac{e^{-\omega_{\mathbf{q}\nu}\tau} + e^{-\omega_{\mathbf{q}\nu}(\hbar\beta-\tau)}}{1 - e^{-\hbar\beta\omega_{\mathbf{q}\nu}}} \\ &= [1 + n_B(\omega_{\mathbf{q}\nu})] e^{-\omega_{\mathbf{q}\nu}\tau} + n_B(\omega_{\mathbf{q}\nu}) e^{-\omega_{\mathbf{q}\nu}(\hbar\beta-\tau)}, \end{aligned} \quad (3.70)$$

where $n_B(\omega_{\mathbf{q}\nu}) = (e^{\hbar\beta\omega_{\mathbf{q}\nu}} - 1)^{-1}$ is the Bose-Einstein distribution function, (ii) the trace over the electronic degrees of freedom introduces a sum over m and $\mathbf{k}$, and (iii) the trace over the phonon degrees of freedom leads to an additional factor of $\mathcal{Z}_{\text{ph}}(\beta) = \text{Tr}[e^{-\beta\hat{H}_{\text{ph}}}]$, the canonical phonon partition function.

The corresponding Feynman diagrams are usually depicted as β -circles shown in Fig. 3.5. However, it is possible to cut the circle at $\tau = 0$ and straighten it out to get a diagram that looks very similar to the one for $G(m\mathbf{k}, \tau)$, cf. Fig. 3.3(4b). In fact, we can immediately reuse the Feynman dictionary from Fig. 3.1 and the recipe from Fig. 3.3 as they are.

Putting everything together, the diagrammatic expansion for $\mathcal{Z}(\beta)$ is given by

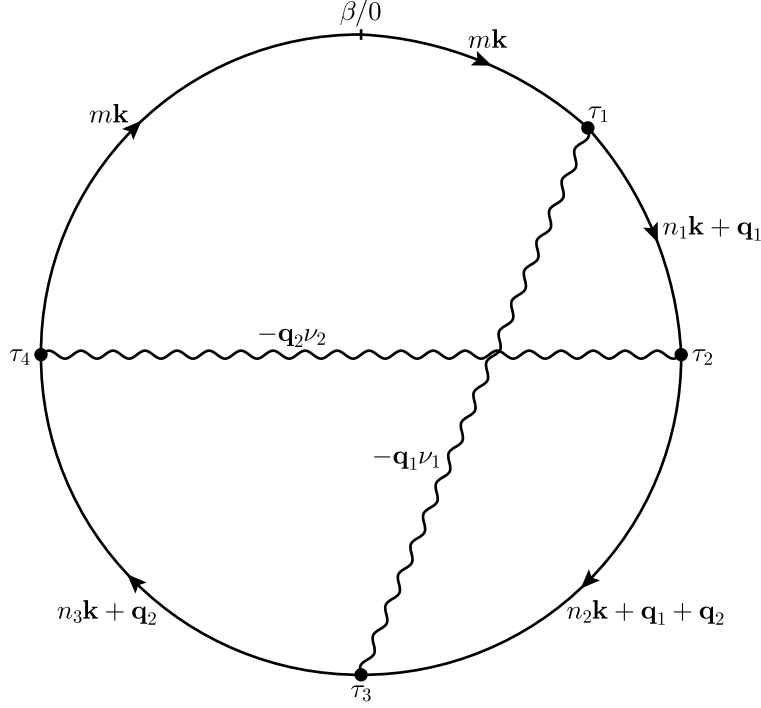
$$\mathcal{Z}(\beta) = \mathcal{Z}_{\text{ph}}(\beta) \sum_{n=0}^{\infty} \sum_{\xi_n=1}^{(n-1)!!} \int \cdots \int d\mathbf{x}_n \mathcal{D}_{n,\xi_n}^{\mathcal{Z}}(\beta; \mathbf{x}_n), \quad (3.71)$$

where summations over n and ξ_n are identical to those in Eq. 3.64 and the diagram weights $\mathcal{D}_{n,\xi_n}^{\mathcal{Z}}(\beta; \mathbf{x}_n)$ have the same functional form as $\mathcal{D}_{n,\xi_n}(m\mathbf{k}, \tau; \mathbf{x}_n)$, except that the zero temperature phonon propagators are replaced by the thermal ones from Eq. 3.70. The integrals over $\mathbf{x}_n$ include the additional sum over m and $\mathbf{k}$ such that

$$\mathbf{x}_n = (\tau_1, \dots, \tau_n, \mathbf{q}_1, \nu_1, \dots, \mathbf{q}_{n/2}, \nu_{n/2}, n_1, \dots, n_{n-1}, m, \mathbf{k}). \quad (3.72)$$

3.4 DiagMC for polarons

With the diagrammatic expansions for $G(m\mathbf{k}, \tau)$, $G_{N_{\text{ph}}}(m\mathbf{k}, n_{\mathbf{q}\nu}, \tau)$, $P(m\mathbf{k}, \tau)$ and $\mathcal{Z}(\beta)$ at hand, we are now in a position to discuss the DiagMC algorithm for polarons. Comparing their expansions in Eqs. 3.64, 3.67, 3.68 and 3.71 to Eq. 2.35, it is clear that DiagMC is capable of tackling this kind of problems. The only missing ingredients are updates to stochastically sample diagram configurations and measurements to extract the relevant polaron properties from the sampled diagrams.

FIGURE 3.5: 4th-order Feynman diagram of the partition function, $\mathcal{Z}(\beta)$.

To make the connection to Sec. 2.2, we can identify the configuration space $\mathcal{C}$ as the space of all Feynman diagrams for a given expansion, i.e. there is a one-to-one mapping between every diagram in the series and a unique configuration $C \in \mathcal{C}$. The weight $\mathcal{W}(C)$ of a configuration C is simply the weight of the corresponding diagram.

Before detailing the updates and measurements, we briefly outline the expansions simulated in the later chapters of this thesis, specify which physical properties are extracted from each expansion, and provide some general remarks on DiagMC implementations:

$P(m\mathbf{k}, \tau)$: The sum of all single-electron-N-phonon Green's functions is used to compute various polaron GS properties relevant to this work. It is related to the polaron dispersion $E_0(\mathbf{k})$ via Eq. 3.42, to the probabilities $Z_{m, n_{\mathbf{q}\nu}}^{(0, \mathbf{k})}$ via Eq. 3.40, and indirectly to the effective mass tensor $m_{ij}^*(\mathbf{k})$ via Eq. 3.12. There is usually no need to simulate individual $G_{N_{\text{ph}}}(m\mathbf{k}, n_{\mathbf{q}\nu}, \tau)$.

Furthermore, since we are only interested in the asymptotic $\tau \rightarrow \infty$ behavior of $P(m\mathbf{k}, \tau)$ and since there exist direct MC estimators for all properties mentioned above (see Sec. 3.4.1), the full τ -dependence is not required. Instead, it is sufficient to run simulations at a fixed, large τ value (how large depends on the model and should be checked carefully).

$G(m\mathbf{k}, \tau)$: The single-electron Green's function is used to compute the spectral

function, $A(\mathbf{k}, \omega)$, via Eq. 3.38. That means $G(m\mathbf{k}, \tau)$ is provided as input to SOCC (see Sec. 2.3). Numerical analytic continuation is a notoriously difficult problem and thus it is crucial to calculate $G(m\mathbf{k}, \tau)$ to very high accuracy. Section 3.4.1 describes an exact MC estimator for Green's functions that eliminates the systematic errors introduced by the binning procedure inherent to histogram-based statistics (cf. Sec. 2.2.3).

In contrast to $P(m\mathbf{k}, \tau)$, the full τ -dependence of $G(m\mathbf{k}, \tau)$ is required for NAC. An update is designed to change τ during the simulation and statistics are collected for $G(m\mathbf{k}, \tau)$ according to some measurement procedure (see Sec. 3.4.1).

To have more control over the τ -behavior, it is common to simulate $e^{\mu\tau}G(m\mathbf{k}, \tau)$ instead of the bare Green's function. μ is a fictitious chemical potential that can be tuned to make the Green's function decay or rise more slowly with τ and so improve the sampling efficiency at large or small τ , respectively.

$\mathcal{Z}(\beta)$: The partition function is used to compute the current-current correlation function, $\Pi_{ij}(\tau)$, and thus the optical conductivity, $\sigma_{ij}(\omega)$, via Eq. 3.44. Since we are interested in the zero temperature limit, simulations are performed for large but fixed β values, which allows us to measure $\Pi_{ij}(\tau)$ at arbitrary τ values in the range $[0, \hbar\beta]$.

The constant factor $\mathcal{Z}_{\text{ph}}(\beta)$ in Eq. 3.71 does not affect calculations of $\Pi_{ij}(\tau)$ and can be ignored.

3.4.1 Measurements

Any measurement done during a DiagMC simulation is based on Eqs. 2.35–2.37. The goal therefore is to write each quantity of interest X as

$$X = \sum_C X_{\text{MC}}(C) p(C) = \sum_C X_{\text{MC}}(C) \frac{\mathcal{W}(C)}{\sum_{C'} \mathcal{W}(C')} \approx \frac{1}{M} \sum_{i=1}^M X_{\text{MC}}(C_i), \quad (3.73)$$

where $X_{\text{MC}}(C)$ is the MC estimator for X , $p(C)$ is the probability of sampling configuration C (or equivalently, the corresponding diagram), C_i are the actual diagrams sampled during the simulation, and M is the total number of samples.

For the rest of this chapter, we will assume units such that $\hbar = 1$.

Green's function

The easiest way to measure $G(m\mathbf{k}, \tau)$ is to use a histogram. The procedure, including the calculation of the normalization $\mathcal{Z}$, is identical to the one described in Sec. 2.2.3 for the function $Q(\tau)$.

Mishchenko *et al.* [50] introduced an exact MC estimator for $G(m\mathbf{k}, \tau)$ that does not suffer from any systematic errors. The derivation is based on a reweighting technique and is applicable in many different contexts. The resulting estimator is given by

$$G_{\text{MC}}(C) = (1 + \eta)^n \frac{\chi_{\mathcal{I}}(\tau')}{|\mathcal{I}|} e^{-\eta E(C)} , \quad (3.74)$$

Here, $\eta = (\tau - \tau')/\tau'$ with τ' the length of the sampled diagram and τ the point at which we want to measure the Green's function, $\chi_{\mathcal{I}}(\tau')$ and $|\mathcal{I}|$ are defined in Sec. 2.2.3 and

$$E(C) = \sum_c \varepsilon_{m_c \mathbf{k}_c} \Delta\tau_c - \sum_a \omega_{\mathbf{q}_a \nu_a} \Delta\tau_a . \quad (3.75)$$

The summations are over all electron ($\sum_c$) and phonon ($\sum_a$) propagators in the diagram and $\Delta\tau_c$ and $\Delta\tau_a$ are their respective lengths.

Phonon distribution

Various phonon distributions in the polaron GS are related to the general probabilities $Z_{m, \underline{n}_{\mathbf{q}\nu}}^{(0, \mathbf{k})}$ as described in Sec. 3.1. Considering Eqs. 3.40 and 3.41, an obvious estimator is given by

$$Z_{\text{MC}}(C) = \delta_{\underline{n}_{\mathbf{q}\nu}, \underline{n}'_{\mathbf{q}\nu}} , \quad (3.76)$$

where $\underline{n}'_{\mathbf{q}\nu}$ is the phonon occupation of the sampled diagram and $\underline{n}_{\mathbf{q}\nu}$ corresponds to the probability $Z_{m, \underline{n}_{\mathbf{q}\nu}}^{(0, \mathbf{k})}$ we want to measure.

In Ref. [50], a circular diagram representation was used to obtain a more effective estimator for $Z_{N_{\text{ph}}}$. The same principles can be applied here to improve Eq. 3.76.

Polaron energy

The derivation of the polaron energy estimator is based on Eq. 3.42 and can also be found in Ref. [50]. If we replace the Fröhlich specific quantities with their more general analogs, $\varepsilon_{m\mathbf{k}}$ and $\omega_{\mathbf{q}\nu}$, we arrive at

$$E_{\text{MC}}(C) = -\frac{1}{\tau} (n - E(C)) , \quad (3.77)$$

where $E(C)$ is defined in Eq. 3.75.

Effective mass

A MC estimator for the Hessian matrix $\mathcal{H}_{E_0}(\mathbf{k} = 0) = \mathcal{H}_{E_0}$, and therefore for the effective mass tensor $m_{ij}^*(\mathbf{k} = 0) = m_{ij}^*$ (see Eq. 3.12), is given in Ref. [115].

The derivation is again based on Eq. 3.42 and assumes that $g_{nm\nu}(\mathbf{k}, \mathbf{q}) = g_{nm\nu}(\mathbf{q})$ is independent of the electron wave vector $\mathbf{k}$ (which is the case for all models considered in this thesis). The resulting estimator is given by

$$\begin{aligned}\mathcal{H}_{\text{MC}} &= \mathcal{H}(C) - \tau \mathbf{v}(C) \otimes \mathbf{v}(C) , \\ \mathbf{v}(C) &= \sum_c \nabla \varepsilon_{m_c \mathbf{k}_c} \frac{\Delta \tau_c}{\tau} , \\ \mathcal{H}(C) &= \sum_c \mathcal{H}_\varepsilon(\mathbf{k}_c) \frac{\Delta \tau_c}{\tau} ,\end{aligned}\tag{3.78}$$

where the sum is over all electron propagators and $\nabla \varepsilon_{m_c \mathbf{k}_c}$ and $\mathcal{H}_\varepsilon(\mathbf{k}_c)$ are the gradient and Hessian of the electron dispersion, respectively, evaluated at the band index and wave vector of the electron propagator c .

Current-current correlation function

The estimator for the current-current correlation function can be derived directly from its definition

$$\Pi_{ij}(\tau) = \langle \hat{j}_i(\tau) \hat{j}_j(0) \rangle = \mathcal{Z}^{-1}(\beta) \text{Tr} \left[e^{-\hat{H}_{\text{pol}} \beta} \hat{j}_i(\tau) \hat{j}_j(0) \right] . \tag{3.79}$$

Plugging Eq. 3.26 for the current operator into the above expression, one finds that the diagrammatic expansion of the numerator is the same as the one for the partition function except for two additional current vertices, one measured at imaginary time 0 and one at τ . This leads to the following estimator for $\Pi_{ij}(\tau)$:

$$[\Pi_{\text{MC}}]_{ij}(C) = e^2 \frac{\partial \varepsilon_{m_0 \mathbf{k}_0}}{\partial k_i} \frac{\partial \varepsilon_{m_\tau \mathbf{k}_\tau}}{\partial k_j} , \tag{3.80}$$

where m_0 and $\mathbf{k}_0$ are the band index and wave vector of the electron propagator at time 0 and m_τ and $\mathbf{k}_\tau$ are the band index and wave vector of the electron propagator at time τ .

Note that this estimator is only valid for the simple current operator from Eq. 3.26. Reference [103] explains how to measure more general (current) operators for polaron like Hamiltonians.

3.4.2 Updates

It is not very difficult to design a set of updates for the diagrammatic expansions introduced in the previous sections that (i) fulfill detailed balance, (ii) are ergodic, and (iii) work for the generic polaron Hamiltonian from Eq. 3.1. However, their

efficiency is very much problem dependent and in the worst case can slow down simulations by orders of magnitude. When running demanding calculations like DiagMC, trading generality for performance is often not a good idea. In practice, it is usually better to optimize updates for a given system to make the sampling procedure as efficient as possible. Since the present thesis is concerned with three very different polaron models, we will therefore not discuss specific implementation details here but rather summarize the updates used in later chapters and point the interested reader to relevant literature.

Add/Remove internal phonon propagator

Adding and removing internal phonon propagators are the most essential updates needed to simulate $G(m\mathbf{k}, \tau)$, $P(m\mathbf{k}, \tau)$ and $\mathcal{Z}(\beta)$. They are type-II updates that either increase (add) or decrease (remove) the diagram order n by 2 (or equivalently, the number of internal phonon lines by 1). Applying these updates allows the Markov chain to transition between the diagrams in Fig. 3.2, i.e. going from 0th- to 2nd-order and back, as well as between the diagram in Fig. 3.2(b) and the ones in Figs. 3.3(a)-(c), i.e. going from 2nd- to 4th-order and back.

Implementation details for specific models are provided in the following references: Fröhlich polaron [50, 81, 105], Holstein polaron [70, 104], general polaron model [103].

Add/Remove external phonon propagator

Adding and removing external phonon propagators are also type-II updates that change the number of external phonon lines N_{ph} by 1 and thus the diagram order n by 2. They are only required for the simulation of $P(m\mathbf{k}, \tau)$ and, for example, enable transitions from the diagram in Fig. 3.3(a) to the diagram in Fig. 3.4.

Implementation details for specific models are provided in the following references: Fröhlich polaron [50], Holstein polaron [104].

Change τ

This type-I update changes the diagram length τ and is only required for the simulation of $G(m\mathbf{k}, \tau)$ to obtain its full τ -dependence. The update is nearly identical to the *Change-length* update in Sec. 2.2.3.

Implementation details for specific models are provided in the following references: Fröhlich polaron [50, 81, 105], Holstein polaron [70, 104].

Change $\mathbf{k}$ and m

Changing the polaron wave vector $\mathbf{k}$ and the electron band m of the initial/final electron propagators in a diagram is a type-I update that is only necessary for simulating the partition function $\mathcal{Z}(\beta)$.

Implementation details for specific models are provided in the following references: general polaron model [103].

Other updates

The updates mentioned above constitute only a minimal ergodic set for the diagrammatic expansions considered in this thesis. It is easy to come up with other updates, such as:

- changing the topology ξ_n of a diagram without changing its order n ,
- changing individual summation or integration variables like phonon wave vectors $\mathbf{q}_i$, phonon modes ν_i , electron band indices n_i , or imaginary time points τ_i ,
- adding or removing multiple internal or external phonon propagators at once,
- stretching or squeezing the diagram as a whole,
- and others.

If and when additional updates are beneficial is very much problem dependent. More updates are not necessarily better as they can increase the complexity of the implementation and slow down simulations if they are not designed carefully or used in the wrong situations.

3.4.3 Further remarks

This chapter has introduced the theory and basic implementation details of a DiagMC algorithm for polaron problems. Our considerations are valid for the Hamiltonian in Eq. 3.1 describing a single electron coupled linearly to phonons. We apply the algorithm to the Fröhlich polaron in Chapter 4 and to the acoustic lattice polaron in Chapter 5. In Chapter 6, we study the quadratic interaction of an electron with phonons. This requires an extension of the theory presented here. The details are given in Secs. 6.4 and 6.8.3.

Chapter 4

Fröhlich polaron dispersion in two and three dimensions

This chapter includes a verbatim copy from the following published article:

T. Hahn, S. Klimin, J. Tempere, J.T. Devreese, C. Franchini, *Diagrammatic Monte Carlo study of Fröhlich polaron dispersion in two and three dimensions*, [Physical Review B 97 \(13\), 134305 \(2018\)](#).

Preamble: The manuscript uses the DiagMC approach discussed in Chapter 3 and applies it to the two- and three-dimensional Fröhlich polaron problem to obtain the following polaron properties:

- Ground state energy $E_0(0, \alpha)$ and effective mass $m_*(\alpha)$ as a function of the coupling strength α for $\mathbf{k} = 0$.
- Polaron dispersion curves $E_0(\mathbf{k}, \alpha)$ for different α values.

The correctness of the author's DiagMC implementation has been verified by comparing the computed ground state energies and effective masses for the 3D model with reference data from Mishchenko *et al.* [50].

Contribution: As the first author of the paper, I developed the methodology, independently implemented the code, conducted the simulations, analyzed the data, prepared the figures, and wrote the manuscript.

4.1 Abstract

We present results for the solution of the large polaron Fröhlich Hamiltonian in 3-dimensions (3D) and 2-dimensions (2D) obtained via the Diagrammatic Monte Carlo (DMC) method. Our implementation is based on the approach by Mishchenko [A.S. Mishchenko *et al.*, Phys. Rev. B **62**, 6317 (2000)]. Polaron ground state

energies and effective polaron masses are successfully benchmarked with data obtained using Feynman's path integral formalism. By comparing 3D and 2D data, we verify the analytically exact scaling relations for energies and effective masses from 3D→2D, which provides a stringent test for the quality of DMC predictions. The accuracy of our results is further proven by providing values for the exactly known coefficients in weak- and strong coupling expansions. Moreover, we compute polaron dispersion curves which are validated with analytically known lower and upper limits in the small coupling regime and verify the first order expansion results for larger couplings, thus disproving previous critiques on the apparent incompatibility of DMC with analytical results and furnishing useful reference for a wide range of coupling strengths.

4.2 Introduction

Ever since the emergence of polaron theory in the 1930s [31], the concept of polarons has been applied to a wide variety of physical systems in which a particle is coupled to its environment, e.g. spin or magnetic polarons [45], exciton polarons [44], BEC-impurity polarons [43], ripplonic polaron [46] etc. The polaron problem in its original form considers a single electron in a polar crystal interacting with the surrounding lattice. Due to Coulomb forces, the electron distorts the ions in its neighbourhood, which creates a polarization that follows the electron as it moves through the crystal. This generated polarization acts back on the electron and so renormalizes electronic properties. The resulting quasiparticle consisting of the electron surrounded by the distorted lattice was termed a "polaron". Nowadays (cf. the review by Alexandrov and Devreese [35]) a more quantum mechanical picture of a polaron is used in which the electron dresses itself with a cloud of phonons.

Polarons may be classified according to the strength of the electron-phonon coupling (weak/strong) and the extension of the lattice distortion around the electron (small/large) [35, 116]. Weak-coupling polarons dress themselves with only a small number of phonons $\bar{N} \ll 1$ leading to a slightly enhanced effective mass compared to the "bare" electron $(m_* - m) \ll m$. Strong-coupling polarons have more phonons in the cloud $\bar{N} \gg 1$ and a much larger effective mass $m_*/m \gg 1$. By $\bar{N}$ we denote the average number of phonons in the cloud, m_* is the effective mass of the polaron and m the mass of the "bare" electron without coupling. Furthermore, a polaron is called a small polaron when the lattice distortion induced by the electron is of the same size as the lattice constant and a large polaron when the distortion extends over several lattice sites. Typically, the description of small polarons requires the treatment of short-range electron-phonon interaction and an

explicit account of the lattice periodicity. Instead, the theory of large polarons assumes long-range forces and relies on the continuum approximation.

Studies of polarons are historically conducted in the framework of quantum field theory using effective quantum Hamiltonians [34, 36]. More recently, first principles methods based on density functional theory turned out to provide an accurate microscopic description of both large and small polarons [117, 118]. The most famous model Hamiltonians go back to the 1950s to Fröhlich [34] and Holstein [36]. Both contain a term for a free particle H_e , a free phonon field H_{ph} and for the particle-phonon interaction $H_{\text{e-ph}}$. While the Holstein Hamiltonian models small polarons, the Fröhlich Hamiltonian, which is the focus of the present study, describes large polarons and is given as

$$H = H_e + H_{\text{ph}} + H_{\text{e-ph}}, \quad (4.1)$$

$$H_e = \sum_{\mathbf{k}} \frac{k^2}{2} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \quad (4.2)$$

$$H_{\text{ph}} = \sum_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}, \quad (4.3)$$

$$H_{\text{e-ph}} = \sum_{\mathbf{k}, \mathbf{q}} \left[V_d(\mathbf{q}) b_{\mathbf{q}}^\dagger a_{\mathbf{k}-\mathbf{q}}^\dagger a_{\mathbf{k}} + V_d^\dagger(\mathbf{q}) b_{\mathbf{q}} a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}} \right]. \quad (4.4)$$

Here $a_{\mathbf{k}}$ and $b_{\mathbf{q}}$ are destruction operators for a particle with wave vector $\mathbf{k}$ and a phonon with wave vector $\mathbf{q}$, respectively. $V_d(\mathbf{q})$ is the coupling function for a system in d dimensions and takes the form

$$V_3(\mathbf{q}) = i \left(\frac{2\sqrt{2}\pi\alpha}{A} \right)^{\frac{1}{2}} \frac{1}{q} \quad (4.5)$$

in 3 dimensions and

$$V_2(\mathbf{q}) = i \left(\frac{\sqrt{2}\pi\alpha}{A} \right)^{\frac{1}{2}} \frac{1}{\sqrt{q}} \quad (4.6)$$

in 2 dimensions [119]. In Eq. 4.5 and 4.6, A is the d -dimensional volume of the system and α is the coupling constant which is material dependent and determines the strength of the electron-phonon interaction. Typical values for real materials are in the range $0 < \alpha < 5$ [120]. Units are chosen such that energy is measured in units of $\hbar\omega_0$ and length in units of $\sqrt{\hbar/m\omega_0}$ which leads to $\hbar = \omega_0 = m = 1$. In deriving and solving the Fröhlich Hamiltonian, it is a common practice to assume certain approximations: (i) the energy dispersion for the electron is parabolic with a band mass m , (ii) the phonon frequency $\omega(\mathbf{q}) = \omega_0$ is dispersionless and constant, (iii) the interaction is only between the electron and long-wavelength

optical, longitudinal phonons and (iv) the spatial extension of the polaron is larger than the lattice constant. In this paper, we exclusively focus on the Fröhlich model and we study the polaron dispersion law, i.e. the dependence of the ground-state energy $E_0(k, \alpha)$ on the modulus of the total polaron momentum $k = |\mathbf{k}|$.

A large body of work [35] exists on solving the Fröhlich Hamiltonian, and most of it concerns the energy of the polaron at rest, $E_0(0, \alpha)$. Yet, so far no exact analytic solution was found. The most successful approach to calculate $E_0(0, \alpha)$ is Feynman's path integral formalism [121, 122], a variational treatment that provides a very accurate upper bound for the polaron ground state energy for all coupling strengths as well as approximate values for the polaron effective mass. Early work on the behavior of the dispersion curve [123, 124] allowed to conclude that the energy-momentum relation starts off quadratically at low k (thus allowing to define a polaron mass) but bends over when approaching the continuum edge $E_c(\alpha) = E_0(0, \alpha) + \hbar\omega_0$. Later it was found that in 3D the dispersion hits the continuum edge whereas for 2D it approaches it asymptotically, and upper and lower bounds for the dispersion were obtained [125–127]. These bounds, as well as some analytically known limits, constitute good benchmarks for any theory of the polaron dispersion.

More recently, the Diagrammatic Monte Carlo method (DMC) was developed and applied to the 3-dimensional Fröhlich polaron [49, 50]. It makes use of diagrammatic expansions of Green's functions and a Metropolis sampling algorithm to perform a random walk in the space of all Feynman diagrams. The DMC not only allows for the calculation of the ground state energies but as well as the polaron dispersion curves, Z-factors (quasiparticle weights) and phonon statistics. However, the DMC results [49, 50] were criticized [125, 126]: the reported results disagree with the analytically known second order coefficient in α for the polaron ground state energy, as well as the large- α expansion coefficient.

The aim of the present paper is the application of our newly implemented DMC code to the solution of the Fröhlich Hamiltonian in both the 3-dimensional (3D) and the 2-dimensional (2D) case. To our knowledge, there do not exist any DMC results for the 2D Fröhlich polaron in the literature. We find that the present DMC results, both in 2D and 3D, agree with the analytically known limits, thus refuting the critique of the DMC method formulated in [125, 126]. In addition, we compare the obtained dispersion relations with analytic upper and lower bounds (where available) and a fitting function [125].

The structure of the paper is as follows. The DMC program is based on the seminal works of Prokof'ev [49] and Mishchenko [50], and is described in Sec. 4.3. The numerical outcome is presented and discussed in Sec. 4.4. We first benchmark our results for the 3D case with the reference data of Prokof'ev *et al.* [49] and

Mishchenko *et al.* [50] as well as with results obtained from Feynman's path integral approach [122]. Furthermore, we show ground state energies $E_0(0, \alpha)$, polaron dispersions $E_0(k, \alpha)$ and effective masses $m_*(\alpha)$ for the 2D Fröhlich polaron and compare them to various scaling relations derived by Peeters and Devreese [128]. We also provide values for the exactly known weak- and strong coupling coefficients. Finally, conclusive remarks are drawn in Sec. 4.5.

4.3 Theory and Methodology

In this section, we introduce the concepts of many-body Green's functions, diagrammatic expansions and corresponding Feynman diagrams as well as the basic concepts of the Diagrammatic Monte Carlo method. Necessary computational details of our code are also given in this section.

4.3.1 Green's functions and Feynman diagrams

To solve the Fröhlich Hamiltonian from Eq. 4.1 for the lowest energy eigenvalues, we make use of the Green's function formalism from many-body physics. In particular, we are interested in the one-electron- N -phonon Green's function in the momentum $(\mathbf{k}, \tilde{\mathbf{q}}_i)$ - imaginary time (τ) representation at zero-temperature, where we assume $\tau > 0$:

$$G^{(N)}(\mathbf{k}, \tau, \{\tilde{\mathbf{q}}_i\}) = \left\langle 0 \left| b_{\tilde{\mathbf{q}}_N}(\tau) \dots b_{\tilde{\mathbf{q}}_1}(\tau) a_{\mathbf{k}_1}(\tau) a_{\mathbf{k}_1}^\dagger(0) b_{\tilde{\mathbf{q}}_1}^\dagger(0) \dots b_{\tilde{\mathbf{q}}_N}^\dagger(0) \right| 0 \right\rangle \quad (4.7)$$

The ket $|0\rangle$ in Eq. 4.7 is the electron and phonon vacuum state [114] and the operators are in the Heisenberg picture $a_{\mathbf{k}}(\tau) = e^{\tau H} a_{\mathbf{k}} e^{-\tau H}$. The total or polaron wave vector is given by $\mathbf{k} = \mathbf{k}_1 + \sum_i \tilde{\mathbf{q}}_i$ and is a conserved quantity [34].

By adding a complete set of polaron eigenstates $|\beta(\mathbf{k})\rangle$ to Eq. 4.7, with $H|\beta(\mathbf{k})\rangle = E_\beta(\mathbf{k})|\beta(\mathbf{k})\rangle$ and $H|0\rangle = E_v|0\rangle = 0$, the Green's function becomes

$$\begin{aligned} G^{(N)}(\mathbf{k}, \tau, \{\tilde{\mathbf{q}}_i\}) &= \sum_{\beta} \left| \left\langle \beta(\mathbf{k}) \left| a_{\mathbf{k}_1}^\dagger b_{\tilde{\mathbf{q}}_1}^\dagger \dots b_{\tilde{\mathbf{q}}_N}^\dagger \right| 0 \right\rangle \right|^2 e^{-(E_\beta(\mathbf{k}) - E_v)\tau} = \\ &= \sum_{\beta} Z_{\beta}^{(N)}(\mathbf{k}, \{\tilde{\mathbf{q}}_i\}) e^{-E_\beta(\mathbf{k})\tau}. \end{aligned} \quad (4.8)$$

The $Z_{\beta}^{(N)}$ -factor measures the squared overlap between the polaron eigenstate $|\beta(\mathbf{k})\rangle$ and a state with one free electron and N free phonons. If $\tau \rightarrow \infty$, Eq. 4.8 shows that the term which contains the state with the lowest energy eigenvalue $E_0(\mathbf{k})$ is the dominant one in the sum. Therefore it is possible to retrieve $E_0(\mathbf{k})$ and the corresponding $Z_0^{(N)}(\mathbf{k}, \{\tilde{\mathbf{q}}_i\})$ -factor for given $\mathbf{k}$ and $\{\tilde{\mathbf{q}}_i\}$ values from the

asymptotic behaviour of the Green's function at long imaginary-times:

$$G^{(N)}(\mathbf{k}, \tau \rightarrow \infty, \{\tilde{\mathbf{q}}_i\}) = Z_0^{(N)}(\mathbf{k}, \{\tilde{\mathbf{q}}_i\}) e^{-E_0(\mathbf{k})\tau}. \quad (4.9)$$

To calculate $G^{(N)}$, we expand the Green's function in a perturbation series [85]. Formally, this leads to an expression of the form

$$G^{(N)}(\mathbf{k}, \tau, \{\tilde{\mathbf{q}}_i\}) = \sum_{n=0}^{\infty} \sum_{\xi_n} \int \cdots \int \mathcal{D}_{n,\xi_n}(\mathbf{k}, \tau, \{\tilde{\mathbf{q}}_i\}; \mathbf{x}) d\mathbf{x}, \quad (4.10)$$

where n labels the order of the perturbation expansion, ξ_n indexes different terms of the same order and $\mathbf{x} = (\tau_1, \dots, \tau_n, \mathbf{q}_1, \dots, \mathbf{q}_n)$ is a vector of integration variables (times of interaction vertices and internal phonon wave vectors). Note the difference between external phonon wave vectors $\{\tilde{\mathbf{q}}_i\}$ appearing in the definition of $G^{(N)}$ and internal phonon wave vectors $\{\mathbf{q}_i\}$ over which is integrated. The integrands $\mathcal{D}_{n,\xi_n}$ are given as a product of free electron Green's functions $G_0(\mathbf{k}, \tau_i - \tau_j)$, free phonon Green's functions $W_0(\mathbf{q}, \tau_i - \tau_j)$ and squared interaction vertices $|V_d(\mathbf{q})|^2$. With the following simple rules it is possible to map all $\mathcal{D}_{n,\xi_n}$ functions to Feynman diagrams:

$$G_0(\mathbf{k}, \tau_i - \tau_j) = \begin{array}{c} \xrightarrow{\quad \mathbf{k} \quad} \\ \tau_j \qquad \tau_i \end{array} = e^{-k^2/2(\tau_i - \tau_j)}, \quad (4.11)$$

$$W_0(\mathbf{q}, \tau_i - \tau_j) = \begin{array}{c} \text{~~~~~} \text{~~~~~} \text{~~~~~} \text{~~~~~} \text{~~~~~} \\ \tau_j \quad \text{~~~~~} \mathbf{q} \quad \text{~~~~~} \tau_i \end{array} = e^{-\omega_0(\tau_i - \tau_j)}, \quad (4.12)$$

$$|V_d(\mathbf{q})|^2 = \begin{array}{c} \mathbf{q} \quad \text{~~~~~} \mathbf{q} \\ \bullet \quad \xrightarrow{\quad} \bullet \\ V_d(\mathbf{q}) \quad V_d^\dagger(\mathbf{q}) \end{array} = \frac{(d-1)\sqrt{2}\pi\alpha}{Aq^{d-1}}. \quad (4.13)$$

This allows us to write the Green's function as an infinite series over Feynman diagrams. Odd orders in the perturbation series evaluate to zero because phonon operators appear linear in the interaction term of the Hamiltonian (Eq. 4.4). A typical diagram is presented in Fig. 4.1. It shows a 8th-order diagram of $G^{(2)}(\mathbf{k}, \tau, \tilde{\mathbf{q}}_1, \tilde{\mathbf{q}}_2)$. All diagrams of $G^{(N)}$ have N external phonon propagators attached to the diagram end. The rules from Eq. 4.11 - 4.13 can be used to translate a diagram back into its functional form. Integration has to be performed over all internal phonon wave vectors $\{\mathbf{q}_i\}$ and over all times $\{\tau_i\}$ so that their chronological order is maintained, e.g. $0 < \tau_1 < \tau_2 < \dots < \tau_8 < \tau$ in Fig. 4.1. The total wave vector $\mathbf{k}$ is always conserved at interaction vertices. For example, the electron propagator between τ_1 and τ_2 in Fig. 4.1 must have the wave vector $\mathbf{k}_2 = \mathbf{k}_1 + \tilde{\mathbf{q}}_1$ so that $\mathbf{k} = \mathbf{k}_2 + \tilde{\mathbf{q}}_2$.

Expressing the Green's function in terms of Feynman diagrams doesn't solve the problem. It merely is a way to rewrite the expansion in a more accessible way. It is still necessary to sum the infinite series of integrals from Eq. 4.10.

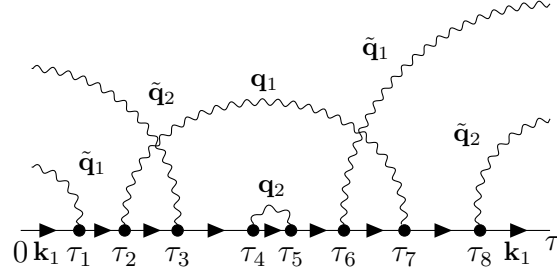


FIGURE 4.1: 8th-order diagram for $G^{(2)}(\mathbf{k}, \tau, \tilde{\mathbf{q}}_1, \tilde{\mathbf{q}}_2)$. Note that diagrams in the expansion of $G^{(2)}$ have two phonon propagators attached to the diagram end. The total polaron wave vector $\mathbf{k} = \mathbf{k}_1 + \tilde{\mathbf{q}}_1 + \tilde{\mathbf{q}}_2$ is conserved at the vertices.

4.3.2 Diagrammatic Monte Carlo

In Ref. [49, 50, 129] it was shown how to use the DMC method to numerically calculate a function $Q(\{y\})$ which is given in a diagrammatic expansion of the form

$$Q(\{y\}) = \sum_{n=0}^{\infty} \sum_{\xi_n} \int \cdots \int \mathcal{D}_{n, \xi_n}(\{y\}; x_1, \dots, x_n) dx_1 \dots dx_n. \quad (4.14)$$

The overall idea behind the DMC method is to interpret $Q(\{y\})$ as a distribution function for the external variables $\{y\}$ [49]. It then uses a Markov chain Monte Carlo (MCMC) procedure to simulate $Q(\{y\})$ by generating diagrams stochastically. This is achieved with a Metropolis-Hastings update scheme to accept or reject new diagrams in which the numerical values of $\mathcal{D}_{n, \xi_n}$ serve as statistical weights. The function $Q(\{y\})$ is obtained by collecting statistics for the external variables $\{y\}$, e.g. in the form of a histogram. At the heart of the DMC algorithm are updates that allow the Markov chain to explore the whole space of Feynman diagrams, i.e. the Markov chain has to be ergodic. It is therefore necessary to implement updates which change the order n , the topology ξ_n , external variables $\{y\}$ and internal variables x_i . Details on basic updating procedures and acceptance probabilities can be found in the Refs. [49, 50, 129, 130].

A general workflow of a DMC application is sketched in Fig. 4.2. Necessary requirements are a diagrammatic expansion of $Q(\{y\})$, updates $\{U_1, \dots, U_k\}$ and probabilities $\{p(U_1), \dots, p(U_k)\}$ with which the updates are chosen. The current diagram in each step is denoted by $\mathcal{D}_{cur}$ and characterized by its parameters values $\mathbf{z} = (\{y\}; x_1, \dots, x_n, n, \xi_n)$. The proposed diagram is called $\mathcal{D}_{new}$ with new parameters $\mathbf{z}' = (\{y'\}; x'_1, \dots, x'_{n'}, n', \xi'_{n'})$. At the beginning, an initial diagram $\mathcal{D}^{(0)}$, e.g. a free electron propagator, is defined and the grid for the histogram is generated. During each Monte Carlo step an update U_i gets selected with probability $p(U_i)$.

Input: initial diagram $\mathcal{D}^{(0)} \leftarrow (\{y^{(0)}\}; x_1^{(0)}, \dots, x_n^{(0)}, n^{(0)}, \xi_n^{(0)})$,
 update procedures $\{U_1, \dots, U_k\}$,
 update probabilities $\{p(U_1), \dots, p(U_k)\}$;
Output: histogram of $Q(\{y\})$;

initialize histogram[];
 initialize diagram $\mathcal{D}_{cur} \leftarrow \mathcal{D}^{(0)}$;
while not converged **do**
 choose an update U_i from $\{U_1, \dots, U_k\}$ with probability $p(U_i)$;
 propose a new diagram $\mathcal{D}_{new} \leftarrow (\{y'\}; x'_1, \dots, x'_{n'}, n', \xi'_{n'})$ according to U_i ;
 calculate acceptance ratio R ;
 draw random uniform number r ;
if $R \geq r$ **then**
 accept the proposed diagram: $\mathcal{D}_{cur} \leftarrow \mathcal{D}_{new}$;
else
 reject the proposed diagram: $\mathcal{D}_{cur} \leftarrow \mathcal{D}_{cur}$;
end if
 histogram[$\{y\}$] $\leftarrow$ histogram[$\{y\}$] + 1;
end while
return histogram;

FIGURE 4.2: General workflow of the DMC algorithm. The algorithm returns the histogram of the function $Q(\{y\})$.

The update U_i proposes a new diagram $\mathcal{D}_{new}$ by changing one or more of the current parameters of $\mathbf{z}$ to $\mathbf{z}'$. Then a Metropolis-Hastings accept/reject step is performed with the following acceptance ratio (detailed balance is assumed)

$$R = \frac{p(U_i^\dagger) \mathcal{D}_{new} P(\mathbf{z}' \rightarrow \mathbf{z})}{p(U_i) \mathcal{D}_{cur} P(\mathbf{z} \rightarrow \mathbf{z}')}, \quad (4.15)$$

where $p(U_i^\dagger)$ is the probability of selecting the inverse update $U_i^\dagger$ of U_i and $P(\mathbf{z} \rightarrow \mathbf{z}')$ is an arbitrary probability density from which the new parameters $\mathbf{z}'$ are chosen. If $R \geq r$, where r is a uniform random number, $\mathcal{D}_{new}$ is accepted otherwise rejected. Finally, the histogram at position $\{y\}$ is updated. These steps are repeated until convergence is achieved. Normalizing the resulting histogram leads to an estimation for $Q(\{y\})$.

4.3.3 DMC for the Fröhlich polaron

With the general procedure of the DMC algorithm at hand, it is fairly easy to apply it to the Fröhlich polaron. Comparing Eq. 4.10 with 4.14 leads to the following identifications:

- (i) $Q \leftrightarrow G^{(N)}$
- (ii) $\{y\} \leftrightarrow \{\mathbf{k}, \tau, \{\tilde{\mathbf{q}}_i\}\}$
- (iii) $\{x_1, \dots, x_n\} \leftrightarrow \{\tau_1, \dots, \tau_n, \mathbf{q}_1, \dots, \mathbf{q}_k\}$

The most straightforward way to obtain the lowest energy eigenvalues $E_0(k, \alpha)$ of the Fröhlich Hamiltonian for a given $\mathbf{k}$ and α with the DMC method is to simulate $G^{(0)}(\mathbf{k}, \tau)$ and fit an exponential function to its long imaginary time behaviour, as can be seen in Eq. 4.9. This was done in the original paper by Prokof'ev [49].

Mishchenko *et al.* [50] provided some improvements to this method. They simulated all $G^{(N)}(\mathbf{k}, \tau, \{\tilde{\mathbf{q}}_i\})$ up to some maximum value $N < N_{max}$ in a single run. It allowed them to introduce direct Monte Carlo estimators for the energy, effective mass, group velocity and Z-factors and to obtain results up to $\alpha = 20$.

In the present paper, we follow the approach by Mishchenko using estimators for the energy $e_{est}(\mathcal{D})$ and inverse effective polaron mass $m_{est}(\mathcal{D})$ making the curve fitting procedure obsolete. A detailed exposition of the workflow can be found in Fig. 4.3. Values for the coupling constant α and the polaron wave vector $\mathbf{k}$ are defined as inputs before the simulation starts. The parameter μ is used as part of a guiding function of the form $e^{\mu\tau}$ to improve the sampling in τ -space. In practice this means that each diagram is multiplied by $e^{\mu\tau}$ or simply by changing the value

of the free electron Green's function to

$$G_0(\mathbf{k}, \tau_i - \tau_j, \mu) = e^{-(k^2/2 - \mu)(\tau_i - \tau_j)}. \quad (4.16)$$

For our calculations, we set μ slightly smaller than the true ground state energy, as recommended in Ref. [49]. We also have specified maximum values for the diagram length τ_{max} , the order n_{max} and for the number of phonon propagators attached to the diagram end N_{max} . The value τ_{min} is used as a cut off, in the sense that we only accumulate estimators if the current diagram length τ is greater than τ_{min} . In our case, $\tau_{max} = 50$ and $\tau_{min} = 5$. Values for n_{max} and N_{max} are dependent on the coupling strength α , τ_{max} and μ and should be chosen sufficiently higher than the average diagram order and average number of external phonons per diagram. The most important ingredients are the updates U_i . We implemented updates for adding and removing internal as well as external phonon propagators, changing the diagram length τ , stretching the diagram as a whole, shifting a single vertex in imaginary time and swapping the phonon propagators of two adjacent vertices. All these updates and a derivation of the estimators are explained in detail in Ref. [50]. We only changed the arbitrary proposal probability distribution $P(\mathbf{z} \rightarrow \mathbf{z}')$ for some of the updates (see Eq. 4.15). Updates are addressed with the same probability $p(U_i) = p(U_j)$.

The basic concept is the same as in the general DMC algorithm, except that we accumulate estimators instead of a histogram (cf. Fig. 4.2 and 4.3). We start from an initial diagram $\mathcal{D}^{(0)}$. The accumulators for the energy E_0^{MC} and inverse effective mass m_*^{MC} as well as the counter c , for the number of diagrams with $\tau > \tau_{min}$, are set to zero. In the main loop, an update U_i is chosen with probability $p(U_i)$ and a new diagram $\mathcal{D}_{new}$ is proposed. It is accepted with probability $\min\{1, R\}$. After the accept/reject step, we check if the current diagram length is greater than τ_{min} . If $\tau > \tau_{min}$, c is increased by 1 and the energy and inverse effective mass estimator for the current diagram $\mathcal{D}_{cur}$ are accumulated. The effective mass is calculated near $\mathbf{k} = 0$ using the quadratic approximation:

$$m_*(\alpha) = \left[\frac{\partial^2 E_0(k, \alpha)}{\partial k^2} \right]_{k=0}^{-1}. \quad (4.17)$$

The loop is repeated until the energy and inverse effective mass estimates have converged. The final estimates are obtained by dividing the accumulators by c .

In Fig. 4.4, we reproduced some of the results from Ref. [50] to verify the correctness of our code. The top graph shows the polaron ground state energy and the bottom graph shows the logarithm of the effective mass as a function of α . Our

Input: initial diagram $\mathcal{D}^{(0)} \leftarrow (\mathbf{k}, \tau^{(0)}, \{\tilde{\mathbf{q}}_i^{(0)}\}; \{\tau_i^{(0)}\}, \{\mathbf{q}_i^{(0)}\}, n^{(0)}, \xi_n^{(0)})$,
 update procedures $\{U_1, \dots, U_k\}$,
 update probabilities $\{p(U_1), \dots, p(U_k)\}$,
 values for: $\alpha, \mu, \mathbf{k}$,
 parameters: $\tau_{max}, \tau_{min}, n_{max}, N_{max}$;
Output: energy $E_0^{MC}(k, \alpha)$,
 inverse effective polaron mass $m_*^{MC}(\alpha)$;

initialize diagram $\mathcal{D}_{cur} \leftarrow \mathcal{D}^{(0)}$;
 $E_0^{MC} \leftarrow 0, m_*^{MC} \leftarrow 0$;
 $c \leftarrow 0$;
while not converged **do**
 choose an update U_i from $\{U_1, \dots, U_k\}$ with probability $p(U_i)$;
 propose a new diagram $\mathcal{D}_{new} \leftarrow (\mathbf{k}, \tau', \{\tilde{\mathbf{q}}_i'\}; \{\tau_j'\}, \{\mathbf{q}_k'\}, n', \xi_{n'})$ according to U_i ;
 calculate acceptance ratio R ;
 draw random uniform number r ;
if $R \geq r$ **then**
 accept the proposed diagram: $\mathcal{D}_{cur} \leftarrow \mathcal{D}_{new}$;
else
 reject the proposed diagram: $\mathcal{D}_{cur} \leftarrow \mathcal{D}_{cur}$;
end if
if $\tau > \tau_{min}$ **then**
 $c \leftarrow c + 1$;
 $E_0^{MC} \leftarrow E_0^{MC} + e_{est}(\mathcal{D}_{cur})$;
 $m_*^{MC} \leftarrow m_*^{MC} + m_{est}(\mathcal{D}_{cur})$;
end if
end while
return $E_0^{MC}/c, m_*^{MC}/c$;

FIGURE 4.3: Detailed workflow of the DMC algorithm as it was used in this paper. The algorithm returns estimates for the lowest eigenenergy $E_0(k, \alpha)$ and the inverse of the effective polaron mass $1/m_*(\alpha)$ for given $\mathbf{k}$ and α values.

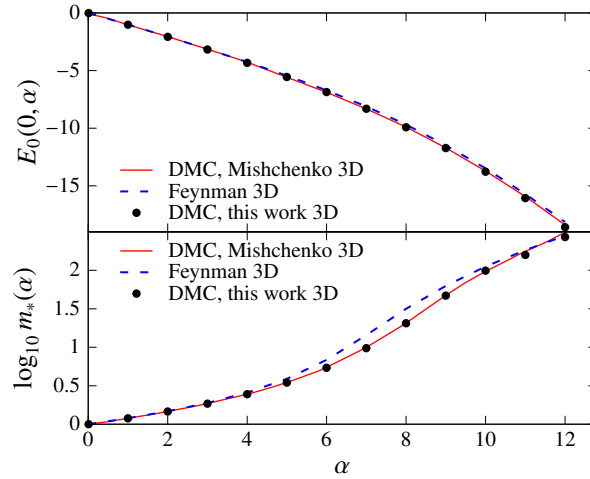


FIGURE 4.4: Comparison of our results (circles) with previous DMC results by Mishchenko [50] (continuous lines) and with results obtained with Feynman’s approach [122] (dashed lines). The top graph shows the polaron ground state energy $E_0(0, \alpha)$ and the bottom graph the logarithm of the polaron effective mass $\log m_*(\alpha)$ as a function of α .

data are in very good agreement with Mishchenko’s data which lets us assume that our code gives reliable DMC results. The figure also displays results obtained with Feynman’s variational treatment [122].

4.4 Results and discussion

In this section, we provide a more extensive discussion of the DMC results for the Fröhlich polaron in 3D and 2D. We show and discuss polaron ground state energies, effective polaron masses and polaron dispersions for different coupling strengths and prove that DMC correctly accounts for the 3D→2D scaling relations. All energies are given in units of $\hbar\omega_0$ and lengths in units of $\sqrt{\hbar/m\omega_0}$.

4.4.1 Polaron ground state energy and effective mass

We first focus on our results for the polaron ground state energy $E_0(0, \alpha)$ (Fig. 4.5), i.e. the minimum of the polaron energy band, and for the effective polaron mass $m_*(\alpha)$ (Fig. 4.6) as a function of α for 3D and 2D systems. Both cases are compared to Feynman’s approach [122] and with available DMC results in 3D [50] (Fig. 4.4). The corresponding numerical values are written in Table 4.1 (3D) and Table 4.2 (2D).

Feynman results in 2D have been obtained from the 3D results via scaling relations [128, 131, 132]. These scaling relations are exact for the Feynman polaron

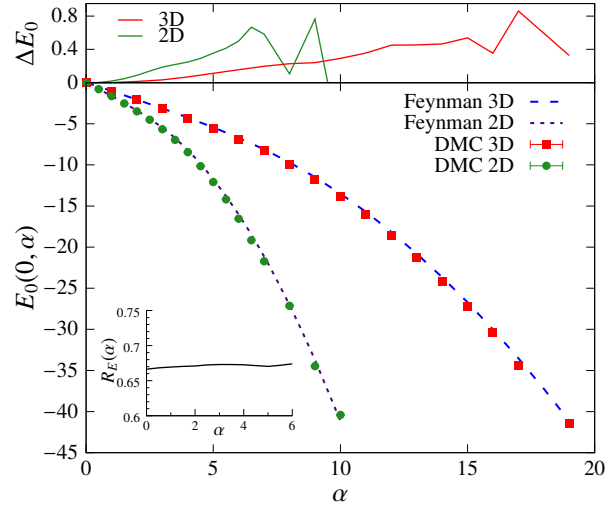


FIGURE 4.5: Polaron energy $E_0(0, \alpha)$ as a function of the coupling constant α . The modulus of the total wave vector is $k = 0$. Results from the Feynman approach are shown as dashed lines. DMC results for 3D systems are depicted as squares and for 2D as circles. ΔE_0 is the difference between Feynman and DMC results. The inset shows the scaling ratio $R_E(\alpha) = E_0^{2D}(0, \alpha)/E_0^{3D}(0, 3\pi\alpha/4)$ between our 2D and 3D DMC results.

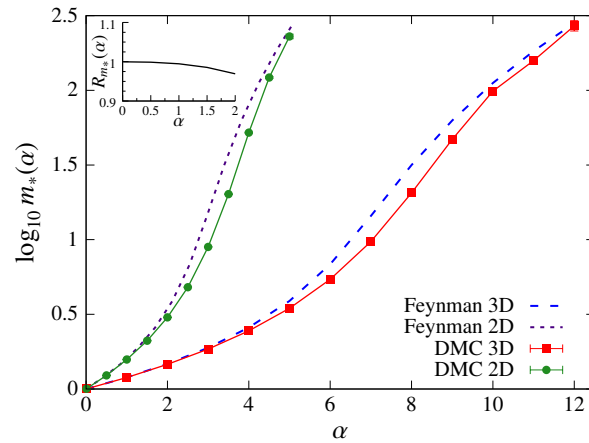


FIGURE 4.6: Logarithm of the polaron effective mass $m_*(\alpha)$ as a function of the coupling constant α . Results from the Feynman approach are shown as dashed lines. DMC results for 3D systems are depicted as squares and for 2D as circles. The inset shows the scaling ratio $R_{m_*}(\alpha) = m_*^{2D}(\alpha)/m_*^{3D}(3\pi\alpha/4)$ between our 2D and 3D DMC results.

energy and Feynman polaron mass:

$$E_0^{2D}(0, \alpha) = \frac{2}{3} E_0^{3D}(0, 3\pi\alpha/4), \quad (4.18)$$

$$\frac{m_*^{2D}(\alpha)}{m^{2D}} = \frac{m_*^{3D}(3\pi\alpha/4)}{m^{3D}}. \quad (4.19)$$

For $\alpha = 0$ the polaron does not form and therefore $E_0 = 0$ and $m_*(0) = m$. As expected, with increasing electron-phonon coupling the polaron energy $E_0(0, \alpha)$ decreases and the effective mass increases as a consequence of the progressive localization of the polaron band. This effect is stronger in 2D than in 3D and explains the steeper curves in 2D.

Overall, our DMC data agree very well with the Feynman results in the entire range of coupling strength, in particular for what concerns the polaron energy (Fig. 4.5). The only sizeable deviation is observed for the effective mass in the intermediate coupling regime, for which Feynman's approach gives considerably higher values than the DMC (Fig. 4.6). Both the DMC results and the variational results obey the scaling laws (4.18) and (4.19). This can be seen in the insets of Figs. 4.5 and 4.6 where we show the ratios $R_E(\alpha) = E_0^{2D}(0, \alpha)/E_0^{3D}(0, 3\pi\alpha/4)$ and $R_{m_*}(\alpha) = m_*^{2D}(\alpha)/m_*^{3D}(3\pi\alpha/4)$ between our DMC results in 2D and 3D. However, the uncertainty in the Monte Carlo calculations of m_*^{2D} for $\alpha > 2$ worsens the stability of the scaling relation of the effective mass at large α . The reason for this low performance is that the effective mass estimator actually calculates the inverse of the effective mass rather than the effective mass itself [50]. Since the polaron mass grows very fast with increasing coupling, its inverse becomes very small, which unavoidably worsens the accuracy of the results.

To test the accuracy of our calculations, we have also retrieved values for the exactly known weak-coupling coefficients q_1 and q_2

$$E_0(0, \alpha) = -q_1\alpha - q_2\alpha^2 + \mathcal{O}(\alpha^3) \quad (4.20)$$

and the strong-coupling coefficient γ

$$\lim_{\alpha \rightarrow \infty} E_0(0, \alpha)/\alpha^2 = -\gamma. \quad (4.21)$$

The exact [126, 132] and DMC values for these coefficients, listed in Table 4.3, are in very good agreement. However, a word of caution is needed here: the coefficients are obtained with a simple curve fitting procedure and the final numerical values are highly sensitive to the range of α values included in the fitting process.

TABLE 4.1: Ground state energies $E_0(0, \alpha)$ and effective masses $m_*(\alpha)$ in 3D from the DMC and Feynman method [122]. Values in brackets stand for the uncertainty in the DMC simulation, e.g $-1.01662(47)$ has a sample standard error of 4.7×10^{-4} .

α	E_0 DMC	E_0 Feynman	m_* DMC	m_* Feynman
1	-1.01662(47)	-1.0130308	1.19396(2)	1.1955147
2	-2.06957(84)	-2.0553559	1.46166(7)	1.4718919
3	-3.16829(136)	-3.1333335	1.85047(13)	1.8889540
4	-4.32490(211)	-4.2564809	2.45196(57)	2.5793104
5	-5.55297(296)	-5.4401445	3.47194(180)	3.8856197
6	-6.86647(287)	-6.7108710	5.41952(625)	6.8383564
7	-8.31039(309)	-8.1126875	9.7130(268)	14.394070
8	-9.92206(606)	-9.6953709	20.55(14)	31.569255
9	-11.72535(701)	-11.485786	46.90(78)	62.751527
10	-13.7820(136)	-13.490437	98.8(3.3)	111.81603
11	-16.0660(127)	-15.709808	158.2(4.6)	183.12497
12	-18.5943(240)	-18.143395	270.1(20.0)	281.62189
13	-21.2434(249)	-20.790681	/	412.78190
14	-24.1151(369)	-23.651278	/	582.58390
15	-27.2629(359)	-26.724904	/	797.49838

TABLE 4.2: Ground state energies $E_0(0, \alpha)$ and effective masses $m_*(\alpha)$ in 2D from the DMC and Feynman method [122]. Values in brackets stand for the uncertainty in the DMC simulation, e.g $-1.64348(23)$ has a sample standard error of 2.3×10^{-4} .

α	E_0 DMC	E_0 Feynman	m_* DMC	m_* Feynman
1	-1.64348(23)	-1.62321	1.57437(8)	1.59966
2	-3.48333(62)	-3.39482	3.01609(21)	3.40982
3	-5.66337(46)	-5.47667	8.94191(730)	15.2085
4	-8.45543(149)	-8.20738	52.108(341)	81.1684
5	-12.08288(610)	-11.7281	229.3(7.8)	257.452
6	-16.5403(269)	-16.0402	601.9(46.0)	609.244
7	-21.7231(566)	-21.1408	/	/
8	-27.1346(802)	-27.0283	/	/
9	-34.4669(370)	-33.7021	/	/
10	-40.4139(379)	-41.1602	/	/

TABLE 4.3: Exactly known (exact) vs. calculated (calc.) expansion coefficients of $E_0(0, \alpha)$ for the weak- and strong coupling limit. The coefficients were obtained using different ranges of α in 2D and 3D. In 2D, we have included $\alpha < 0.2$ for computing q_1 and q_2 and $4 \leq \alpha < 9$ for γ . The corresponding 3D ranges are $\alpha < 0.85$ (q_1 and q_2) and $9 \leq \alpha < 18$ (γ).

	q_1 exact	q_1 calc.	q_2 exact	q_2 calc.
3D	1.0	$0.9999 \pm 3.8 \times 10^{-4}$	0.01592	$0.01588 \pm 9.1 \times 10^{-4}$
2D	1.5708	$1.57084 \pm 1.7 \times 10^{-4}$	0.06397	$0.06483 \pm 2.8 \times 10^{-3}$
	γ exact	γ calc.		
3D	0.1085	$0.10805 \pm 7.7 \times 10^{-4}$		
2D	0.4047	$0.40236 \pm 3.8 \times 10^{-3}$		

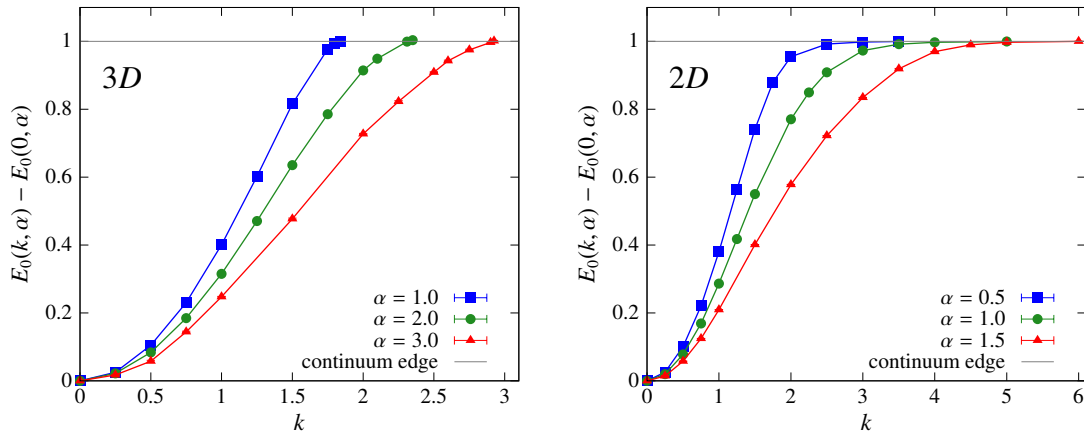


FIGURE 4.7: Polaron energy $E_0(k, \alpha) - E_0(0, \alpha)$ as a function of the modulus of the total wave vector k in 3D (left, for coupling constants $\alpha = 1.0, 2.0$ and 3.0) and 2D (right, $\alpha = 0.5, 1.0$ and 1.5). The continuum edge is shown at $E_c(k) = 1$.

We have computed q_1 and q_2 using $\alpha < 0.85$ and $\alpha < 0.2$, in 3D and 2D respectively, whereas for γ we have included values in the range $9 \leq \alpha < 18$ (3D) and $4 \leq \alpha < 9$ (2D).

Gerlach, Kalina and Smondyrev [126] correctly point out that the (3D) second order perturbative result $q_2 = 0.0126$ obtained by Mishchenko using DMC [50] deviates from Röseler's [133] exact result $q_2 = 0.01592\dots$, but we surmise that they incorrectly concluded that the DMC results $E_0(0, \alpha)$ are incompatible with Röseler's results. Here, we resolve this issue by providing the calculated DMC values explicitly, showing that there is no discrepancy. Both for the 3D and the 2D case, it can be seen in Table 4.3 that the DMC technique yields accurate estimates for q_2 , as well as for the other analytically known expansion coefficients q_1 and γ .

4.4.2 Polaron dispersion

In Fig. 4.7, we display some dispersion curves in 3D and 2D for selected values of α . The results have been shifted so that the ground state energy at $k = 0$ is $E_0(0, \alpha) = 0$. This makes a comparison between different α values easier. As expected, $E_0(k, \alpha)$ increases monotonically as a function of k and becomes more flat with increasing coupling. This reflects the tendency to form more localized bands as the electron-phonon coupling strength becomes stronger, an effect that is more intense in the more-localized 2D limit, where the dispersion curves bend over more sharply. Clearly, this behavior correlates with the polaron effective mass since it is defined as the inverse of the curvature of the energy band at $k = 0$ (see Fig. 4.6).

For large k , the energy curve approaches the so called "continuum edge" $E_c(\alpha)$ defined as the energy value:

$$E_c(\alpha) = E_0(0, \alpha) + \hbar\omega_0 = E_0(0, \alpha) + 1, \quad (4.22)$$

i.e. the energy value which is one phonon excitation quantum or unity (in our units) above the ground state energy. An important difference between the 3D and 2D case is that in 3D the dispersion curve crosses the continuum edge at a finite critical wave vector length $k_c(\alpha)$. Instead, in 2D, it has been proven that this edge constitutes an asymptote and is approximated from below as $k \rightarrow \infty$ [125–127].

For small α , there exist rigorous upper and lower bounds for the polaron dispersion [127] that restrict this dispersion to a narrow domain. In the top row of Fig. 4.8, the DMC results are shown together with these bounds for $\alpha = 0.068$, the value of the coupling strength for GaAs. Our results lie in between the bounds, close to the upper bound, both in 3D (upper left panel of Fig. 4.8) and 2D (upper right panel). The strict lower bound only exists for small values of the coupling strength: $\alpha = 0.5$ already lies outside the range where this lower bound can be found.

Gerlach and Smondyrev [127] propose a fitting function for the dispersion. This fit is based on a re-scaling of the upper bound formula, to obtain the correct gap between bottom of the band and the continuum edge, while maintaining the effective mass. As shown in the lower left panel of Fig. 4.8, the DMC results for the 3D case for $\alpha = 0.5$ lie below both the variational upper bound and the Gerlach-Smondyrev dispersion. The same conclusion can be drawn for the 2D case, shown in the lower right panel of Fig. 4.8.

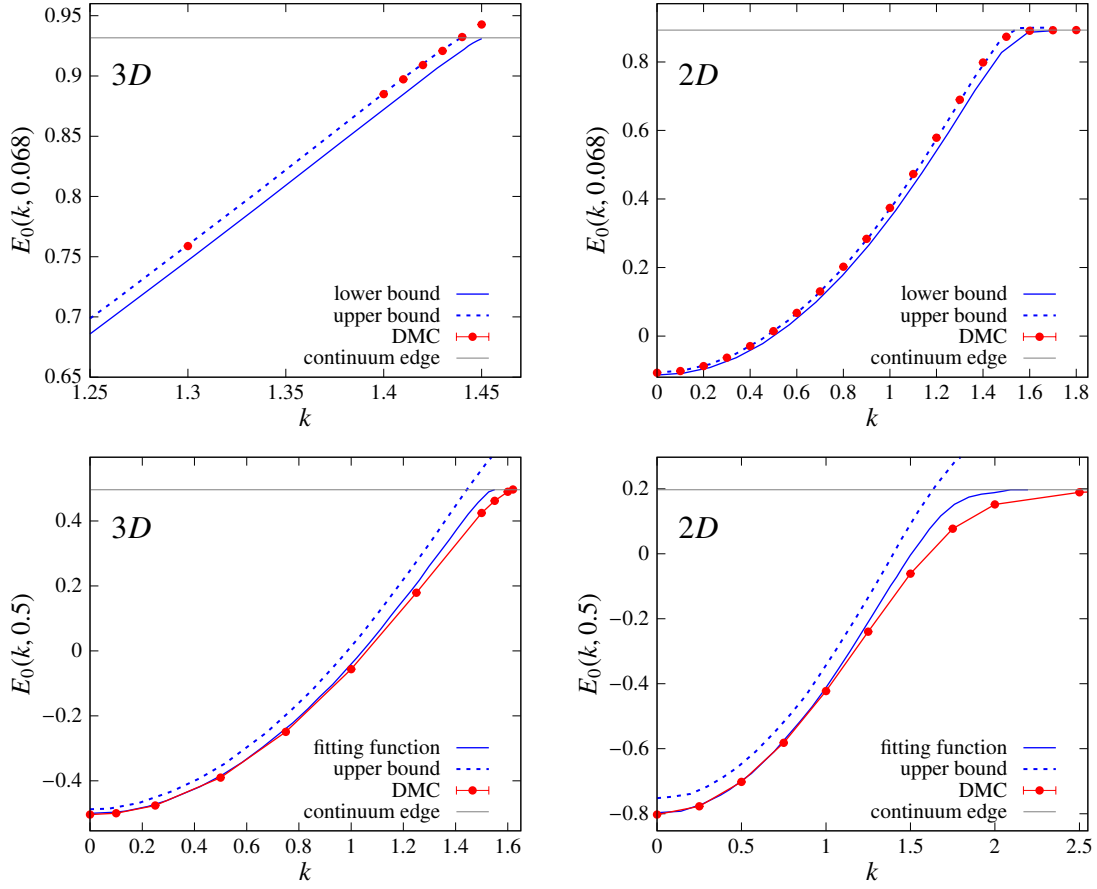


FIGURE 4.8: Polaron energy $E_0(k, \alpha)$ in 3D (left) and 2D (right) as a function of the modulus of the total wave vector k for coupling constant $\alpha = 0.068$ (top row) and $\alpha = 0.5$ (bottom row). Lower and upper bounds, and a fitting function to the dispersion are taken from Ref. [127].

TABLE 4.4: Critical wave vectors $k_c(\alpha)$ for coupling constants $\alpha = 0.068$, $\alpha = 0.5$ and $\alpha = 1.0$. Listed are results from our DMC calculations, from Eq. 4.23 which is valid up to first order in α , as well as from the fitting function from Ref. [127].

	$\alpha = 0.068$	$\alpha = 0.5$	$\alpha = 1.0$
DMC, this work	1.440	1.615	1.833
Result to order α , Eq. (4.23)	1.442	1.616	1.818
Gerlach and Smondyrev, Ref. [127]	1.442	1.570	1.697

We now focus on the 3D case, in which the dispersion reaches the continuum edge at a given k_c . Up to lowest order in α ,

$$k_c(\alpha) = \sqrt{2} + \left(\frac{\pi}{2} - 1\right) \frac{\alpha}{\sqrt{2}} + \mathcal{O}(\alpha^2). \quad (4.23)$$

In Table 4.4, we compare for several α values the critical wavenumber obtained (i) with DMC, (ii) with the first order approximation, Eq. 4.23, and (iii) using the Gerlach-Smondryev dispersion. At small coupling strength $\alpha = 0.068$, all three approaches yield the same result. However, as α is increased slightly (remaining in the regime where the lowest order approximation can be expected to be valid), the result obtained from the Gerlach-Smondryev dispersion drops below the value found by the other two approaches. The value of k_c in the Gerlach-Smondryev approach is 3% resp. 8% smaller than the DMC result for $\alpha = 0.5$ and 1.

Previously [127], this discrepancy was blamed on the fact that the DMC method supposedly failed to reproduce even the known q_2 parameter (the coefficient of α^2), whereas the fitting function is claimed to be good up to order α^3 . However, as we have shown in the previous subsection, this explanation cannot hold since contrary to what was believed earlier, the DMC does reproduce the q_2 value with high accuracy. The Gerlach-Smondryev dispersion is not the result of variational minimization, nor is it a rigorous lower bound: rather it is an ad hoc proposal that rescales the best variational upper bound to give the correct known limits. Keeping in mind that the DMC calculation takes many phonons into account (i.e. goes well beyond order α in the diagrams), we can conclude that the DMC results indicate that this fitting procedure is not appropriate for $\alpha \geq 0.5$.

4.5 Summary and Conclusion

The Diagrammatic Monte Carlo is a powerful method which has proven to work in many applications for many different systems [51, 63, 83, 106, 134, 135]. For this paper, we have implemented a DMC code based on the Refs. [49, 50] and applied it to the solution of the large polaron Fröhlich Hamiltonian in 3D and 2D. We benchmarked our code with existing DMC results for the 3D case to verify its correctness and then computed polaron ground state energies, effective polaron masses and polaron dispersion curves in 2D and 3D.

In summary, our data confirm that the effect of electron-phonon coupling is enhanced in 2D compared to 3D, and this is reflected in all computed physical quantities. Concerning the ground state energies, the DMC results are in very good agreement with those obtained by Feynman's approach [122] and we have

demonstrated that they obey the scaling relations between 3D and 2D [128]. The reliability of the DMC procedure is further corroborated by the calculations of the coefficients used for the weak- and strong-coupling regime, which are almost identical to the exactly known values. This refutes a claim [126] that the DMC technique is not able to correctly obtain the q_2 coefficients. Regarding the effective polaron mass, the DMC performance becomes slightly less satisfactory at stronger coupling. This inaccuracy should be traced back to the numerical errors involved in the calculation of the inverse of the effective mass. Alternative definitions of the polaron effective mass have been proposed in literature, which could be possibly tested in future work to assess and compare the performance of DMC and path-integrals approaches [136, 137].

One of the most interesting outcomes of the present study are the polaron dispersion curves. The DMC calculations reproduce very well the different behaviour seen in 2D and 3D: in 2D the energy curve approaches the continuum edge asymptotically from below, whereas in 3D it reaches the continuum edge at a finite critical k_c . For small α ($=0.068$, a realistic value for a material like GaAs), the DMC dispersion as well as the k_c are in very good agreement with the known lower and upper limits derived from the variational approach of Gerlach and Smondyrev [127]. For larger α ($\alpha = 0.5, 1.0$), the DMC data agree well with the first order expansion results, but deviate from the values based on a proposed fitting function for the dispersion. While the DMC technique cannot validate the fitting procedure proposed by Gerlach and Smondyrev for $\alpha \geq 0.5$, it does suggest that up to $\alpha \approx 1$ the first order expansion result of Eq. 4.23 already provides an accurate estimate of k_c .

4.6 Acknowledgements

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Chapter 5

Acoustic lattice polaron

This chapter includes a verbatim copy from the following published article:

T. Hahn, N. Nagaosa, C. Franchini, A.S. Mishchenko, *Diagrammatic quantum Monte Carlo study of an acoustic lattice polaron*, *Physical Review B* **104** (16), L161111 (2021).

Preamble: The manuscript uses the DiagMC + SOCC approach discussed in Chapters 2 and 3 and applies it to an acoustic lattice polaron model in three dimensions. The model Hamiltonian describing the acoustic lattice polaron has been derived as part of the study and the following polaron properties are presented (as functions of the coupling strength λ and Debye frequency Ω_0):

- Ground state energy E_{GS} , effective mass m^* , quasiparticle weight Z_0 , average phonon number $\langle N_{\text{ph}} \rangle$, and phonon distribution function $Z(n)$.
- Spectral function $A(\omega)$ and first excited state energy.
- Optical conductivity $\sigma(\omega)$.

The correctness of the author's DiagMC implementation has been verified by comparing the computed polaron properties to weak- and strong-coupling perturbation theory results (not shown in the thesis).

Contribution: As the first author of the paper, I developed the methodology, independently implemented the code, conducted the simulations, analyzed the data, and wrote part of the manuscript.

5.1 Abstract

We present a diagrammatic Monte Carlo study of a lattice polaron interacting with an acoustic phonon branch through the deformation potential. Weak and strong coupling regimes are separated by a self-trapping region where quantum resonance

between various possible lattice deformations is seen in the ground state properties, spectral function, and optical conductivity. This study shows that the acoustic lattice polaron represents a distinct quantum object with unique features, markedly different from any previously considered polaron model. In particular, the acoustic lattice polaron exhibits an interplay between long- and short wavelength acoustic vibrations resulting in a composite phonon cloud which leads to the formation of multiple competing polaron states with a complex spectral response.

5.2 Introduction

The fundamental conception of a polaron, an electron interacting with phonons and increasing its mass by dragging the accompanying phonon cloud with it, was formed long ago [31, 32]. Depending on the type of phonon involved and on the mechanism used to model the electron-phonon coupling [41, 42, 101, 138–141], it is possible to distinguish between optical [34] vs. acoustic [38, 142] and lattice [36] vs. continuum [143] polarons. Optical polaron models have been studied extensively over the years. The gap in the spectrum of optical phonons makes them accessible to approximate approaches [55, 144, 145], approximation free numerical techniques [146–154], and even analytic methods [155]. On the contrary, acoustic polaron models have received much less attention. Due to their gapless phonon spectrum, many techniques, which work well for the optical case, either fail [155] or are effective only at weak coupling [156]. This lack of reference studies in the polaron literature is in contrast to the growing evidence that realistic calculations require a thorough treatment of electron-acoustic phonon interactions [20, 26, 157–166].

In general, a typical polaron model describes an electron interacting with a single phonon branch ($\hbar = 1$):

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \sum_{\mathbf{q}} \omega(\mathbf{q}) b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + N^{-1/2} \sum_{\mathbf{k}, \mathbf{q}} V(\mathbf{q}, \mathbf{k}) c_{\mathbf{k}+\mathbf{q}}^{\dagger} c_{\mathbf{k}} (b_{-\mathbf{q}}^{\dagger} + b_{\mathbf{q}}) . \quad (5.1)$$

Here, the operator $c_{\mathbf{k}}^{\dagger}/b_{\mathbf{q}}^{\dagger}$ creates an electron/phonon with momentum $\mathbf{k}/\mathbf{q}$. The Hamiltonian is fully determined by the electron dispersion $\epsilon_{\mathbf{k}}$, the phonon frequency $\omega(\mathbf{q})$, and the interaction vertex $V(\mathbf{q}, \mathbf{k})$. In lattice models, N specifies the number of unit cells and sums over momenta are restricted to the first Brillouin zone (BZ).

Every polaron eigenstate $|\nu, \mathbf{k}\rangle$ of Eq. (5.1) with energy $E_{\nu}(\mathbf{k})$ can be written as a linear combination of states in which an electron with momentum $\mathbf{k} - \mathbf{q}_1 - \dots - \mathbf{q}_n$

is accompanied by n phonons with momenta $\mathbf{q}_1, \dots, \mathbf{q}_n$:

$$|\nu, \mathbf{k}\rangle = \sum_{n=0}^{\infty} \sum_{\mathbf{q}_1 \dots \mathbf{q}_n} \Theta_{\mathbf{q}_1 \dots \mathbf{q}_n}^{\nu, \mathbf{k}} c_{\mathbf{k}-\mathbf{q}_1-\dots-\mathbf{q}_n}^\dagger b_{\mathbf{q}_1}^\dagger \dots b_{\mathbf{q}_n}^\dagger |\emptyset\rangle. \quad (5.2)$$

$|\emptyset\rangle$ denotes the electron and phonon vacuum and $\Theta_{\mathbf{q}_1 \dots \mathbf{q}_n}^{\nu, \mathbf{k}}$ are expansion coefficients. For a fixed polaron momentum $\mathbf{k}$, we can identify the eigenstate $|\nu = 0, \mathbf{k}\rangle$ with the lowest energy $E_0(\mathbf{k})$. The ground state (GS) $\langle 0, \mathbf{k}_{\text{GS}} \rangle$, which is usually located at $\mathbf{k} = \mathbf{k}_{\text{GS}} = 0$, has an energy $E_{\text{GS}} = E_0(\mathbf{k} = \mathbf{k}_{\text{GS}})$ and effective mass $m^* = (d^2 E_0(\mathbf{k}_{\text{GS}})/d\mathbf{k}^2)^{-1}$. The structure of the phonon cloud is described by the probabilities of finding n -phonons in the GS, $Z(n) = \sum_{\mathbf{q}_1 \dots \mathbf{q}_n} |\Theta_{\mathbf{q}_1 \dots \mathbf{q}_n}^{0, \mathbf{k}=\mathbf{k}_{\text{GS}}}|^2$, and their average number $\langle N_{\text{ph}} \rangle = \sum_n n Z(n)$. More information is contained in the spectral function $A_{\mathbf{k}}(\omega) = \sum_{\nu} \delta(\omega - E_{\nu}(\mathbf{k})) |\langle \emptyset | c_{\mathbf{k}} | \nu, \mathbf{k} \rangle|^2$, which has poles (sharp peaks) at energies of stable (metastable) states of the polaron.

Optical polaron models with phonon dispersion $\omega(\mathbf{q}) = \omega_0 > 0$ and interaction vertex $V(\mathbf{q}, \mathbf{k}) = V(\mathbf{q})$ are well understood. In the case of lattice models, it is common practice to quantify the electron-phonon coupling strength with a single parameter

$$\tilde{\lambda} = \sum_{\mathbf{q}} \frac{2|V(\mathbf{q})|^2}{W\omega(\mathbf{q})}, \quad (5.3)$$

where W is the width of the electronic band. Polaron states for $\tilde{\lambda} \ll 1$ and $\tilde{\lambda} \gg 1$ show profound differences. In the weak coupling regime (WCR) at $\tilde{\lambda} \ll 1$, the GS is light $m^*/m^*(\tilde{\lambda} = 0) \approx 1$ with a slightly distorted lattice $\langle N_{\text{ph}} \rangle \ll 1$ around the electron, whereas in the strong coupling regime (SCR) at $\tilde{\lambda} \gg 1$, the GS is heavy $m^*/m^*(\tilde{\lambda} = 0) \gg 1$ because of a large phonon cloud $\langle N_{\text{ph}} \rangle \gg 1$ surrounding the electron.

At $\tilde{\lambda} = \tilde{\lambda}_{\text{cr}} \approx 1$, one may observe the self-trapping (ST) phenomenon. ST, as it was defined in the pioneer works [31, 167–169], refers to an apparent quantum resonance between WCR and SCR. There are two indicators for ST: (i) a two-peak structure in the phonon distribution function $Z(n)$, and (ii) a clear avoided crossing behavior of the GS and first excited state (FES) in the spectral response. These two fingerprints are very spectacular when the optical phonon frequency ω_0 is sufficiently small $\omega_0 \ll W$, but they are hardly observed at large ω_0 [170].

The phonon spectrum of the acoustic polaron model dramatically changes the situation because the energy gap $\omega_0 > 0$, inherent to optical phonons, is missing and there is no *a priori* knowledge whether the Debye frequency Ω_0 of the acoustic phonon dispersion can be a good substitute. It so happened that all previous non-perturbative studies were restricted to a simplified continuum model [39, 63,

142, 171–173]. The electronic band in the continuum model is approximated by $\epsilon_{\mathbf{k}} = k^2/2$ while the phonon dispersion and interaction vertex are set to $\omega(\mathbf{q}) = v_s q$ and $V(\mathbf{q}) \sim \sqrt{q}$, with v_s a sound velocity [40]. A momentum cutoff $q \leq k_0$ is introduced to establish the maximal Debye frequency $\Omega_0 = v_s k_0$. Surprisingly, it was shown [39, 63, 142, 171, 174] that the WCR to SCR crossover is sharper for *larger* values of Ω_0 . This is clearly opposite to what is found in optical polaron models, where the crossover is sharper for *smaller* ω_0 .

With the present Letter, we fill a gap in the polaron literature by providing a reference study of an acoustic lattice polaron model using approximation free diagrammatic Monte Carlo [49–51, 175] and stochastic optimization consistent constraints (SOCC) [50, 92, 93] analytic continuation methods. SOCC does not involve any approximation and does not assume any predefined shape of the real frequency spectra because the procedure is based solely on the imaginary time input data [92].

5.3 Model

We consider a three dimensional primitive cubic lattice with the tight binding dispersion for the electron

$$\epsilon(\mathbf{k}) = 2t \sum_i^{x,y,z} [1 - \cos(k_i)] , \quad -\pi \leq k_i < \pi , \quad (5.4)$$

(t is the nearest-neighbor hopping amplitude) and an acoustic phonon spectrum due to nearest-neighbor force constants and with Debye frequency Ω_0

$$\omega(\mathbf{q}) = \Omega_0 \sqrt{\sum_i^{x,y,z} \sin^2 \{q_i/2\}} , \quad -\pi \leq q_i < \pi . \quad (5.5)$$

Estimating the deformation potential $D = \sigma \text{div}(\mathbf{u}(\mathbf{r})) = \sigma \sum_i^{x,y,z} \partial u_i / \partial x_i$, as the energy proportional to the change of the unit cell volume $D \sim \sum_i^{x,y,z} | \mathbf{u}_i(\mathbf{r} + \hat{\mathbf{a}}_i) - \mathbf{u}_i(\mathbf{r}) |$, where $\hat{\mathbf{a}}_i$ is a primitive unit vector of the 3D cubic lattice and $\mathbf{u}_i(\mathbf{r}) \sim \hat{\mathbf{a}}_i \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} (b_{\mathbf{q}} + b_{-\mathbf{q}}^\dagger) / \sqrt{\omega(\mathbf{q})}$ is a displacement due to the acoustic phonon mode, one arrives at the interaction vertex

$$V(\mathbf{q}) = \gamma \sum_i^{x,y,z} \sin \{|q_i/2|\} \left[\sum_i^{x,y,z} \sin^2 \{q_i/2\} \right]^{-1/4} . \quad (5.6)$$

As is usually the case, we define a dimensionless coupling constant $\lambda = \gamma^2/(6t\Omega_0)$ which corresponds to $\tilde{\lambda} \approx 2.5\lambda$ as follows from Eqs. (5.3)–(5.6). The lattice constant a and the hopping amplitude t are set to unity throughout.

5.4 Results

Figures 5.1(a)–5.1(d) show the ground state properties (effective mass, energy, quasiparticle weight and average number of phonons) as functions of the coupling strength λ . In contrast to the acoustic continuum polaron, the transition from WCR to SCR is sharper for smaller values of the Debye energy cutoff Ω_0 . This behavior is similar to what is observed in optical lattice models, where the crossover is more abrupt for smaller ratios ω_0/W . Moreover, it is interesting to note that the value of $\tilde{\lambda}_{\text{cr}} \approx 2.5\lambda_{\text{cr}}$ in the adiabatic limit is in good agreement in both optical and acoustic lattice models. In Fig. 5.1(e), we show $\lambda_{\text{cr}}(\Omega_0)$ determined from derivatives of various GS properties with respect to λ (see the caption for more details). Although the values of $\lambda_{\text{cr}}(\Omega_0)$ slightly depend on the kind of derivative, this discrepancy becomes negligible at small values of Ω_0 allowing us to extrapolate to the adiabatic limit $\lambda_{\text{cr}}(\Omega_0 \rightarrow 0) = 0.355 \pm 0.01$. Using Eq. (5.3), we can compare this value for the acoustic polaron $\tilde{\lambda}_{\text{cr}}^{\text{ac}}(\Omega_0 \rightarrow 0) = 0.895 \pm 0.03$ to the one obtained for the optical polaron $\tilde{\lambda}_{\text{cr}}^{\text{op}}(\Omega_0 \rightarrow 0) = 0.9$ [176, 177].

The general features of the phonon distribution function $Z(n)$ in Figs. 5.1(f) and 5.1(g) are very similar to the optical polaron case [55, 57, 178]. In the WCR, the free electron contribution to the expansion of the polaron GS in Eq. (5.2) is the dominant one and so $Z(n=0) \approx 1$ while $Z(n>0) \approx 0$. In the SCR, $Z(n)$ resembles a Poisson distribution with its mean located at $\approx 13.47\lambda/\Omega_0$. For the nearly adiabatic case $\Omega_0 = 0.5$ [Fig. 5.1(f)], $Z(n)$ develops a two-peak structure close to the critical coupling $\lambda_{\text{cr}} \approx 0.41$. This self-trapping indicator is not seen in the nearly anti-adiabatic case $\Omega_0 = 2$ [Fig. 5.1(g)], where we always observe a single peak.

It is thus no surprise that for $\Omega_0 = 0.5$, in agreement with the resonant behavior of $Z(n)$, the spectral function in Fig. 5.2(a) demonstrates the avoided crossing phenomenon representative for self-trapping. At $\lambda = 0.1$, the FES is still well separated $\approx 0.2t$ from the GS, which contains nearly all of the weight, i.e. $Z_0 \approx 1$. With increasing coupling, this gap becomes smaller and the weight is slowly transferred to the FES, as can be seen from Figs. 5.2(b) and 5.2(c). At the crossover point $\lambda = \lambda_{\text{cr}}$, the energy gap between GS and FES is minimal and their weights become equal.

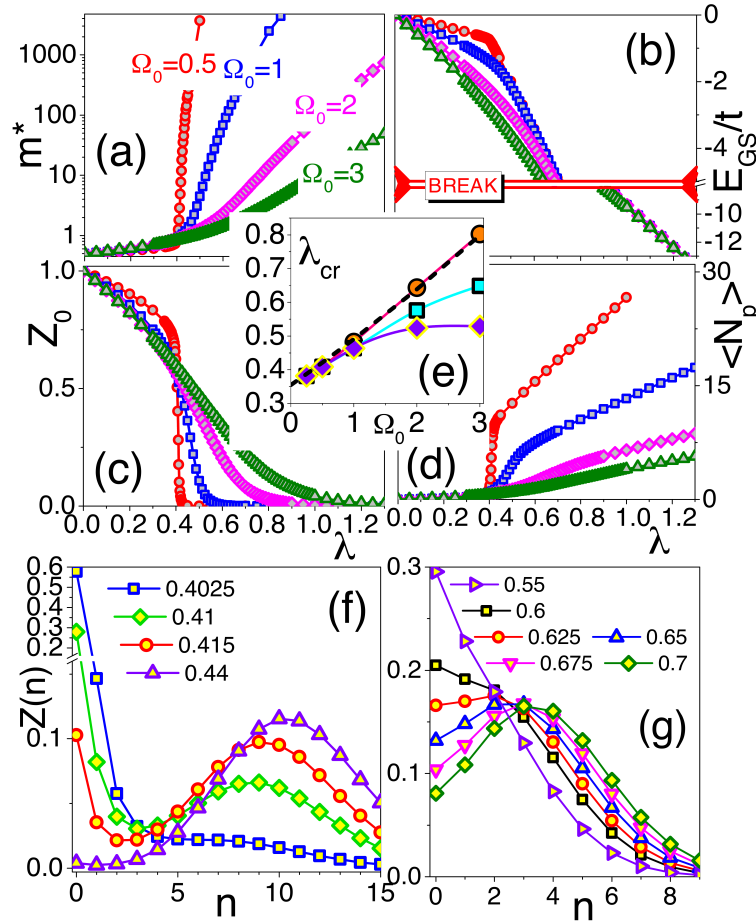


FIGURE 5.1: (a-d) Polaron ground state properties for $\Omega_0 = 0.5$ (red circles), $\Omega_0 = 1$ (blue squares), $\Omega_0 = 2$ (magenta rhomboids), and $\Omega_0 = 3$ (olive triangles): (a) effective mass m^* , (b) ground state energy E_{GS} [horizontal red double line shows a break in the y -axis from -5 to -8 separating two different energy scales], (c) quasiparticle weight Z_0 , and (d) average phonon number $\langle N_{ph} \rangle$ in the phonon cloud. (e) Ω_0 -dependence of the critical values λ_{cr} determined from the condition $d^2 Z_0 / d\lambda^2 = 0$ (rhomboids), $\text{Min}[d^2 E_{GS} / d\lambda^2]$ (squares), and $d^2 \langle N_{ph} \rangle / d\lambda^2 = 0$ (circles). Dashed line shows extrapolation to zero Debye frequency $\Omega_0 \rightarrow 0$. (f-g) Distribution $Z(n)$ of the number n of phonons in the GS for different λ (in legend) for (f) $\Omega_0 = 0.5$ and (g) $\Omega_0 = 2$.

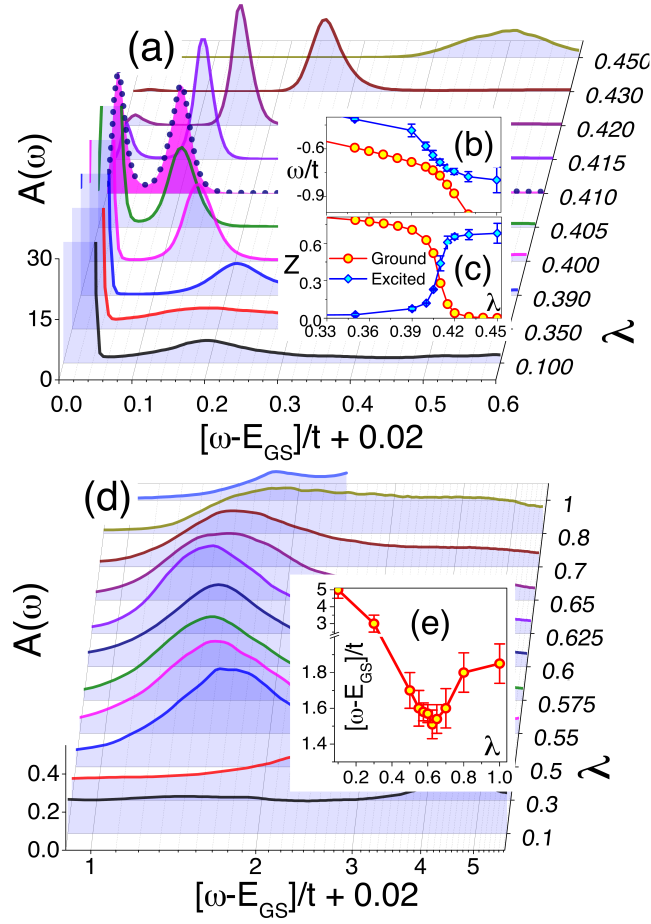


FIGURE 5.2: (a-c) $\Omega_0 = 0.5$: (a) Spectral functions $A(\omega)/\kappa$ [κ with increasing λ is 0.006, 0.02, 0.08, 0.12, 0.23, 0.44, 0.61, 0.65, 0.67, 0.68], (b) energy, and (c) weight of the GS (red circles) and FES (blue squares) peaks. The spectrum at $\lambda_{\text{cr}} \approx \lambda = 0.41$ is highlighted by a dotted line. (d-e) $\Omega_0 = 2$: (d) Incoherent part of spectral functions $A(\omega)/\kappa$ [κ with increasing λ is 0.04, 0.21, 0.45, 0.6, 0.75, 0.8, 0.8, 0.9, 0.95, 0.65, 0.2] and (e) energy of the excited state peaks counted from E_{GS} .

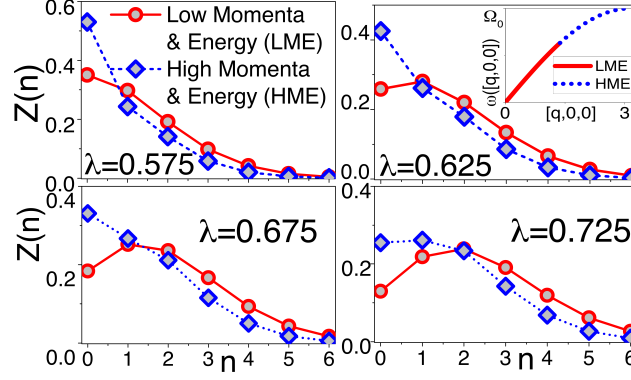


FIGURE 5.3: Distribution of the number n of phonons in the ground state for $\Omega_0 = 2$. Phonons are grouped into LME/HME (circles/rhomboids). Inset in the upper right corner shows the division into LME and HME.

On the other hand, it seems surprising that we can see the avoided crossing hybridization behavior for $\Omega_0 = 2$ [Figs. 5.2(d) and 5.2(e)], since there is no corresponding two-peak structure in the phonon distribution function $Z(n)$ [see Fig. 5.1(g)].

However, the unique feature of the acoustic lattice polaron is the presence of two distinctive groups of phonons whose properties are significantly different. Considering the dispersion in Eq. (5.5) and the interaction vertex in Eq. (5.6), one can distinguish between low momenta and energy (LME) phonons close to the Γ point and high momenta and energy (HME) phonons near the BZ boundary. We tentatively divide the phonons into LME/HME by using a sphere with radius $q_{f=1/2} = (3\pi^2)^{1/3}$, where f is the fraction of the volume of the BZ [see inset in Fig. 5.3]. Phonons with momenta inside the sphere belong to LME otherwise to HME. Figure 5.3 shows their different behavior for $\Omega_0 = 2$. The LME phonon cloud transfers from WCR to SCR at $\lambda \approx 0.6$, while the HME cloud makes the crossover at a considerably stronger coupling $\lambda \approx 0.725$. Depending on λ , it is thus possible to observe three qualitatively different situations in the GS: (i) LME and HME are both in the WCR, (ii) LME is in the SCR while HME is still in the WCR and (iii) LME and HME are both in the SCR. It is important to note that the number of possible GS regimes is the same as for the self-trapping phenomenon observed for optical polarons. Moreover, the situations in (i) and (iii) simply correspond to the standard WCR and SCR. However, regime (ii) is specific to the acoustic lattice polaron. It shows an additional fine structure in the LME/HME phonon clouds which is not present in the total phonon distribution $Z(n)$ [see Fig. 1(g)]. We observed no qualitative difference between LME and HME phonons for different fractions f because LME enters the SCR at smaller values of λ both for $f = 1/4$

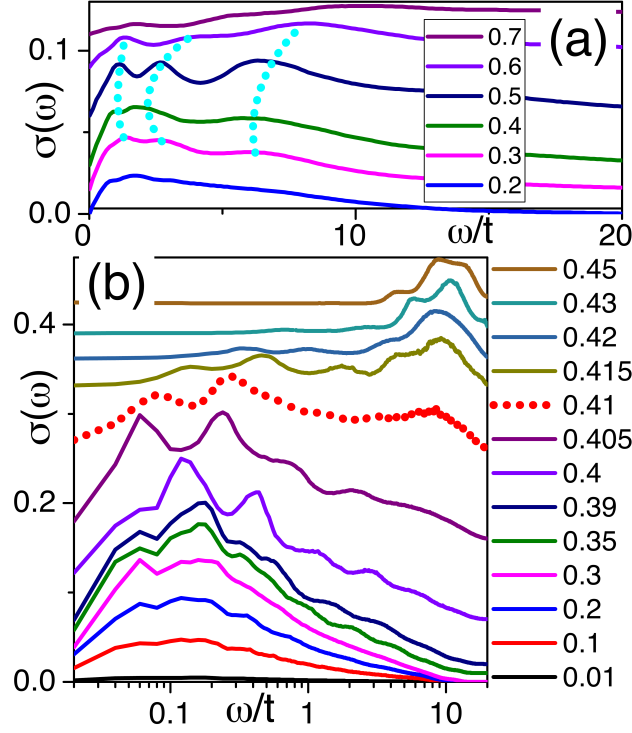


FIGURE 5.4: Optical conductivity $\sigma(\omega) + \chi$ for different λ given in the legend. χ is an artificially added onset to discern the curves for different values of λ : (a) $\Omega_0 = 2$ [χ with increasing λ is 0, 0.015, 0.03, 0.06, 0.09, 0.11] and (b) $\Omega_0 = 0.5$ [χ with increasing λ is 0, 0, 0, 0, 0.01, 0.02, 0.07, 0.16, 0.26, 0.33, 0.36, 0.39, 0.42]. Dotted blue lines in (a) follow peaks to guide the eye. The spectrum in (b) at $\lambda_{\text{cr}} \approx \lambda = 0.41$ is highlighted by the dotted red line.

and $f = 3/4$ (Fig. S1 and Fig. S2 in Supplementary material 5.7). Besides, the LME cloud transfers for $\lambda = 0.625$ from WCR to SCR in the range $f \in [1/4, 3/4]$, whereas HME always stays in the WCR (Fig. S3 Supplementary material 5.7). The configuration (iv) when LME is in the WCR and HME is in the SCR, is not seen in the GS but might be realized in some excited states. Furthermore, the very nature of acoustic phonons implies that there is always a group of soft phonons present, namely LME, which are responsible for the manifestations of the self-trapping phenomenon even for large Debye frequencies Ω_0 , see Figs. 5.2(d) and 5.2(e). For $\Omega_0 = 0.5$, both LME and HME show a two-peak structure while the number of phonons n at maximal $Z(n)$ is, indeed, larger for LME (Fig. S4 in Supplementary material 5.7).

The anomalously rich structure of the phonon cloud leads to the existence of multiple competing states. For example, a third competing state is clearly seen in the spectral function $A(\omega)$ for $\Omega_0 = 0.5$ (see Fig. S5 in Supplementary material 5.7). To reveal more details on the excited spectrum, one can look at the zero temperature optical conductivity (OC) $\sigma(\omega)$, since the symmetry selection rules

for $A(\omega)$ and $\sigma(\omega)$ are different [55, 112]. We are aware of only one pioneering variational study which investigated the optical response of the acoustic continuum polaron [179]. Figure 5.4 presents approximation free results for $\sigma(\omega)$ for our lattice model. Numerous excited states, which were never observed in the OC of optical polarons, can be identified for $\Omega_0 = 2$ (Fig. 5.4(a)) and $\Omega_0 = 0.5$ (Fig. 5.4(b)). This is a reflection of the unique composite phonon cloud of the acoustic polaron containing a combination of differently behaving LME and HME phonons.

5.5 Conclusions

In conclusion, we have shown that the lattice polaron interacting with an acoustic phonon branch via the deformation potential is an object whose complexity is going far beyond the previously studied optical and acoustic continuum polarons. Its most interesting feature is the existence of two groups of phonons which can interact with the quasiparticle in different ways. These two phonon clouds are responsible for the rich structure in the optical response showing multiple excited states and for the persistent self-trapping phenomenon even at large values of the Debye frequency. Furthermore, the sharpness of the crossover between weak and strong coupling has a different dependence on the Debye/cut-off frequency in the acoustic continuum polaron compared to our lattice model. This shows that these two models are not simply two limiting cases of each other but that they describe very different objects. Our results constitute the first comprehensive account of the fundamental properties of an acoustic polaron. They will be useful in detecting characteristic features of electron-acoustic phonon coupling in experiments and can further guide the exploration of polaron physics in real materials.

5.6 Acknowledgements

We are grateful to O. Barišić and S. N. Klimin for fruitful discussions. This work was supported by JST CREST Grant Number JPMJCR1874, Japan and by the joint FWO-FWF Grant No. I 2460-N36 and Grant No. I 4506. The computational results presented have been achieved in part using the Vienna Scientific Cluster (VSC).

5.7 Supplemental Material

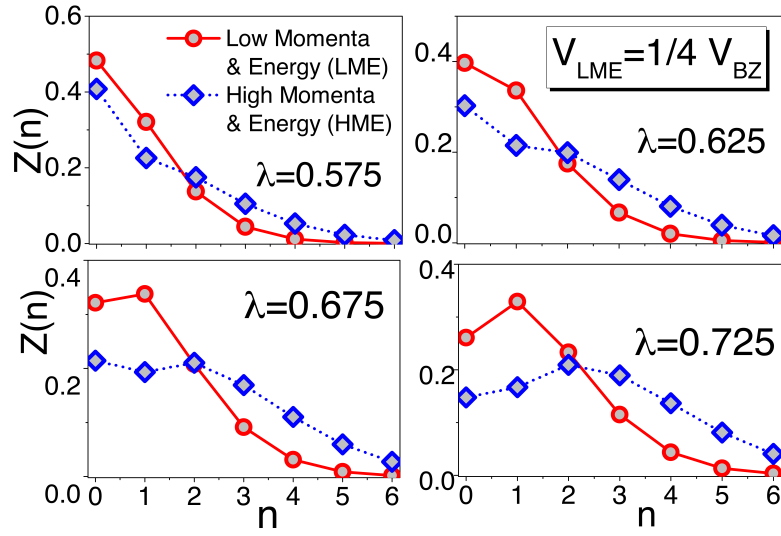


FIGURE 5.5: Distribution of the number n of phonons in the ground state for $\Omega_0 = 2$. Phonons are grouped into LME/HME (circles/rhomboids) with the threshold $q_{1/4}$.

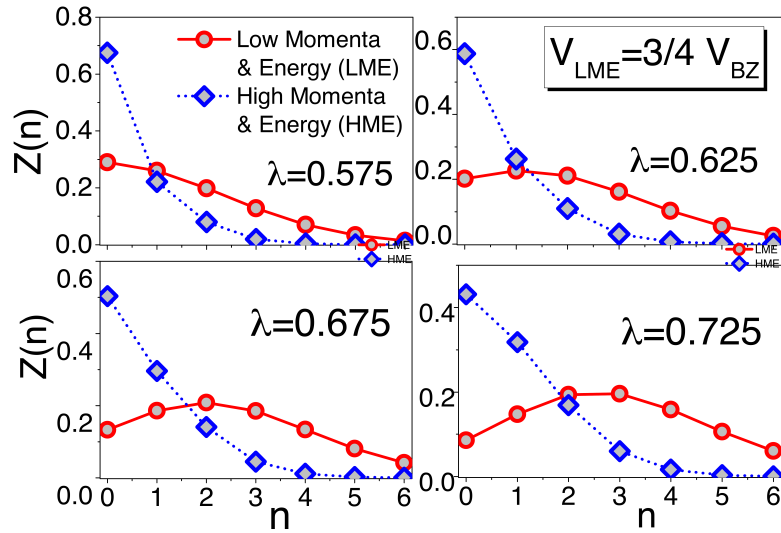


FIGURE 5.6: Distribution of the number n of phonons in the ground state for $\Omega_0 = 2$. Phonons are grouped into LME/HME (circles/rhomboids) with the threshold $q_{3/4}$.

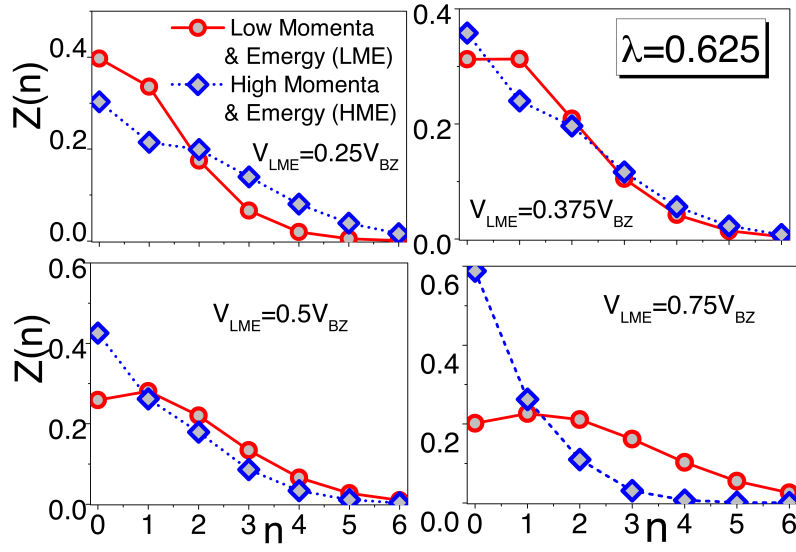


FIGURE 5.7: Distribution of the number n of phonons in the ground state for $\Omega_0 = 2$ and coupling constant is $\lambda = 0.625$. Phonons are grouped into LME/HME (circles/rhomboids) with different thresholds $q_{0.25}$, $q_{0.375}$, $q_{0.5}$, and $q_{0.75}$.

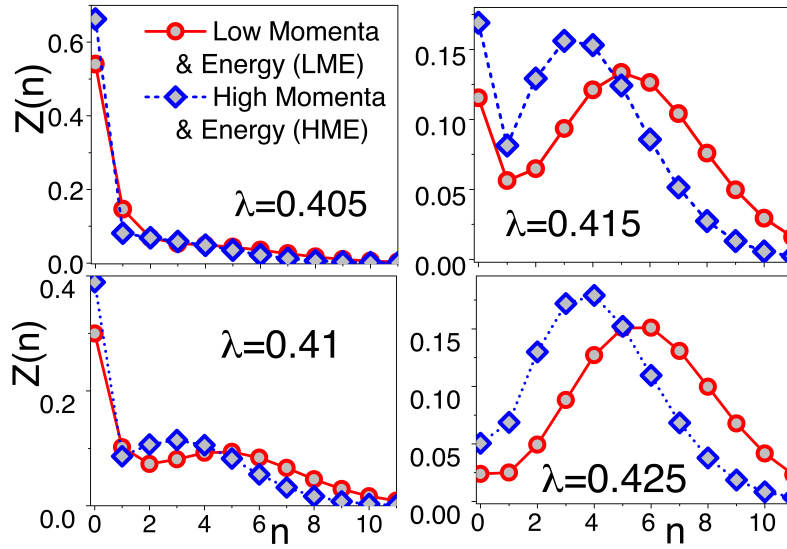


FIGURE 5.8: Distribution of the number n of phonons in the ground state for $\Omega_0 = 0.5$. Phonons are grouped into LME/HME (circles/rhomboids) with the threshold $q_{1/4}$.

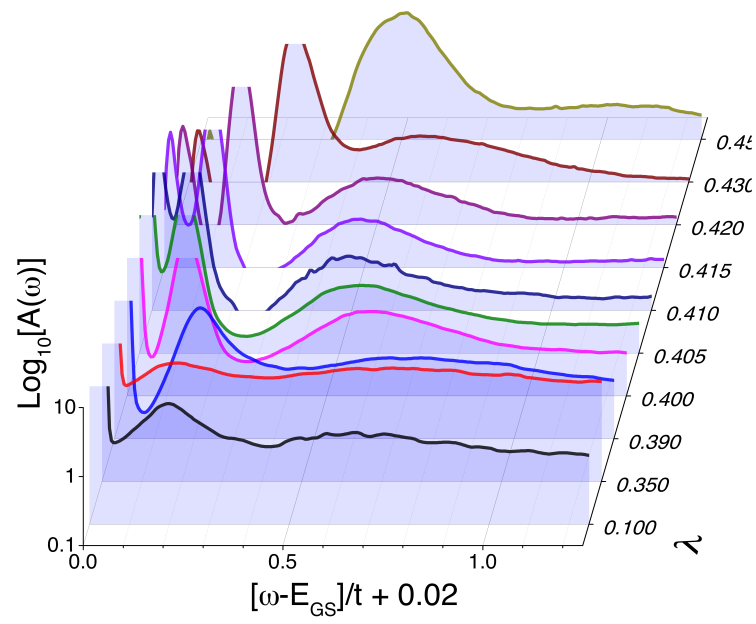


FIGURE 5.9: Spectral functions $A(\omega)/\kappa$ for $\Omega_0 = 0.5$ and different coupling strengths λ . κ with increasing λ is 0.006, 0.02, 0.08, 0.12, 0.23, 0.44, 0.61, 0.65, 0.67, 0.68.

Chapter 6

Quadratic electron-phonon interaction

This chapter includes a verbatim copy from the following published article:

S. Ragni, [T. Hahn](#), Z. Zhang, N. Prokof'ev, A. Kuklov, S. Klimin, M. Houtput, B. Svistunov, J. Tempere, N. Nagaosa, C. Franchini, A. S. Mishchenko, *Polaron with quadratic electron-phonon interaction*, [Physical Review B 107 \(12\), L121109 \(2023\)](#).

Preamble: The manuscript extends the DiagMC + SOCC approach described in Chapters [2](#) and [3](#) to nonlinear electron-phonon coupling and applies it to a Holstein-like polaron model with purely quadratic interactions to obtain the following polaron properties (as functions of the coupling strength g_2 and the adiabatic ratio Ω/W):

- Ground state energy E , effective mass m^* , quasiparticle weight Z , average number of phonons $\langle N_{\text{ph}} \rangle$, and phonon distribution function Z_n .
- Spectral function $A(\omega)$ and first excited state energy.

The updates and estimators used in the DiagMC algorithm have been developed in close collaboration with the first author of the publication. Implementation details can be found in Sec. [6.8.3](#) and in Stefano Ragni's PhD thesis [[115](#)]. The correctness of the algorithm has been verified by comparing with another numerically exact method, the x -representation approach, and with analytically known atomic limit results.

Contribution: As a co-author of the paper, I collaborated with the first author in developing the theory, supervised the development of the DiagMC code, and contributed to the writing of the manuscript.

6.1 Abstract

We present the first numerically exact study of a polaron with quadratic coupling to the oscillator displacement, or X^2 -polaron, using two alternative methodological developments. Our results cover both anti-adiabatic and adiabatic regimes and the entire range of electron-phonon coupling g_2 , from the system's stability threshold at attractive $g_2 = -1$ to arbitrary strong repulsion at $g_2 \gg 1$. Key properties of X^2 -polarons prove dramatically different from their linear counterparts. They (i) are insensitive even to large quadratic coupling except in the anti-adiabatic limit near the threshold of instability at attraction; (ii) depend only on the adiabatic ratio but are insensitive to the electron dispersion and dimension of space; (iii) feature weak lattice deformations even at the instability point. Our results are of direct relevance to properties of electrons at low densities in polar materials, including recent proposals for their superconducting states.

6.2 Introduction

The first results on polarons with quadratic coupling to phonons were reported in Refs. [180, 181], which explored properties of large-radius solitons in the adiabatic limit at strong coupling. Indications that nonlinear coupling to atomic displacements is important were found in several materials such as doped manganites [182], halide perovskites [183], and quantum paraelectrics [184–186]. Most notable is the unusual T^2 dependence of resistivity at high temperature, which was explained by considering electron-phonon interactions (EPI) with quadratic dependence on the phonon coordinates [184, 187]. The soft vibrational modes in these materials are transverse optical (TO) phonons for which the linear EPI is suppressed in the long-wave limit. However, local electron density changes the potential acting on nearby atoms and this change may increase or decrease the local spring constants. Early suggestions that bi-phonon exchange could be an important pairing mechanism at low doping [188] were recently revisited by quantifying and employing them for explaining the superconducting properties of SrTiO_3 [189–191]. While the treatment of the problem was perturbative, the dimensionless coupling constant was estimated to be of order unity, raising the question of consistency.

In the low-density limit—when the polaron physics is most relevant [107]—the key assumption on which the Migdal-Eliashberg theory is based (irrelevance of vertex corrections at strong coupling), namely $E_F \gg \Omega$, where E_F is the Fermi energy and Ω is the characteristic phonon frequency, fails. Thus, any quantitative study of strong EPI effects in this limit should start from precise calculations of

basic polaron properties such as its energy, E , effective mass, m^* , and the quasi-particle residue, Z . We are aware of only few theoretical attempts to account for quadratic EPI beyond perturbation theory. The original work [180, 181] was based on a variational approach for large-radius soliton-type solutions. A nonperturbative momentum average approximation [144] was used to study the interplay between linear (Holstein model [36]) and non-linear EPI at zero temperature in Refs. [192, 193]. Effects of non-linear EPI on the formation of charge density waves, superconductivity, and quasi-particle properties were investigated in a series of papers [194–196]. These determinant Monte Carlo [197] studies considered finite clusters (up to $N = 8 \times 8$ sites) in two dimensions at high electron density and finite temperature. More recently, the interplay between linear and quadratic EPI in the Fröhlich model of continuous space polarons was studied at zero temperature in Ref. [198] using variational Feynman’s path integral method [121].

All studies find that quadratic interaction with positive/negative coupling constant decreases/increases the effective strength of the linear EPI. However, none of the previous work was able to treat effects of strong quadratic coupling in the thermodynamic limit without approximations, or was investigating polaron properties for purely quadratic interaction. Meanwhile, as was mentioned above, there exist important cases when coupling to soft transverse phonons has no linear terms in the long-wave limit, e.g. quantum paraelectrics [184] and optically pumped systems [199, 200].

In this Letter, we employ two complementary numerically exact methods to solve the polaron model with quadratic coupling to atomic displacements, or X^2 -polaron, at zero temperature. The first one is based on Feynman diagrams and is best suited for studying dispersive phonons in the regimes of weak and intermediate coupling. The second method—performing best at strong coupling and becoming particularly simple in the dispersionless regime—works with the path-integral representation for both the electron and atomic displacements. The two methods are new methodological advances that go well beyond previous developments. We explore both adiabatic and non-adiabatic limits and find that X^2 -polarons remain well-defined all the way to the instability threshold and possess the remarkable ability (especially in the adiabatic case) to resist renormalization even in the extreme strong coupling limit.

6.3 Model

The key difference between our Hamiltonian and the well-studied Holstein model [36] is the quadratic, instead of linear, coupling to the local oscillator coordinates,

$X_i = [b_i^\dagger + b_i]/\sqrt{2M\Omega} \equiv x_i/\sqrt{2M\Omega}$, where M and Ω are the oscillator mass and frequency, respectively (we use standard notation for on-site creation/annihilation operators for harmonic modes and electrons):

$$H = -t \sum_{\langle ij \rangle} a_j^\dagger a_i + \Omega \sum_i b_i^\dagger b_i + \frac{\Omega}{4} g_2 \sum_i n_i [b_i^\dagger + b_i]^2. \quad (6.1)$$

Here $n_i = a_i^\dagger a_i$ is the electron occupation number. The first two terms describe the electron hopping between nearest neighbor sites on the simple cubic lattice (in what follows we take t as the unit of energy) and the local vibration modes, respectively. We count oscillator energies from their ground states, and use the dimensionless constant g_2 to parameterize the coupling. By writing the local potential energy for $n_i = 1$ as $M\Omega^2[1 + g_2]X_i^2/2$, we observe that (i) the model becomes unstable at $g_2 \leq -1$, implying that the radius of convergence for a perturbative treatment in powers of g_2 is unity, (ii) the oscillator frequency is renormalized to

$$\tilde{\Omega} = r\Omega, \quad r = \sqrt{1 + g_2}, \quad (6.2)$$

and (iii) its ground state energy shifts to $\Omega(r - 1)/2$.

6.4 Momentum-space representation

See also Supplemental material in Sec. 6.8 and references [50, 201] therein. The first scheme is based on the Diagrammatic Monte Carlo (DiagMC) technique introduced in Ref. [49] and further developed in Ref. [50]. The imaginary-time Green's function, $G(\mathbf{k}, \tau)$, for momentum state $\mathbf{k}$ is sampled stochastically from the series expansion in powers of g_2 expressed as Feynman diagrams in terms of bare electron and phonon propagators. This method is convergent for $|g_2| < 1$ where all results are identical with those of the second approach within the statistical error bars. The difference between linear and quadratic coupling is a more complex set of diagram topologies consisting of a set of n -phonon loops because now each interaction vertex involves two phonons (instead of one) being emitted or absorbed (see Eq. (6.1)).

Figure 6.1 shows typical low-order diagrams. The simplest self-energy diagram is given by the 1-loop; its series, see Fig. 6.2, is absorbed into the “bare” electronic propagator, $G_0 \rightarrow \tilde{G}_0$, by shifting the tight-binding dispersion $\epsilon_{\mathbf{k}} \rightarrow \tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + g_2\Omega/4$:

$$\tilde{G}_0(\mathbf{k}, \tau) = e^{-\tilde{\epsilon}_{\mathbf{k}}\tau}, \quad D_0(\mathbf{q}, \tau) = e^{-\Omega\tau}. \quad (6.3)$$

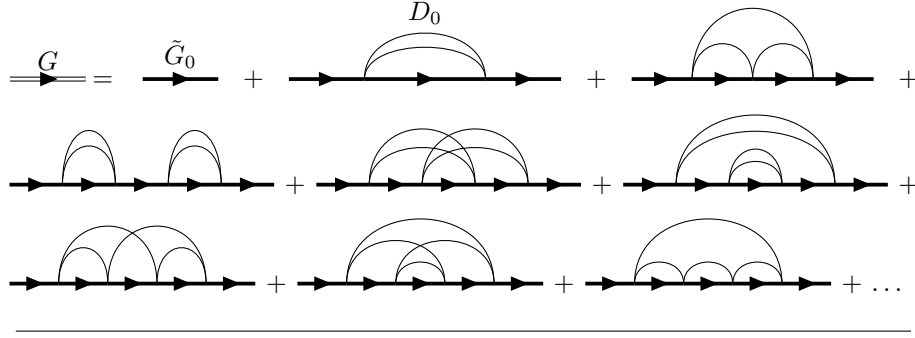


FIGURE 6.1: Momentum-space diagrams for the Green's function up to fourth order in the quadratic coupling.

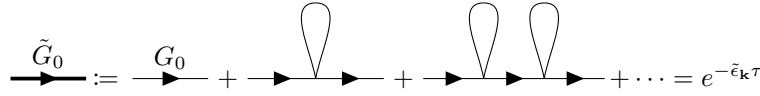


FIGURE 6.2: The geometric series of the 1-loop diagrams defines the “Hartree” renormalized electron propagator.

The remaining high-order loops display a wide variety of topologies that increase dramatically with the order of the diagram. In addition, there exist multiple Wick pairings that are topologically equivalent and result in the same contribution, meaning that each diagram comes with the combinatorial factor $2^{N_V - N_2}$, where N_V is the total number of vertices and N_2 is the number of 2-phonon loops, i.e. loops consisting of two phonon propagators. The sign of the diagram is given by $(-g_2)^{N_V}$, meaning that the expansion is sign-positive for $g_2 < 0$.

An ergodic sampling scheme includes the following updates:

Add/remove 2-loop: Seed time, τ_1 and τ_2 , and momentum, $\mathbf{q}_1$ and $\mathbf{q}_2$, variables for new vertices to be added to the diagram and balance this proposal by suggesting to remove any of the existing 2-loops.

Add/remove 3-loop: This update is a straightforward generalization of the previous one, but for 3-loops. It is required for the generation of odd-order diagrams.

Relink: Pick any two phonon propagators across the whole diagram at random such that they do not share vertices, i.e. they start and end on four different vertices. Propose a new diagram topology by connecting the four vertices with the two phonon propagators randomly.

Additional updates, such as changing time and/or momentum variables of the diagram, are introduced to improve the autocorrelation time.

Following Ref. [50], the simulation is extended to the N -phonon Green's function, which allows one to collect information about the structure of the phonon cloud. We employ standard procedures to extract the ground state energy, E ,

quasiparticle weight, Z , average number of phonons, $\langle N_{\text{ph}} \rangle$, and effective mass, m^* , of the polaron.

6.5 X-representation approach

As discussed in Ref. [66], see also the Supplemental Material in Sec. 6.8, any non-linear coupling to local vibration modes can be dealt with exactly and efficiently by specifying dimensionless atomic coordinates x_i for all sites connected by the electron hopping transitions. The only new ingredient required for adapting the scheme of Ref. [66] to the model in Eq. (6.1) is the imaginary-time oscillator propagator in the presence of the electron

$$\begin{aligned}\tilde{U}(y, x, \tau) &= e^{(1/2)\Omega\tau - \tilde{Q}(y, x, \tau)} \sqrt{\frac{r}{4\pi \sinh(\tilde{\Omega}\tau)}} , \\ \tilde{Q}(y, x, \tau) &= \frac{r[\cosh(\tilde{\Omega}\tau)(x^2 + y^2) - 2xy]}{4 \sinh(\tilde{\Omega}\tau)} .\end{aligned}\quad (6.4)$$

For empty sites, the “bare” propagator $U(y, x, \tau)$ has the same functional form as $\tilde{U}(y, x, \tau)$ but with $r = 1$ and $\tilde{\Omega} = \Omega$. Thus, for any electron’s lattice path and any set of atomic displacements on sites connected by hopping transitions, one has an exact sign-positive expression for the system’s evolution operator subject to stochastic sampling without a bias.

In the so-called atomic limit (AL), $t = 0$, the solution for the Green’s function immediately follows from the Gaussian integral $G_A(\tau) = \int dx dy U(x) \tilde{U}(x, y, \tau) U(y)$ leading to

$$G_A(\tau) = Z_A e^{-E_A \tau} \left[1 - \left(\frac{1-r}{1+r} \right)^2 e^{-2\tilde{\Omega}\tau} \right]^{-1/2}, \quad (6.5)$$

where

$$Z_A = \frac{2\sqrt{r}}{1+r}, \quad E_A = \frac{\Omega}{2}(r-1). \quad (6.6)$$

The spectral density, defined by $G_A(\tau) = \int_0^\infty d\omega A_A(\omega) e^{-\omega\tau}$, is readily obtained by Taylor expanding $G_A(\tau)$ in powers of $e^{-2\tilde{\Omega}\tau}$:

$$A_A(\omega) = \sum_{k=0}^{\infty} Z_{2k} \delta(\omega - E_{2k}). \quad (6.7)$$

It is a set of δ -functions at frequencies $E_{2k} = E_A + 2k\tilde{\Omega}$ with Z_{2k} -factors equal to

$$Z_{2k} = Z_A \frac{(2k-1)!!}{(2k)!!} \left[\frac{1-r}{1+r} \right]^{2k}. \quad (6.8)$$

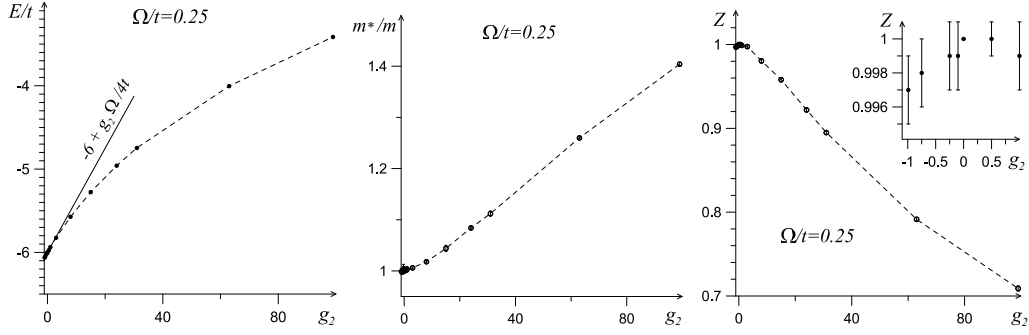


FIGURE 6.3: Polaron properties (energy, effective mass, and Z -factor) in the adiabatic regime $\Omega/W = 1/48$ (bandwidth $W = 12t$ in 3D) as functions of EPI coupling.

Finally, the atomic limit admits an exact solution for the average number of phonons in the polaron cloud defined as in Ref. [50]

$$\langle N_{\text{ph}} \rangle = \sum_{k=0}^{\infty} (2k) Z_{2k} = \frac{(1-r)^2}{4r}. \quad (6.9)$$

If both $\tilde{\Omega}$ and Ω are much larger than t (meaning that to the leading approximation the oscillators always remain in the ground state as the electron moves), then the finite- t effects can be fully characterized by the overlap integral squared between the bare and renormalized ground states equal to Z_A :

$$E = -6Z_A t + E_A, \quad m^*/m = Z_A^{-1}. \quad (6.10)$$

6.6 Results

In sharp contrast to conventional polarons, properties of X^2 -polarons strongly depend on the sign of g_2 , see Figs. 6.3 and 6.4. The effective mass (quasiparticle weight) goes through a minimum (maximum) at $g_2 = 0$, while the energy is an increasing function of g_2 . The asymmetry is especially notable in the anti-adiabatic case $\Omega/W = 4$, see Fig. 6.4, and is directly linked to the fact that at $g_2 \rightarrow -1$ the local phonon frequency undergoes a dramatic change and ultimately softens to zero. Correspondingly, as long as the condition $\tilde{\Omega} > W$ is satisfied, the atomic-limit expressions featuring square-root singularities, see Eqs. (6.5)–(6.10), provide an accurate description of the polaron properties. However, on approach to the stability threshold, this condition ultimately gets violated and the singularity is removed because an electron moves away before the slow phonon mode has a chance

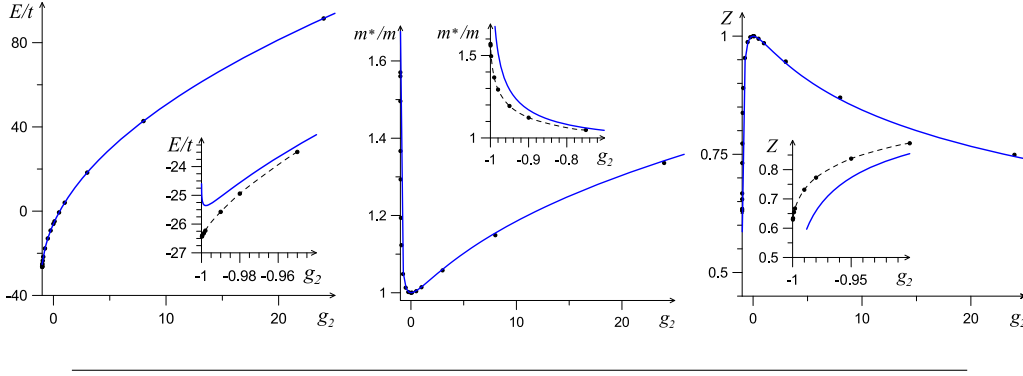


FIGURE 6.4: Polaron properties (energy, effective mass, and Z -factor) in the anti-adiabatic regime $\Omega/W = 4$ in 3D as functions of EPI coupling. Solid lines are the analytic predictions based on the atomic limit (6.6)–(6.10); dashed lines connecting data points are used to guide an eye.

to adjust to its interacting ground state. This explains the remarkable fact, that all polaron properties remain well defined and regular in the $g_2 \rightarrow -1$ limit for any finite value of t , see Figs. 6.4 and 6.5.

For positive g_2 , all properties change gradually even at $g_2 \gg 1$. Moreover, in the adiabatic limit $\Omega/W = 1/48$, see Fig. 6.3, both Z and m^*/m remain close to unity with sub percent accuracy for any $|g_2| \leq 1$. One way to interpret the data is to make a connection with the linear problem where the crossover from weak to strong coupling takes place when the dimensionless coupling λ , defined as the ratio between the coupling strength squared and the product of $W/2$ and Ω , is of the order of unity. Introducing a similar parameter for model (6.1) we get $\lambda = 2(g_2\Omega/4)^2/(W\Omega) = (g_2^2\Omega)/(8W)$. Its value for $|g_2| = 1$ is $\lambda = 1/384$ for the adiabatic case shown in Fig. 6.3 and $\lambda = 1/2$ for the anti-adiabatic case shown in Fig. 6.4.

Another stark difference between linear and quadratic couplings is found in the structure of the lattice distortion dragged along by polarons. It is quantified through probabilities Z_n of having n virtual phonons in the ground state [for AL it is given by Eq. (6.8)]. In the linear case, the peak in Z_n shifts from $n = 0$ at weak coupling to large finite values of n at strong coupling [50, 202]. In contrast, Z_n for X^2 -polarons is peaked at $n = 0$ and decreases exponentially at large n (Fig. 6.5b) for any value of negative g_2 , including the close vicinity of the instability point $(1+g_2) < 10^{-3}$ when the average phonon number of phonons $\langle N_{\text{ph}} \rangle$ is already large (Fig. 6.5a). Somewhat counter-intuitively, $Z_{n=0}$ for the moving particle ($t > 0$) is larger than for the localized particle in the AL ($t = 0$), whereas for large n the opposite is true, see inset in Fig. 6.5a. Only for large g_2 in the deep adiabatic limit $\Omega/t \ll 1$ it is possible that Z_n has a peak at finite n due to formation of the soliton state [180].

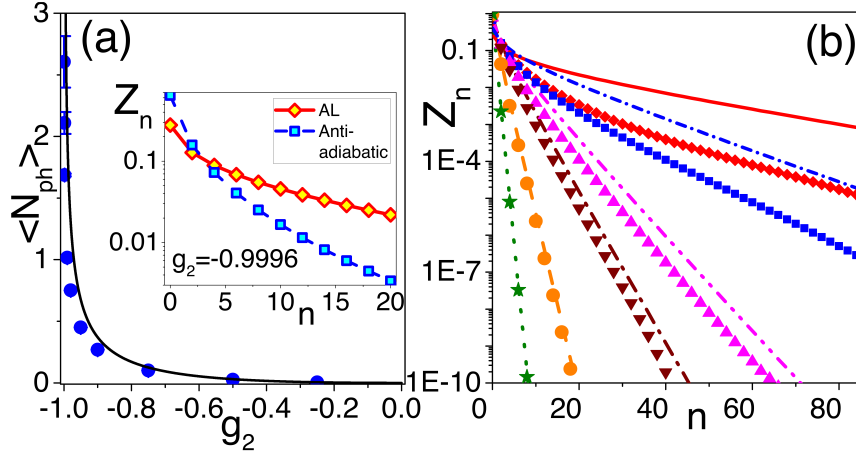


FIGURE 6.5: Phonon cloud in the anti-adiabatic limit in 3D at $\Omega/W = 4$. (a) Average number of phonons $\langle N_{\text{ph}} \rangle$ (blue circles) and the AL prediction (line), Eq. (6.9), for negative coupling constant. (b) Phonon distributions Z_n in the polaron cloud (symbols) and the AL prediction (lines, Eq. (6.8)), $g_2 =$: -0.25 (stars, dotted line), -0.75 (circles, dashed line), -0.95 (triangles down, dash-dot line), -0.98 (triangles up, dash-dot-dot line), -0.998 (squares, short-dash-dot line), and -0.9996 (diamonds, solid line). Inset in panel (a) shows the phonon distribution (squares) and Eq. (6.8) (diamonds) for $g_2 = -0.9996$ on a smaller scale.

We also find that properties of X^2 -polarons mostly depend on the particle bandwidth, and are rather insensitive to the form of the dispersion relation and even the dimension of space, e.g., E , Z , $\langle N_{\text{ph}} \rangle$, and m^* are practically indistinguishable between the 3D and 1D cases provided the bandwidth is the same (see Supplemental material).

To complete the picture, we performed analytic continuation of the Green's function spectral density, $A(\omega)$, in the anti-adiabatic limit by the Stochastic Optimization with Consistent Constraints method [50, 92]. In Figure 6.6b, we show the extracted positions of excited states and how they compare with the AL predictions (Fig. 6.6a). One can see in Fig. 6.6b that the onsets of high energy peaks are well described by energies E_{2k} in Eq. (6.7).

6.7 Conclusions

We find that properties of X^2 -polarons are dramatically different from those based on the intuition gained during a long history of Holstein polaron studies. In the adiabatic regime, X^2 -polarons are nearly indistinguishable from bare particles for any coupling with $|g_2| \sim 1$. In the anti-adiabatic regime, particle properties are renormalized more strongly (but saturate to finite values) when approaching the instability threshold at $g_2 = -1$, but remain small for positive g_2 except in the

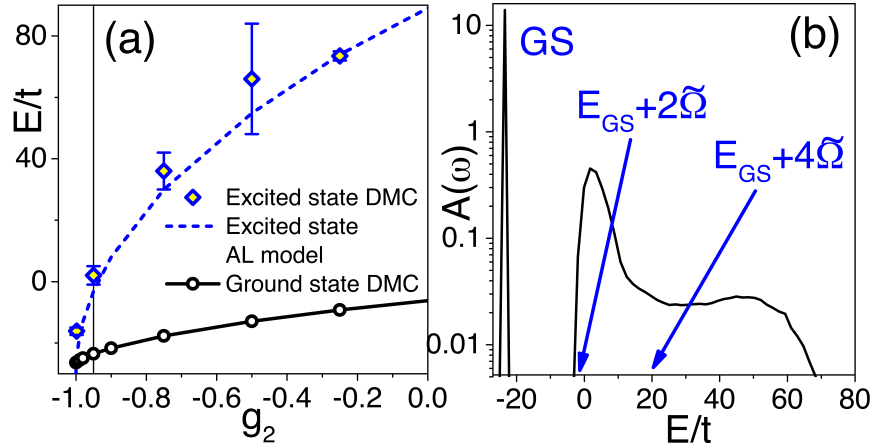


FIGURE 6.6: Anti-adiabatic limit in 3D at $\Omega/W = 4$. (a) Ground state energy (circles connected by the black line) and that of the first excited state (blue diamonds). Blue dashed line is the first excited state energy in the AL. Vertical line at $g_2 = -0.95$ corresponds to the coupling for which the spectral function $A(\omega)$ in panel (b) is shown. (b) Spectral function $A(\omega)$ at $g_2 = -0.95$ for which Eq. (6.2) predicts $\tilde{\Omega} \approx 10.7$. Arrows show energies of 2-phonon $2\tilde{\Omega}$ and 4-phonon $4\tilde{\Omega}$ thresholds above the ground state energy.

limit of large coupling. Perhaps the most unexpected result is that the lattice deformation around the X^2 -polaron remains weak even at the threshold. This outcome explains the success of recent work on superconductivity in SrTiO_3 [189–191] which treated electrons as bare particles.

We established that the adiabatic ratio Ω/W is the key parameter to pay attention to for this problem, while other microscopic details and even the system dimension are less relevant. This fact can be used for the development of approximate schemes, such as momentum average [144], dynamical mean field theory [203], or many body approach [106] in the low density limit, that can then be validated against our numerically exact results.

The soliton-type solutions [180] cannot form for model parameters simulated in this work. The minimal requirement is to have $m^*/m \gg 1$ at $\Omega \ll \tilde{\Omega} \leq t$, which is not satisfied even for the $(\Omega/t = 0.1, \tilde{\Omega} = 30\Omega)$ parameter set, for which we find $m^*/m \approx 3$. Future work should address the soliton problem under the assumption that the crystal is in close proximity to the quantum critical point when $\Omega \rightarrow 0$ and the electron contribution to the local vibrational energy is finite when $\tilde{\Omega} \rightarrow \text{const}$.

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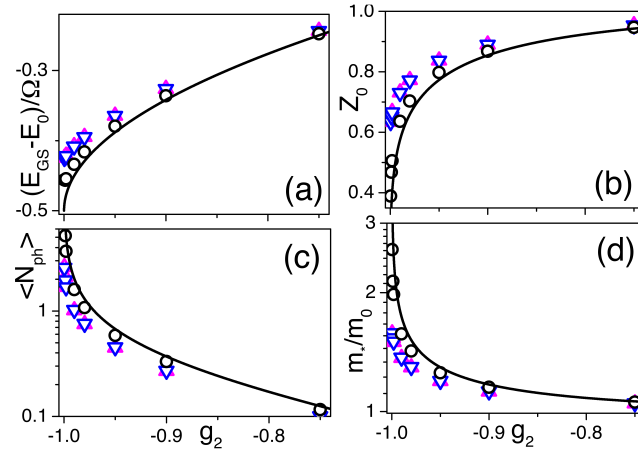


FIGURE 6.7: (a) Energy shifts, (b) Z_0 -factors, (c) average number of phonons $\langle N_{\text{ph}} \rangle$, and (d) effective masses m^*/m_0 for models 1 (triangles up), 2 (triangles down), and 3 (circles). Solid lines show the analytic results in the AL.

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6.8 Supplemental material

6.8.1 Sensitivity to the microscopic details of the electron spectrum

Figure 6.7 demonstrates that the renormalization of X^2 -polaron properties depends only on the electronic bandwidth and is rather insensitive to the details of the electron dispersion and dimension of space. We consider the anti-adiabatic regime for which all properties change most dramatically with coupling. Model 1 is the three dimensional simple cubic lattice with $\Omega/W = 4$ and Model 2 is the one dimensional chain with the same adiabatic ratio. Model 3 is the one dimensional chain with the bandwidth reduced by a factor of three, $\Omega/W = 12$. Since the three models have different bandwidths W we compare the ground state energy shifts $(E_{GS} - E_0)/\Omega \equiv (E_{GS} - W/2)/\Omega$ in units of Ω .

One can see that ground state energies, Z -factors, average number of phonons in the phonon cloud $\langle N_{\text{ph}} \rangle$, and effective masses in Models 1 and 2 are nearly impossible to distinguish whereas the results for the Model 3 are different and, as expected, closer to the AL predictions.

6.8.2 Implementation of the x -representation approach

Here we work in the representation of the eigenstates of local oscillator coordinates X_i (the so-called x -representation). A convenient “visual” starting point is the coordinate path-integral formulation for both the particle and the (local) oscillators. The particle path starts at $\tau = 0$ and ends at a certain finite τ . It is used to sample the ground-state imaginary-time polaron Green’s function

$$G(\tau, r) = \langle a_r(\tau) a_0^\dagger(0) \rangle. \quad (6.11)$$

The next step is a massive integration over the oscillator paths leaving behind only (i) the finite-time propagators in the coordinate representation, (ii) the oscillator ground-state wavefunction, and—only in the case of dispersive phonons—(iii) interaction vertices between (otherwise local) oscillator coordinates.

In the case of dispersionless phonons—like the one we deal with in the present work, a dramatic simplification comes with the observation that the paths for phonon modes on different sites are disconnected. Hence, we need to sample oscillators paths only for the sites reached by the particle’s worldline and need not be sampled for time periods when the particle occupation number remains constant.

Without loss of generality, one can count oscillator energies from their ground state and write

$$H_i^{(\text{ph})} = \Omega b_i^\dagger b_i. \quad (6.12)$$

Now one may assume that oscillator paths start at $\tau = -\infty$ and end at $\tau = +\infty$. This way the “boundary conditions” at $\pm\infty$ become irrelevant: an infinitely long oscillator path is τ -independent and equivalent to the ground-state projector, yielding, upon the integration, the value $U_0(x)$ of the oscillator ground-state wave function at the coordinate x corresponding to the fixed end of the infinite path:

$$U_0(x) = \frac{e^{-x^2/4}}{(2\pi)^{1/4}}. \quad (6.13)$$

Further integration converts the path of the i -th oscillator—interacting with the given particle path—into a string of x -propagators, $\Pi(x'', x', \tau'' - \tau')$, sandwiched between two functions U_0 (for clarity, we suppress the site subscript i):

$$U_0(x_1) \Pi(x_2, x_1, \tau_2 - \tau_1) \dots \Pi(x_n, x_{n-1}, \tau_n - \tau_{n-1}) U_0(x_n).$$

There are two types of x -propagators: the ones corresponding to the free oscillators,

$$U(x_2, x_1, \tau) = \langle x_2 | e^{-\tau H^{(\text{ph})}} | x_1 \rangle, \quad (6.14)$$

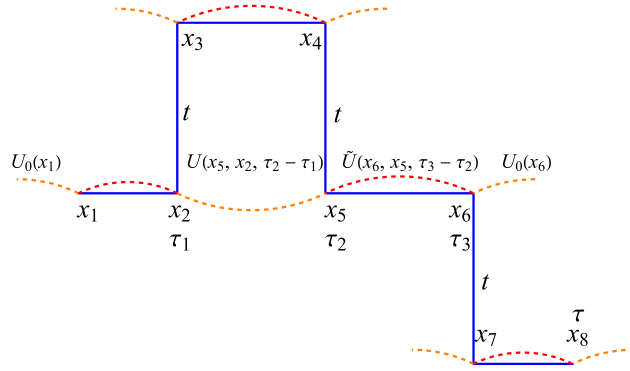


FIGURE 6.8: A typical diagram for the ground-state Green's function $G(\tau, r)$. Site subscripts are suppressed for clarity. The solid (blue) line represents particle's path, each hopping event of which contributes a factor of t . Dashed lines with free ends represent the functions U_0 . Dashed lines with both ends attached to the particle's path represent x -propagators, the choice between U or $\tilde{U}$ is dictated by the absence or presence of the solid line.

and the ones corresponding to the oscillators whose potential energy is changed by the presence of the particle,

$$\tilde{U}(x_2, x_1, \tau) = \langle x_2 | e^{-\tau \tilde{H}^{(\text{ph})}} | x_1 \rangle, \quad (6.15)$$

$$\tilde{H}^{(\text{ph})} = H^{(\text{ph})} + g_2 \frac{M\Omega^2}{2} X^2. \quad (6.16)$$

This way we arrive at the configuration space illustrated in Fig. 6.8. To compensate for an exponential decrease of $G(\tau, r)$ with τ , we use a standard trick of introducing an auxiliary chemical potential μ_τ .

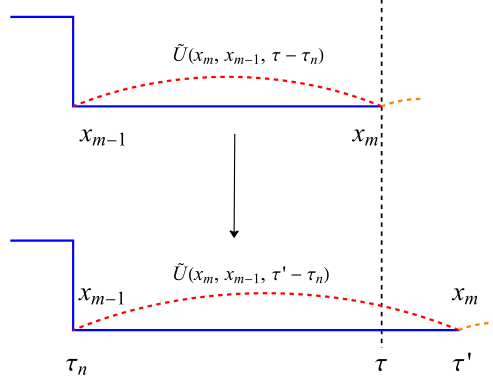
Our MC scheme includes three updates:

Change the τ value. A new value, τ' , is generated within the interval $[\tau_n, \tau_{\max}]$ as shown in Fig. 6.9, where τ_n is the time of the last hopping transition and $\tau_{\max}$ is a preset maximum value of τ . The acceptance ratio for this update is given by

$$R = \frac{P(\tau)}{P(\tau')} \frac{\tilde{U}(x_m, x_{m-1}, \tau' - \tau_n)}{\tilde{U}(x_m, x_{m-1}, \tau - \tau_n)} e^{-\mu_\tau(\tau' - \tau)}, \quad (6.17)$$

where $P(\tau')$ is the distribution function for generating τ' . We choose the exponential distribution $P(\tau') = \mu_p e^{-\mu_p(\tau' - \tau_n)}$ optimizing the value of μ_p to make sure that $R \sim 1$.

Change x -value. A new x -value x'_j is generated at a randomly chosen hopping kink. Fig. 6.10 shows two possible cases:

FIGURE 6.9: An illustrative diagram for the τ -update.

Case 1. Here the coordinate x_j is shared between propagators U_0 and $\tilde{U}$. The acceptance ratio is

$$R = \frac{P(x_j) U_0(x'_j) \tilde{U}(x'_j, x_k, \Delta\tau)}{P(x'_j) U_0(x_j) \tilde{U}(x_j, x_k, \Delta\tau)} \quad (6.18)$$

where $P(x'_j)$ is the probability distribution function for generating x'_j .

We use the Gaussian distribution

$$P(x'_j) = (2\pi\sigma^2)^{-1/2} \exp \left[- (x'_j - \mu)^2 / (2\sigma^2) \right], \quad (6.19)$$

$$\mu = \frac{r\sigma^2}{2} x_k \operatorname{csch}(\tilde{\Omega}\Delta\tau), \quad (6.20)$$

$$\sigma^2 = 2 \left[1 + r \coth(\tilde{\Omega}\Delta\tau) \right]^{-1}, \quad (6.21)$$

in which case $R = 1$, and the update is always accepted.

Case 2. Here the coordinate x_j is shared between propagators U and $\tilde{U}$. The acceptance ratio is

$$R = \frac{P(x_j) U(x_l, x'_j, \Delta\tau_2) \tilde{U}(x'_j, x_k, \Delta\tau_1)}{P(x'_j) U(x_l, x_j, \Delta\tau_2) \tilde{U}(x_j, x_k, \Delta\tau_1)}, \quad (6.22)$$

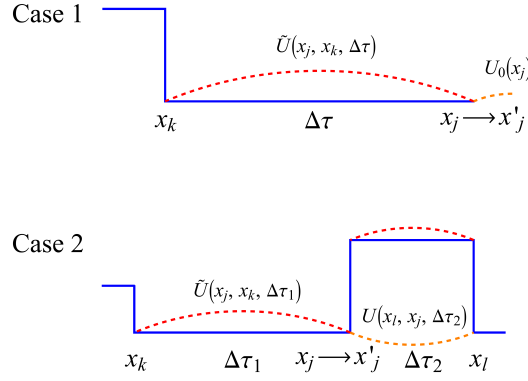
Similarly to Case 1, we achieve $R = 1$ by using the Gaussian distribution (6.19), now with

$$\mu = \frac{\sigma^2}{2} \left[x_l \operatorname{csch}(\Omega\Delta\tau_2) + r x_k \operatorname{csch}(\tilde{\Omega}\Delta\tau_1) \right], \quad (6.23)$$

$$\sigma^2 = 2 \left[\coth(\Omega\Delta\tau_2) + r \coth(\tilde{\Omega}\Delta\tau_1) \right]^{-1}. \quad (6.24)$$

Add/delete a hopping kink. In this update (illustrated in Fig. 6.11), we first choose to add a hopping kink with probability P_{add} or delete one with $1 - P_{\text{add}}$.

Add a kink. This update adds a hopping transition to any of the N_{nb} nearest-neighbor sites (for 3D cubic lattice, $N_{\text{nb}} = 6$) at the end of the diagram at time τ

FIGURE 6.10: An illustrative diagram for the x -update.

and extends the path's imaginary time variable to $\tau' > \tau$. This procedure generates two x -values, x' and x'' , for the new propagator $\tilde{U}(x'', x', \tau' - \tau)$. The acceptance ratio is

$$R_{\text{add}} = \frac{1 - P_{\text{add}}}{P_{\text{add}}} \frac{N_{\text{nb}}}{P(\tau') f(x', x'')} t e^{-\mu_\tau(\tau' - \tau)} \times \frac{\tilde{U}(x'', x', \tau' - \tau) U(x', x_k, \Delta\tau) U_0(x'')}{U_0(x_k)}, \quad (6.25)$$

where $P(\tau')$ and $f(x', x'')$ are the distribution functions for generating τ' , x' and x'' .

There is a special case: if the added hopping transition moves the particle to a site that it never visited before, one should replace $U(x', x_k, \Delta\tau)/U_0(x_k)$ with $U_0(x')$ in the acceptance ratio.

One possible choice for $P(\tau')$ and $f(x', x'')$ is $P(\tau') = \mu_p e^{-\mu_p(\tau' - \tau_n)}$ and $f(x', x'') = f(x')f(x'')$ with $f(x) = (2\pi\sigma^2)^{-1/2} \exp[-x^2/(2\sigma^2)]$, where $\sigma^2 = 2/(1+r)$.

Delete a kink. This update deletes the last hopping kink and changes the imaginary time from τ' to τ . The acceptance ratio is the reciprocal of the one for the add update:

$$R_{\text{delete}} = R_{\text{add}}^{-1} \quad (6.26)$$

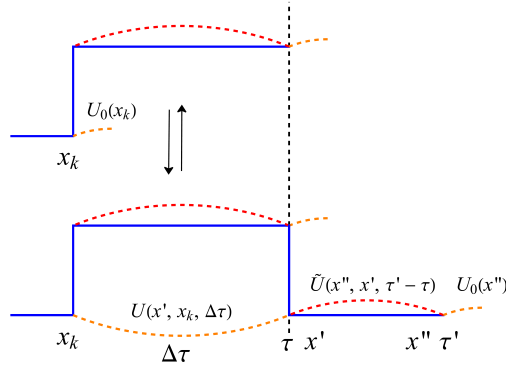


FIGURE 6.11: An illustrative diagram for adding and deleting hopping kinks.

6.8.3 Implementation of the momentum-space representation approach

By applying the Fourier transform to the electron and phonon creation/annihilation operators, the Hamiltonian is written in momentum space:

$$\begin{aligned}
 H = & \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \Omega \sum_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} \\
 & + \frac{\Omega}{4} \frac{g_2}{N} \sum_{\mathbf{k}, \mathbf{q}_1, \mathbf{q}_2} a_{\mathbf{k}+\mathbf{q}_1+\mathbf{q}_2}^{\dagger} a_{\mathbf{k}} (b_{-\mathbf{q}_1}^{\dagger} + b_{\mathbf{q}_1}) (b_{-\mathbf{q}_2}^{\dagger} + b_{\mathbf{q}_2}),
 \end{aligned} \tag{6.27}$$

where N is the number of unit cells and the lattice constant is set to $a = 1$. The electron dispersion is

$$\epsilon_{\mathbf{k}} = -2t \sum_{i=1}^3 \cos(k_i), \quad -\pi \leq k_i < \pi. \tag{6.28}$$

We work in the thermodynamic limit, so that momentum sums are turned into integrals:

$$\sum_{\mathbf{k}} \rightarrow \frac{V}{(2\pi)^3} \int_{\text{BZ}} d\mathbf{k}, \quad V = Na^3. \tag{6.29}$$

Feynman diagrams in the momentum-space representation are mathematically represented by a diagram weight denoted by the symbol $\mathcal{D}_{\text{diag}}$. The diagram weight is given by the product of all diagram elements, translated by substituting lines with the electron and phonons propagators presented in Eq. (3) of the main text. Each interaction vertex is translated to a factor of $(g_2\Omega/4)/(2\pi)^3$, with the factor $(2\pi)^3$ coming from the thermodynamic limit included for convenience.

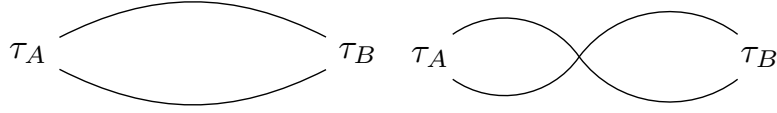


FIGURE 6.12: Diagram representation of the two possible Wick pairings for two vertices.

Combinatorial factors

In the S -matrix expansion, the time-ordered phonon bracket generates many possible Wick pairings. Some of them link the vertices in different ways, so that they are topologically different terms and we represent them as different diagrams. But there are also multiple pairings that are topologically equivalent, and evaluate to the same expression, which means that each diagram may appear more than once in the expansion: that is, it carries a combinatorial factor.

Let us take the simplest case of two vertices at τ_A and τ_B :

$$\langle |\mathcal{T} B_{\mathbf{q}_1}(\tau_A) B_{\mathbf{q}_2}(\tau_A) B_{\mathbf{q}_3}(\tau_B) B_{\mathbf{q}_4}(\tau_B)| \rangle, \quad (6.30)$$

where $B_{\mathbf{q}}(\tau) = b_{\mathbf{q}}(\tau) + b_{-\mathbf{q}}^\dagger(\tau)$. In this case there are two possible Wick pairings (neglecting equal time pairings, which would result in two 1-loops):

$$\langle |\mathcal{T} B_{\mathbf{q}_1}(\tau_A) B_{\mathbf{q}_2}(\tau_A) B_{\mathbf{q}_3}(\tau_B) B_{\mathbf{q}_4}(\tau_B)| \rangle, \quad (6.31)$$

$$\langle |\mathcal{T} B_{\mathbf{q}_1}(\tau_A) B_{\mathbf{q}_2}(\tau_A) B_{\mathbf{q}_3}(\tau_B) B_{\mathbf{q}_4}(\tau_B)| \rangle. \quad (6.32)$$

Both translate to the 2-loop diagram, which then gets a combinatorial factor of 2.

It is possible to represent these different Wick pairings graphically if we always distinguish between the two “sockets” in which we can plug the phonon line, for example above or below the horizontal (see Fig. 6.12).

In a general diagram consisting of $N_V = \sum_{n=2}^{\infty} n N_n$ quadratic vertices linked together into N_n n -phonon loops, the combinatorial factor associated with such diagram is

$$\boxed{2^{N_V - N_2}}. \quad (6.33)$$

This result can be shown as follows. Consider first the vertices that are linked in 2-loops. Each 2-loop has 2 possible Wick pairings: (a) and (b) from Fig. 6.12. If there are N_2 2-loops, the number of possibilities is 2^{N_2} .

Consider now a loop of n vertices, with $n > 2$. Start by connecting two of them: this can be done in 4 ways (Fig. 6.13a). Then, for each further vertex added to the

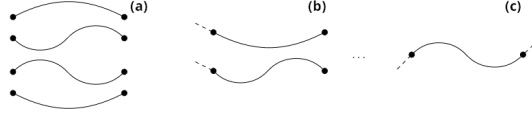


FIGURE 6.13: Graphical representation of the factors in Eq. (6.34).

loop, there are 2 possibilities (without or with a twist, Fig. 6.13b). The last one is constrained to just 1 possibility, because it must reattach to the beginning of the n -loop (Fig. 6.13c). Putting it all together:

$$4 \times 2^{n-2} \times 1 = 2^n. \quad (6.34)$$

Multiplying together the contributions from the N_2 2-loops and from higher order loops:

$$2^{N_2} \times (2^3)^{N_3} \times (2^4)^{N_4} \dots = 2^{N_V - N_2}. \quad (6.35)$$

The result (Eq. (6.33)) is in agreement with the rule based on diagram symmetries presented in [201].

Updates

Add/remove 2-loop. The addition of a 2-loop to the diagram is proposed. First, one of the $N_V + 1$ electron propagators is selected at random, and its initial and final times are labeled as τ_l and τ_r . The initial time τ_1 of the 2-loop is chosen uniformly between τ_l and τ_r , and the final time τ_2 is chosen from the exponential distribution $P(\tau_2) \propto e^{-2\Omega(\tau_2 - \tau_1)}$. The phonon momenta $\mathbf{q}_1$ and $\mathbf{q}_2$ are chosen inside the 1st BZ from the uniform distribution $U(\mathbf{q}_1, \mathbf{q}_2) = (2\pi)^{-6}$.

The update is balanced by proposing the removal of one of the $N_2 + 1$ 2-loops from the diagram, which is chosen uniformly. The acceptance ratio for the add update is

$$R_{\text{add-2}} = \frac{N_V + 1}{N_2 + 1} \frac{\tau_r - \tau_l}{P(\tau_2)} \frac{1}{U(\mathbf{q}_1, \mathbf{q}_2)} \frac{\mathcal{D}_{\text{add-2}}}{\mathcal{D}_{\text{cur}}} \times 2, \quad (6.36)$$

where $\mathcal{D}_{\text{cur}}$ and $\mathcal{D}_{\text{add-2}}$ are the weights of the current and proposed diagram, respectively. The factor of 2 arises from Eq. (6.33) because the proposed configuration contains one 2-loop more than the current configuration. The diagram weight ratio is given by

$$\frac{\mathcal{D}_{\text{add-2}}}{\mathcal{D}_{\text{cur}}} = \frac{(g_2 \Omega / 4)^2}{(2\pi)^6} \exp \{ -\Sigma_{\tau_1 \rightarrow \tau_2}(\mathbf{q}_1 + \mathbf{q}_2) \}, \quad (6.37)$$

$$\Sigma_{\tau_a \rightarrow \tau_b}(\mathbf{q}) = \sum_{i \in \tau_a \rightarrow \tau_b} [\tilde{\epsilon}_{\mathbf{k}_i - \mathbf{q}} - \tilde{\epsilon}_{\mathbf{k}_i} + 2\Omega] \Delta \tau_i, \quad (6.38)$$

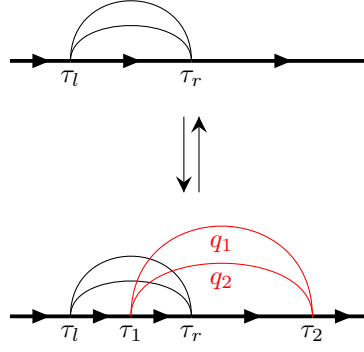


FIGURE 6.14: An illustrative diagram for adding and removing 2-phonon loops.

where the sum is over all electron propagators between time points τ_a and τ_b , $\mathbf{k}_i$ is the electron momentum of the i -th propagator and $\Delta\tau_i$ its length.

The acceptance ratio of the *Remove 2-loop* update is the reciprocal of the one for the *Add 2-loop* update.

Add/remove 3-loop. The addition of a 3-loop to the diagram is proposed. First, one of the $N_V + 1$ electron propagators is selected at random, and its initial and final times are labeled as τ_l and τ_r . The initial time τ_1 of the 3-loop is chosen uniformly between τ_l and τ_r , the middle time τ_m is chosen from the exponential distribution $P(\tau_m) \propto e^{-2\Omega(\tau_m - \tau_1)}$ and the final time τ_2 is chosen from the exponential distribution $P(\tau_2) \propto e^{-2\Omega(\tau_2 - \tau_m)}$. The phonon momenta $\mathbf{q}_1$, $\mathbf{q}_2$ and $\mathbf{q}_3$ are chosen inside the 1st BZ from the uniform distribution $U(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = (2\pi)^{-9}$.

The update is balanced by proposing the removal of one of the $N_3 + 1$ 3-loops from the diagram, which is chosen uniformly. The acceptance ratio for the add update is

$$R_{\text{add-3}} = \frac{N_V + 1}{N_3 + 1} \frac{\tau_r - \tau_l}{P(\tau_m)P(\tau_2)} \frac{1}{U(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)} \frac{\mathcal{D}_{\text{add-3}}}{\mathcal{D}_{\text{cur}}} \times 8, \quad (6.39)$$

where the factor of 8 arises from Eq. (6.33) because the proposed configuration contains one 3-loop more than the current configuration. The diagram weight ratio is given by

$$\frac{\mathcal{D}_{\text{add-3}}}{\mathcal{D}_{\text{cur}}} = \frac{(g_2\Omega/4)^3}{(2\pi)^9} \exp\{-(\Sigma_{12} + \Sigma_{13})\}, \quad (6.40)$$

$$\Sigma_{12} = \Sigma_{\tau_l \rightarrow \tau_m}(\mathbf{q}_1 + \mathbf{q}_2), \quad \Sigma_{13} = \Sigma_{\tau_m \rightarrow \tau_2}(\mathbf{q}_1 + \mathbf{q}_3), \quad (6.41)$$

with $\Sigma_{\tau_a \rightarrow \tau_b}(\mathbf{q})$ defined in Eq. (6.38).

The acceptance ratio of the *Remove 3-loop* update is the reciprocal of the one for the *Add 3-loop* update.

Relink. Randomly pick two phonon propagators across the whole diagram. If the two propagators have any vertex in common, the update is rejected, so that 4

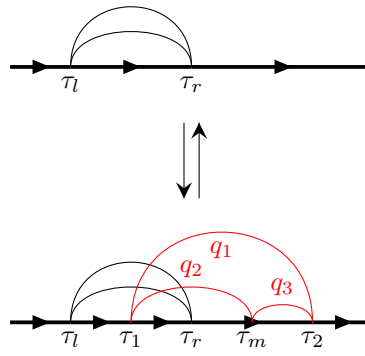


FIGURE 6.15: An illustrative diagram for adding and removing 3-phonon loops.

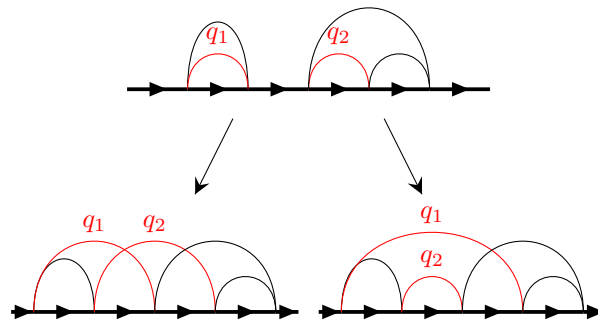


FIGURE 6.16: *Relink* update on a diagram containing one 2-loop and one 3-loop. A possible choice for the phonon propagators to relink is highlighted in red, and the possible transitions are shown.

distinct vertices can be identified. The vertices can be connected in 3 different ways with the phonon propagators leading to 3 distinct diagram topologies (including the topology of the current diagram): we propose at random one of the other two (see Fig. 6.16).

When evaluating the acceptance ratio, we observe that, unlike in higher order loops, the two phonons in a 2-loop are indistinguishable in the sense that they connect the same vertices. Picking any of them is an equivalent choice for the purpose of the *relink* update, yielding the same final state. For this reason, the probability to switch between configurations with a different number of 2-loops is not balanced.

To satisfy detailed balance, we find the following transition ratio: $2^{\Delta N_2}$, where $\Delta N_2 = N'_2 - N_2$ is the difference in the number of 2-loops between the proposed and current diagram. This ratio exactly compensates the combinatorial factors, so that only the diagram weight ratio is left to compute:

$$R_{\text{rel}} = 2^{\Delta N_2} \frac{\mathcal{D}_{\text{rel}}}{\mathcal{D}_{\text{cur}}} \times \frac{2^{N_V - N'_2}}{2^{N_V - N_2}} = \frac{\mathcal{D}_{\text{rel}}}{\mathcal{D}_{\text{cur}}} . \quad (6.42)$$

External phonons

Within the momentum-space approach, information about the phonon cloud can be obtained by extending the simulation to generate diagrams of the irreducible N -phonon Green's function [50]. To this end, we generalize the updates previously described in a simple way. When proposing the final time in the *add 2-loop* update, and when proposing the middle and final time in the *add 3-loop* update, we allow them to go beyond the total diagram length τ . The resulting phonon is regarded as an external phonon, as if the representation were circular. Moreover, the *relink* update is generalized to allow phonon propagators to cross the origin in order to create topologies with external phonons.

Chapter 7

Summary and conclusion

This thesis presents a comprehensive theoretical and numerical investigation of polaron physics across a range of interaction mechanisms and model Hamiltonians. Its primary objective has been to understand how different forms of electron-phonon coupling give rise to distinct quasiparticle behavior and how the corresponding properties can be accessed using numerically exact many-body techniques. To this end, different continuum and lattice polaron models have been studied, characterized by their specific interaction vertices, electron band structures and phonon dispersion relations.

The first part of this work is devoted to the analytical derivation of the theory underlying these models and to the development of the numerical infrastructure required for their solution. After introducing the polaron concept and deriving the general electron-phonon Hamiltonian in Chapter 1, it focuses in Chapter 2 on the two main numerical methods utilized in this thesis: (i) Diagrammatic Monte Carlo, and (ii) stochastic optimization with consistent constraints for numerical analytic continuation. Both methods are described in a pedagogical way with special emphasis on the DiagMC approach.

Chapter 3 starts with a summary of various polaron properties and their relation to many-body correlation functions. Using a perturbation expansion of the time-evolution operator in imaginary time, it is shown how these correlation functions can be expressed as infinite sums of Feynman diagrams. The last section of the chapter discusses the details of a DiagMC implementation for polaron Hamiltonians in the form of Eq. 1.29, with a particular focus on the Monte Carlo updates and estimators used to efficiently sample the configuration space of all Feynman diagrams and to extract physical observables.

The overall strategy for studying polaron problems in this thesis can be summarized as follows: (i) Use DiagMC to obtain ground state properties like energies, effective masses, quasiparticle weights or average number of phonons in the polaron cloud, and to compute imaginary time correlation functions, such as the

single-particle Green's function or current-current correlation function. (ii) Perform numerical analytic continuation to reconstruct dynamical quantities such as spectral functions and optical conductivity from the imaginary time data. (iii) Analyze the obtained results and interpret them in terms of the underlying physical mechanisms.

In the remaining chapters, this strategy has been applied to three representative polaron models, each illustrating distinct aspects of electron-phonon physics.

The first study in Chapter 4 addresses the Fröhlich large polaron in two and three spatial dimensions [175]. The simulations reproduce ground state energies and effective masses with high accuracy compared to other DiagMC results and confirm exact scaling relations connecting two- and three-dimensional systems. Furthermore, the calculated weak and strong coupling expansion coefficients agree with their analytically known values, thereby validating the numerical procedure. The computed polaron dispersion relations reveal characteristic differences between 2D and 3D systems: in two dimensions the spectrum approaches the continuum edge asymptotically, while in three dimensions it reaches the continuum at a finite critical momentum. These results provide a stringent validation of the DiagMC approach. They clarify earlier discussions concerning its accuracy in describing Fröhlich polarons, and they give us the confidence to extend our studies to less conventional cases.

The second study in Chapter 5 investigates a lattice polaron interacting with an acoustic phonon branch through deformation-potential coupling [202]. In contrast to previously studied optical or continuum polarons, this system exhibits a significantly richer physical structure. The numerical results reveal the existence of a self-trapping region separating weak and strong coupling regimes, characterized by quantum resonance between competing lattice distortions. A key aspect of this model is the presence of two distinct phonon contributions that interact with the quasiparticle in different ways, leading to the formation of a composite phonon cloud. This mechanism produces a complex spectral and optical response with multiple excited states and demonstrates that the acoustic lattice polaron represents a qualitatively distinct quasiparticle compared with both optical and acoustic continuum polarons. The results presented here provide the first systematic characterization of this system and offer useful guidance for identifying signatures of electron-acoustic phonon coupling in experimental studies.

The final part of the thesis, Chapter 6, examines polarons with quadratic coupling to lattice displacements [204]. This interaction leads to quasiparticle properties that differ substantially from models with linear electron-phonon coupling. The numerical results show that, in the adiabatic regime, the quadratic polaron

remains nearly indistinguishable from a bare particle even for relatively strong coupling strengths. In the anti-adiabatic regime, stronger renormalization effects are observed near the instability threshold. However, these effects stay in a moderate range and saturate to finite values. An unexpected outcome of the simulations is that lattice deformations remain weak even close to the instability point. These findings help explain why electrons in certain polar materials, such as SrTiO_3 , can often be successfully treated as nearly free particles in theoretical descriptions of superconductivity. Moreover, the study identifies the adiabatic ratio as the key parameter controlling the system's behavior, indicating that simplified theoretical approaches may be constructed and validated against the numerically exact results from this work. Our results obtained with momentum-space DiagMC have been compared with an alternative X-representation (i.e. atomic coordinates representation) approach working with a path-integral representation for both the electron and atomic displacements. This method, originally developed by Prokof'ev and Svistunov [66], was further extended by the first author of our quadratic polaron paper, Stefano Ragni, to treat polarons with arbitrary nonlinear electron-phonon interactions [205]. A more detailed description of the method and other similar applications can be found in Stefano Ragni's PhD thesis [115]. In parallel, complementary analytical approaches were developed by incorporating quadratic interactions into the method of squeezed phonon states [206].

In addition to developing the theory, running the simulations and analyzing the data of the three main studies mentioned above, a significant part of the author's PhD work has been devoted to the implementation of a high-quality C++ Monte Carlo library that forms the core of all DiagMC codes developed and used in the present thesis. The library has been designed with robustness, modularity, and extensibility in mind, enabling users to efficiently implement different Monte Carlo algorithms. Owing to space and time limitations, the details of this effort have not been discussed as part of the dissertation. They will be presented in a forthcoming technical publication, accompanied by an open-source release of the software including dedicated documentation and tutorial material. This initiative aims to support the growing interest in Diagrammatic Monte Carlo and to provide standardized benchmark implementations that can facilitate future research in the field.

In conclusion, this thesis demonstrates that DiagMC, together with numerical analytic continuation methods, provides a powerful and versatile framework for investigating polaron Hamiltonians. By combining analytical derivations, algorithmic development, and extensive numerical simulations, the work establishes

a coherent approach to study polaron physics across different interaction mechanisms and model systems. The results presented here deepen our understanding of electron-phonon interactions in both continuum and lattice environments and provide reliable reference data for future research. At the same time, the methodological advances and computational tools developed for this dissertation open new perspectives for the application of DiagMC techniques to more complex quantum many-body polaron problems, including their integration into first-principles electronic structure codes.

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