Polaron action for multimode dispersive phonon systems

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Path-integral approach to the tight-binding polaron is extended to multiple optical phonon modes of arbitrary dispersion and polarization. The non-linear lattice effects are neglected. Only one electron band is considered. The electron-phonon interaction is of the density-displacement type, but can be of arbitrary spatial range and shape. Feynman’s analytical integration of ion trajectories is performed by transforming the electron-ion forces to the basis in which the phonon dynamical matrix is diagonal. The resulting polaron action is derived for the periodic and shifted boundary conditions in imaginary time. The former can be used for calculating polaron thermodynamics while the latter for the polaron mass and spectrum. The developed formalism is the analytical basis for numerical analysis of such models by path-integral Monte Carlo methods.

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I. INTRODUCTION

In the last two decades, quantum Monte Carlo (MC) simulation methods proved to be a powerful theoretical tool in analyzing models with strong electron-phonon interactions. The pioneering works by Hirsch and Fradkin on the many-polaron one-dimensional Holstein model and the Su-Schrieffer-Heeger polaron, by de Raedt and Lagendijk on the Holstein polaron and bipolaron, and by Alexandrou and Rosenfelder on the Fröhlich polaron, were followed more recently by the continuous-time path-integral MC, diagrammatic MC, and the Lang-Firsov MC methods. The new methods have expanded the list of calculable polaron properties, both static and dynamic. However, expansion in terms of analysis of more complex polaron models has been slow. The bulk of new literature is still devoted to the two canonical polaron models: Fröhlich model of the ionic solid and Holstein model of molecular crystal. While these models are important, the new MC methods are powerful and versatile enough to study others. Notable exceptions from this trend are the investigations of the Su-Schrieffer-Heeger model, Jahn-Teller polaron, and of the $tJ$ model with electron-phonon interaction.

We recently started a series of generalizations of the continuous-time path integral MC method away from the standard Holstein interaction with localized phonons on cubic lattices. A long-range electron-phonon interaction was investigated in Refs. 14, and different Bravais lattices in Ref. 15. In this paper, we take the first step toward generalizing the method on dispersive and multimode phonon systems. A critical element of the method is analytical integration over ion trajectories in the path-integral expression for the polaron partition function. This leads to a polaron action, expressed as a functional over the electron path, which includes all the effects of the phonon dynamics and electron-phonon interaction. For the Einstein phonons, the integration results in the single-oscillator formula derived by Feynman. In more complex cases, the electron-ion forces must be first transformed to the basis of the lattice normal modes, then the normal modes integrated out using the Feynman formula, and then the final result transformed back to the original basis. To our knowledge, the only investigation of this kind in the polaron MC literature was done by de Raedt and Lagendijk who studied the one-dimensional Holstein polaron with dispersive optical phonons by the discrete-time path-integral MC. They found that the transition into a self-trapped state always takes place for for dispersive phonons as well as for dispersionless phonons but the transition point depends on the details of the phonon dispersion. Their derivation now needs to be repeated for continuous imaginary time and generalized to multiple phonon modes. Recently, Zoli calculated the phonon path integral for the Holstein model in the semiclassical approximation where the retarded nature of the phonon action was neglected.

Phonon dispersion is expected to affect polaron properties, most notably the polaron effective mass and hence mobility. The forces acting between the ions spread out the deformation even if the electron-phonon interaction is local. When the electron hops between the lattice cells, partial deformation already exists, which increases the phonon overlap integral. Thus in general, dispersion reduces the polaron mass. In this sense, the dispersion is analogous to a long-range electron-phonon interaction.

The purpose of the present paper is to carry out general phonon integration to enable MC studies of novel polaron models. The main analytical result is given below in equations (34)-(36) and (31)-(32). The expressions are rather complex, however, and the practical impact of the formalism will depend on the efficiency of numerical methods used to evaluate the polaron action at each MC update. This is likely to become the subject of future work.
II. SHIFT PARTITION FUNCTION

Consider the general problem of a lattice electron interacting with an arbitrary system of ions via a density-displacement interaction. In the path integral formalism\textsuperscript{16}, the electron is described by an imaginary-time path $r(\tau)$, where $r$ is the discrete lattice coordinate at “time” $\tau$, and $0 \leq \tau \leq \beta = (k_B T)^{-1}$. In this paper, only one Wannier state per unit cell is assumed. The ion system is represented by $p \geq 1$ continuous degrees of freedom $\xi_{ns}$ (displacements) where $n$ numbers the unit cells, and $1 \leq s \leq p$. The mass of $s$-th degree of freedom is $m_s$. Ions interact with each other via pairwise force constants $v_{n,n'}$, which are functions of the difference $n - n'$ only. Cubic and higher terms in the lattice potential energy are neglected. A displacement $\xi_{ns}$ is acted upon by the electron with force $f_{ns}(\tau) = f_{ns}[r(\tau)]$, so that the interaction potential is $-f_{ns}(\tau)\xi_{ns}$. The imaginary time action of such a system is given by

$$A[r(\tau), \xi_{ns}(\tau)] = T[r(\tau)] + A_{\text{ph}}[\xi_{ns}(\tau)] + A_{\text{e-ph}}[r(\tau), \xi_{ns}(\tau)]$$

$$= T[r(\tau)] - \sum_{n,s} \int_0^\beta \frac{m_s \xi_{ns}^2(\tau)}{2\hbar^2} d\tau - \frac{1}{2} \sum_{n,n',s'} \int_0^\beta v_{n,n',s'} \xi_{ns}(\tau) \xi_{n's'}(\tau) d\tau + \sum_{n,s} \int_0^\beta f_{ns}[r(\tau)] \xi_{ns}(\tau) d\tau. \quad (1)$$

Here the first term $T$ represents the kinetic energy of the electron. It is not the subject of the present work, see instead Refs. \textsuperscript{6,12}. Note that the action $A$ is dimensionless. The statistical weight of a configuration is given by $\exp(A)$. The central object of the polaron path-integral quantum Monte Carlo method is the shift partition function

$$Z_{\Delta r} = \sum_{r_0} \int \prod_{n,s} d\xi_{ns,0} \int_{r(0)=r_0; \xi_{ns}(0)=\xi_{ns,0}}^{r(\tau)\equiv r_0+\Delta r; \xi_{ns}(\tau)\equiv \xi_{ns,\tau}+\xi_{ns,0}} D\tau(r) D\xi_{ns}(\tau) e^{A[r(\tau), \xi_{ns}(\tau)]}. \quad (2)$$

Here the inner path integral is taken under shifted boundary conditions in imaginary time. This means that the entire real-space configuration at the end point $\tau = \beta$ (which comprises the electron and phonon coordinates) is identical to the configuration at the end point $\tau = 0$ up to a parallel shift by a real space vector $\Delta r$. The outer boundary integral is over all possible configurations at $\tau = 0$.

Since the ion coordinates enter the action linearly and quadratically, path integration over $\xi_{ns}(\tau)$ in $\text{(1)}$ can be done analytically. We first calculate a more general path integral

$$W[\xi_{ns,0}; \xi_{ns,\tau}; r(\tau)] = \int_{\xi_{ns}(0)\equiv \xi_{ns,0}}^{\xi_{ns}(\tau)\equiv \xi_{ns,\tau}} D\xi_{ns}(\tau) e^{A_{\text{ph}}[\xi_{ns}(\tau)] + A_{\text{e-ph}}[r(\tau), \xi_{ns}(\tau)]}. \quad (3)$$

Here, in contrast to eq. $\text{(2)}$, the end coordinates of ions are not restricted in any way. $W$ is a function of the end coordinates $\xi_{ns,0}$, $\xi_{ns,\tau}$, and a functional of the whole electron path. Path integration is performed by a method devised by Feynman$\textsuperscript{12}$. Variation of the exponent with respect to $\xi_{ns}(\tau)$ subjected to fixed boundary conditions yields a Euler-Lagrange equation for the stationary path $\tilde{\xi}_{ns}(\tau)$

$$\frac{m_s}{\hbar^2} \tilde{\xi}_{ns}(\tau) - \sum_{n,n',s'} v_{n,n',s'} \tilde{\xi}_{ns}(\tau) + f_{ns}(\tau) = 0. \quad (4)$$

This is a system of $pN$ coupled second order ordinary inhomogeneous differential equations for functions $\xi(\tau)$ with boundary conditions

$$\tilde{\xi}_{ns}(0) = \xi_{ns,0},$$

$$\tilde{\xi}_{ns}(\beta) = \xi_{ns,\beta}. \quad (5)$$

The inhomogeneous terms $f_{ns}(\tau)$ are functions of the electron path $r(\tau)$ and as such are arbitrary functions of imaginary time $\tau$. When the solution of eq. $\text{(4)}$ is found, $W$ is calculated by performing a path shift in $\text{(3)}$:

$$\xi_{ns}(\tau) = \tilde{\xi}_{ns}(\tau) + \eta_{ns}(\tau),$$

$$\eta_{ns}(0) = \eta_{ns,\beta} = 0. \quad (7)$$

Upon substitution of $\text{(4)}$ in $\text{(3)}$ the action $A_{\text{ph}} + A_{\text{e-ph}}$ separates in three terms: $A_1$ that depends only on $\tilde{\xi}$, $A_2$ that depends only on $\eta$, and the mixed term $A_3$ that depends on both $\xi$ and $\eta$. The mixed term vanishes identically by virtue of the classical equations $\text{(4)}$. $W$ becomes

$$W[\xi_{ns,0}; \xi_{ns,\tau}; r(\tau)] = e^{A_1[\xi_{ns}(\tau)]} \int_{\eta_{ns}(0)=0}^{\eta_{ns}(\beta)=0} D\eta_{ns}(\tau) e^{A_2[(\eta_{ns}(\tau)]} = Z_{\text{ph}} e^{A_1[\tilde{\xi}_{ns}(\tau)]}. \quad (9)$$
The path integral over $\eta(\tau)$ does not depend on any dynamical variables and therefore can be assigned a multiplicative constant $Z_{ph}$. It represents the incomplete thermodynamic partition function of freely vibrating ions. [The partition function will become complete after the final integration over the end ion coordinates in (2).] The functional $A_1$ in eq. (3) has the following form:

$$A_1[\xi_n(\tau)] = \sum_{n,s} \left\{ \frac{m_s}{2\hbar^2} \left[ \dot{\xi}_{ns}(0)\xi_{ns}(0) - \dot{\xi}_{ns}(\beta)\xi_{ns}(\beta) \right] + \frac{1}{2} \int_0^{\beta} f_{ns}(\tau')\dot{\xi}_{ns}(\tau')d\tau' \right\} .$$  \hspace{1cm} (10)

As soon as the solution of system (4) is known, $W$ is calculated explicitly using eqs. (9) and (10).

### III. SOLUTION OF CLASSICAL EQUATIONS

In this section we solve the classical equations (4) under the boundary conditions (5)-(6). The strategy is to transform $\xi_n$ to normal coordinates, in which the system is diagonal, and then apply the formula for a single harmonic oscillator. The first step is a Fourier-mass transformation

$$\tilde{\xi}_{ns}(\tau) = \frac{1}{N} \sum_k a_{ks}(\tau) e^{ikn},$$  \hspace{1cm} (11)

$$a_{ks}(\tau) = \sqrt{m_s} \sum_n \tilde{\xi}_{ns}(\tau) e^{-ikn},$$  \hspace{1cm} (12)

where $N$ is the number of unit cells and $k$ spans the Brillouin zone of the reciprocal lattice. Substituting (11) into (4), multiplying by $e^{-ik\cdot n}$ and summing over $n$, equation (4) is transformed into the following:

$$-\ddot{a}_{ks}(\tau) + \hbar^2 \sum_{s'} w_{ss'}(k) a_{ks'}(\tau) = \frac{\hbar^2}{\sqrt{m_s}} \sum_n e^{-ikn} f_{ns}(\tau),$$  \hspace{1cm} (13)

$$w_{ss'}(k) = w^*_{s's}(k) = \sum_{n-n'} \tilde{\xi}_{ns.n's'} \sqrt{m_s m_{s'}} e^{ik(n-n')}.$$

The new $p \times p$ matrix $w(k)$ is Hermitian. The latter property is a consequence of the factor $\sqrt{m_s}$ in the above transformations. This is of course a standard device of the classical theory of lattice vibrations. The dimensionality of $w(k)$ is frequency squared. On the next step, consider an eigenvalue problem for the matrix $w(k)$:

$$\sum_{s'} w_{ss'}(k) u^k_{s'\lambda} = \omega^2_{k\lambda} u^k_{s\lambda}.$$

Since $w$ is Hermitian, the eigenvalues $\omega^2_{k\lambda}$ are real. We also assume that $\omega^2_{k\lambda}$ are positive which implies no structural phase transition. Further, since $w^*_{s's'}(-k) = w_{ss'}(k)$ then $\omega_{-k\lambda} = \omega_{k\lambda}$. The index $\lambda$ numbers different eigenvalues, that is phonon modes. The eigenvector $u^k_{s\lambda}$ defines the phonon polarization. The eigenvectors are orthogonal, $\sum_{\lambda} u^k_{s\lambda} u^k_{s'\lambda} = \delta_{ss'}$. In $k$-points of high symmetry, the eigenvectors can be made orthogonal by a proper procedure. In addition, $u^{-k*}_{s\lambda} = u^k_{s\lambda}$. Next, expand the functions $a_{ns}(\tau)$ in the basis of $w$:

$$a_{ks}(\tau) = \sum_{\lambda=1}^{p} c_{k\lambda}(\tau) u^k_{s\lambda},$$  \hspace{1cm} (16)

$$c_{k\lambda}(\tau) = \sum_{s=1}^{p} a_{ks}(\tau) u^k_{s\lambda},$$  \hspace{1cm} (17)

where $c_{k\lambda}(\tau)$ are new complex functions of imaginary time. Substituting (16) into (13), using the definition (15), multiplying the resulting equation by $u^k_{s\lambda}*$ and summing over $s$ one obtains

$$-\ddot{c}_{k\lambda}(\tau) + (\hbar \omega_{k\lambda})^2 c_{k\lambda}(\tau) = \hbar^2 \sum_{s} \frac{u^k_{s\lambda} u^k_{s\lambda}^*}{\sqrt{m_s}} \sum_n e^{-ikn} f_{ns}(\tau).$$  \hspace{1cm} (18)
Thus, the system of equations is fully diagonalized, with a transformed inhomogeneous term on the right hand side. The problem is reduced to the well studied case of one harmonic oscillator under an arbitrary external force. Before applying the corresponding formulas the boundary conditions must be recalculated in the new basis. Combining eqs. (18)-(20), the transformed boundary conditions read

\[ c_{k\lambda}(0) = \sum_{n_s} \sqrt{m_s} u_{s\lambda} e^{i\kappa n_s} e^{-ikn}, \]  

\[ c_{k\lambda}(\beta) = \sum_{n_s} \sqrt{m_s} u_{s\lambda} \xi_{ns\beta} e^{-ikn}. \]  

To proceed further we recall the following result from the harmonic oscillator theory. A real function \( H(\tau) \) satisfying the equation

\[ -\dddot{\bar{\xi}}(\tau) + (\hbar \omega_{k\lambda})^2 \ddot{\bar{\xi}}(\tau) = f(\tau), \]

with the boundary conditions \( H(0) = H_0 \) and \( H(\beta) = H_\beta \), is given by the expression

\[ H(\tau) = H_0 \frac{\sinh \hbar \omega_{k\lambda}(\beta - \tau)}{\sinh \hbar \omega_{k\lambda} \beta} + H_\beta \frac{\sinh \hbar \omega_{k\lambda} \tau}{\sinh \hbar \omega_{k\lambda} \beta} + \int_0^\beta G_{k\lambda}(\tau, \tau') f(\tau') d\tau', \]

where

\[ G_{k\lambda}(\tau, \tau') = \frac{1}{\hbar \omega_{k\lambda} \sinh \hbar \omega_{k\lambda} \beta} \left\{ \begin{array}{ll} \sinh \hbar \omega_{k\lambda} \tau \cdot \sinh \hbar \omega_{k\lambda}(\beta - \tau') & \tau < \tau' \\ \sinh \hbar \omega_{k\lambda}(\beta - \tau) \cdot \sinh \hbar \omega_{k\lambda} \tau' & \tau > \tau' \end{array} \right. \]

is the Green’s function of the equation (22) under the zero boundary conditions. Separating eqs. (18)-(20) into real and imaginary parts and applying formula (22) one obtains

\[ c_{k\lambda}(\tau) = \frac{\sinh \hbar \omega_{k\lambda}(\beta - \tau)}{\sinh \hbar \omega_{k\lambda} \beta} \sum_{n_s} \sqrt{m_s} u_{s\lambda} \xi_{ns0} e^{-ikn} + \frac{\sinh \hbar \omega_{k\lambda} \tau}{\sinh \hbar \omega_{k\lambda} \beta} \sum_{n_s} \sqrt{m_s} u_{s\lambda} \xi_{ns\beta} e^{-ikn} \]

\[ + \int_0^\beta d\tau' G_{k\lambda}(\tau, \tau') h^2 \sum_s \frac{u_{s\lambda}^*}{\sqrt{m_s}} \sum_n e^{-ikn} f_{ns}(\tau'). \]

Restoration of the classical displacement \( \bar{\xi}_{ns} \) from eq. (11) yields the complete solution of the original Cauchy problem (4)-(6)

\[ \bar{\xi}_{ns}(\tau) = \frac{1}{N} \sum_{k\lambda} \frac{\sinh \hbar \omega_{k\lambda}(\beta - \tau)}{\sinh \hbar \omega_{k\lambda} \beta} \sum_{n's'} \frac{m_{s'}}{m_s} u_{s'\lambda}^* u_{s\lambda} e^{i(k(n-n'))} \xi_{n's'0} \]

\[ + \frac{1}{N} \sum_{k\lambda} \frac{\sinh \hbar \omega_{k\lambda} \tau}{\sinh \hbar \omega_{k\lambda} \beta} \sum_{n's'} \frac{m_{s'}}{m_s} u_{s'\lambda}^* u_{s\lambda} e^{i(k(n-n'))} \xi_{n's'\beta} \]

\[ + \frac{1}{N} \sum_{k\lambda} \int_0^\beta d\tau' G_{k\lambda}(\tau, \tau') \sum_{n's'} \frac{h^2}{\sqrt{m_s m_{s'}}} u_{s'\lambda}^* u_{s\lambda} e^{i(k(n-n'))} f_{n's'}(\tau'). \]

Note that because

\[ u_{s'\lambda}^* u_{s\lambda} e^{-ik(n-n')} = u_{s'\lambda}^* u_{s\lambda} e^{-ik(n-n')} = \left[ u_{s'\lambda}^* u_{s\lambda} e^{i(k(n-n'))} \right]^*, \]

the summation over \( k \) in equation (25) makes the displacements purely real, as expected. Finally, substituting the classical solution in eq. (10), after some algebra, one obtains the polaron action \( A_1 \) as a function of the end ion
coordinates and a functional of the forces

\[ A_1[\xi_{n_0}, \xi_{n_s}; f_{n_s}(\tau)] = \]

\[ \frac{1}{2N} \sum_{k\lambda} \frac{\omega_{k\lambda}}{h \sinh \omega_{k\lambda} \beta} \sum_{n_n's'} \sqrt{m_{s'} m_s} \Re \left[ u_{k\lambda}^{*} u_{k\lambda} e^{i(k(n'-n))} \right] \times \]

\[ \left\{ -\left( \xi_{n_0} \xi_{n's'} + \xi_{n_s} \xi_{n's'} \right) \cosh \omega_{k\lambda} \beta + \xi_{n_0} \xi_{n's'} \beta + \xi_{n_s} \xi_{n's'} \beta \right\} \]

\[ + \frac{1}{2N} \sum_{k\lambda} \sum_{n_n's'} \Re \left[ u_{k\lambda}^{*} u_{k\lambda} e^{i(k(n'-n))} \right] \int_0^\beta d\tau' \sinh \omega_{k\lambda}(\beta - \tau') \left\{ \sqrt{m_{s'} / m_s} \xi_{n_0} f_{n's'}(\tau') + \sqrt{m_{s'} / m_s} \xi_{n_s} f_{n's'}(\tau') \right\} \]

\[ + \frac{1}{2N} \sum_{k\lambda} \sum_{n_n's'} \Re \left[ u_{k\lambda}^{*} u_{k\lambda} e^{i(k(n'-n))} \right] \int_0^\beta d\tau' \sinh \omega_{k\lambda}(\tau') \left\{ \sqrt{m_{s'} / m_s} \xi_{n_s} f_{n's'}(\tau') + \sqrt{m_{s'} / m_s} \xi_{n_0} f_{n's'}(\tau') \right\} \]

\[ + \frac{1}{2N} \sum_{k\lambda} \sum_{n_n's'} \frac{\hbar^2}{m_{s'} m_s} \Re \left[ u_{k\lambda}^{*} u_{k\lambda} e^{i(k(n'-n))} \right] \int_0^\beta d\tau' \int_0^\beta d\tau'' G_{k\lambda}(\tau, \tau') f_{n_s}(\tau) f_{n's'}(\tau') . \]

Equations 21 and 27 provide an explicit solution for the quantity \( W \) defined in eq. 3.

IV. POLARON ACTION

In accordance with the general ideas of the continuous time polaron Monte Carlo, the end points in the action 27 must be related by \( \xi_{n_0} = \xi_{n_0} - \Delta \tau s_0 \). Then \( W = Z_{n_0} e^{A_1} \) should be integrated over all \( \xi_{n_0} \) from minus to plus infinity, see eqs. 2, 3, and 4. To perform the integration, it is convenient to employ the same series of transformations that enabled calculation of the path integral, that is

\[ \xi_{n_0} = \frac{1}{N} \sum_{k\lambda} \frac{1}{\sqrt{m_s}} u_{k\lambda}^* e^{i k n} g_{k\lambda} = \frac{1}{N} \sum_{k\lambda} \frac{1}{\sqrt{m_s}} u_{k\lambda}^* e^{-i k n} g_{k\lambda} , \]

\[ \xi_{n_s} = \frac{1}{N} \sum_{k\lambda} \frac{1}{\sqrt{m_s}} u_{k\lambda}^* e^{i k (n-\Delta \tau)} g_{k\lambda} = \frac{1}{N} \sum_{k\lambda} \frac{1}{\sqrt{m_s}} u_{k\lambda}^* e^{-i k (n-\Delta \tau)} g_{k\lambda} . \]

Here \( g_{k\lambda} = b_{k\lambda} + i d_{k\lambda} \) is a new complex variable. Substituting the expansions into eq. 27 one obtains the action as a function of amplitudes \( a \) and \( d \)

\[ A_1[b_{k\lambda}, d_{k\lambda}; f_{n_s}(\tau)] = \frac{1}{N} \sum_{k\lambda} \frac{\omega_{k\lambda}}{h \sinh \omega_{k\lambda} \beta} \left( \cosh \omega_{k\lambda} \beta - \cos k \Delta \tau \right) \left( -b_{k\lambda}^2 - d_{k\lambda}^2 \right) \]

\[ + \frac{1}{N} \sum_{k\lambda} b_{k\lambda} \sum_{n_s} \frac{1}{\sqrt{m_s}} \left\{ \Re \left[ u_{k\lambda}^* e^{i k n} \right] B_{k\lambda n_s} + \Re \left[ u_{k\lambda}^* e^{i k (n-\Delta \tau)} \right] C_{k\lambda n_s} \right\} \]

\[ - \frac{1}{N} \sum_{k\lambda} d_{k\lambda} \sum_{n_s} \frac{1}{\sqrt{m_s}} \left\{ \Im \left[ u_{k\lambda}^* e^{i k n} \right] B_{k\lambda n_s} + \Im \left[ u_{k\lambda}^* e^{i k (n-\Delta \tau)} \right] C_{k\lambda n_s} \right\} \]

\[ + \frac{1}{2N} \sum_{k\lambda} \sum_{n_n's'} \frac{\hbar^2}{m_{s'} m_s} \Re \left[ u_{k\lambda}^* u_{k\lambda} e^{i(k(n'-n))} \right] \int_0^\beta d\tau'' \int_0^\beta d\tau' G_{k\lambda}(\tau, \tau') f_{n_s}(\tau) f_{n's'}(\tau') . \]

where

\[ B_{k\lambda n_s} = \int_0^\beta \int_0^\beta d\tau d\tau' \sinh \omega_{k\lambda} \beta \left( \cosh \omega_{k\lambda} \beta - \cosh \omega_{k\lambda} \beta \right) f_{n_s}(\tau') , \]

\[ C_{k\lambda n_s} = \int_0^\beta \int_0^\beta d\tau d\tau' \sinh \omega_{k\lambda} \beta \left( \cosh \omega_{k\lambda} \beta - \cosh \omega_{k\lambda} \beta \right) f_{n_s}(\tau') , \]

and \( \Re \) and \( \Im \) denote the real and imaginary parts, respectively. The final step is gaussian integration of \( e^{A_1} \) over the real \( b \) and \( d \) from minus to plus infinity. The reality of \( \xi \) and the property \( u_{k\lambda} = u_{k\lambda}^* \) ensure that \( b_{-k\lambda} = b_{k\lambda} \).
and $d_{-k\lambda} = -d_{k\lambda}$. Thus the domain of integration is limited to half of the Brillouin zone. The integration is straightforward, and leads to the result $const \cdot e^{A_{\Delta r}}$ where $const$ completes the partition function of free phonons while the polaron action $A_{\Delta r}$ is given by

$$A_{\Delta r}[f_{ns}(\tau)] = \frac{1}{N} \sum_{k\lambda} \frac{h \sinh \hbar \omega_{k\lambda} \beta}{4 \omega_{k\lambda} (\cosh \hbar \omega_{k\lambda} \beta - \cos k\Delta r)} \sum_{\mathbf{n},\mathbf{n}'s'} \frac{1}{\sqrt{m_s m_{s'}}} \times$$

$$\times \left\{ \Re \left[ u_{s\lambda}^* e^{i\mathbf{k} \cdot \mathbf{r}_s} e^{-i\mathbf{k}' \cdot \mathbf{r}_{s'}} B_{k\lambda ns} B_{k\lambda ns'} + \Re \left[ u_{s\lambda}^* e^{i\mathbf{k} \cdot \mathbf{r}_s} e^{-i\mathbf{k}' \cdot \mathbf{r}_{s'}} B_{k\lambda ns} C_{k\lambda ns'} + \Re \left[ u_{s\lambda}^* e^{i\mathbf{k} \cdot \mathbf{r}_s} e^{-i\mathbf{k}' \cdot \mathbf{r}_{s'}} C_{k\lambda ns} B_{k\lambda ns'} \right] \right] \right\}$$

$$+ \frac{1}{2N} \sum_{k\lambda} \sum_{\mathbf{n},\mathbf{n}'s'} \frac{h^2}{\sqrt{m_s m_{s'}}} \Re \left[ u_{s\lambda}^* u_{s\lambda} e^{i\mathbf{k} \cdot \mathbf{r}_s} e^{-i\mathbf{k}' \cdot \mathbf{r}_{s'}} \right] \int_0^\beta \int_0^\beta d\tau d\tau' G_{k\lambda}(\tau, \tau') f_{ns}(\tau) f_{ns'}(\tau') \right]. \quad (33)$$

To simplify this expression consider first the case $\Delta r = 0$. This corresponds of course to the periodic boundary conditions in imaginary time. Taking into account the explicit forms of $B$, $C$, and $G$, the periodic action can be brought into the form

$$A_0[f_{ns}(\tau)] = \frac{1}{N} \sum_{k\lambda} \frac{h}{4 \omega_{k\lambda}} \int_0^\beta \int_0^\beta d\tau d\tau' \frac{\cosh \hbar \omega_{k\lambda} \beta}{\sinh \hbar \omega_{k\lambda} \beta} \sum_{\mathbf{n},\mathbf{n}'s'} \frac{1}{\sqrt{m_s m_{s'}}} \Re \left[ u_{s\lambda}^* u_{s\lambda} e^{i\mathbf{k} \cdot \mathbf{r}_s} e^{-i\mathbf{k}' \cdot \mathbf{r}_{s'}} \right] f_{ns}(\tau) f_{ns'}(\tau') \right. \quad (34)$$

Comparing this result with an analogous expression for independent oscillators\(^{17}\) shows that eq. (34) involves the forces transformed to the basis in which the phonon subsystems is diagonal. This is of course exactly what is expected intuitively.

Returning to the general action \(^{33}\), one can calculate the correction to the periodic action by taking the difference between $A_{\Delta r}$ and $A_0$. The general expression is rather complicated. However, nonzero $\Delta r$ are needed only in calculation of the polaron mass and spectrum, which are the properties of zero temperature partition functions. Thus the action correction is needed only in the $\beta \to \infty$ limit. Then $\cos k\Delta r$ is negligible compared to $\cosh \hbar \omega_{k\lambda} \beta$, and tanh $\hbar \omega_{k\lambda} \beta \approx 1$ with exponential accuracy. Thus the correction becomes

$$\Delta A_{\Delta r}(\beta \to \infty) = \frac{1}{N} \sum_{k\lambda} \frac{h}{4 \omega_{k\lambda}} \sum_{\mathbf{n},\mathbf{n}'s'} \frac{1}{\sqrt{m_s m_{s'}}} \left\{ \Re \left[ u_{s\lambda}^* u_{s\lambda} e^{i\mathbf{k} \cdot \mathbf{r}_s} e^{-i\mathbf{k}' \cdot \mathbf{r}_{s'}} \right] e^{i\mathbf{k} \cdot \mathbf{r}_s} e^{-i\mathbf{k}' \cdot \mathbf{r}_{s'}} \right\} B_{k\lambda ns} B_{k\lambda ns'} +$$

$$+ \Re \left[ u_{s\lambda}^* u_{s\lambda} e^{i\mathbf{k} \cdot \mathbf{r}_s} e^{-i\mathbf{k}' \cdot \mathbf{r}_{s'}} \right] C_{k\lambda ns} B_{k\lambda ns'} \right\} =$$

$$= \frac{1}{N} \sum_{k\lambda} \frac{h}{2 \omega_{k\lambda}} \sum_{\mathbf{n},\mathbf{n}'s'} \frac{1}{\sqrt{m_s m_{s'}}} \Re \left[ u_{s\lambda}^* u_{s\lambda} e^{i\mathbf{k} \cdot \mathbf{r}_s} e^{-i\mathbf{k}' \cdot \mathbf{r}_{s'}} \right] e^{i\mathbf{k} \cdot \mathbf{r}_s} e^{-i\mathbf{k}' \cdot \mathbf{r}_{s'}} B_{k\lambda ns} C_{k\lambda ns'} \right]. \quad (35)$$

To summarize the results, the shift partition function \(^{24}\) reduces to a path integral over only the electron coordinates

$$Z_{\Delta r} = Z_{ph} \sum_{\mathbf{r}(\beta)=\mathbf{r}_0+\Delta \mathbf{r}} D\mathbf{r}(\tau) e^{T[\mathbf{r}(\tau)] + A_0[\mathbf{r}(\tau)] + \Delta A_{\Delta r}[\mathbf{r}(\tau)]}. \quad (36)$$

Here $Z_{ph} = \prod_{k\lambda} [2 \sinh (\frac{\theta}{2} \hbar \beta \omega_{k\lambda})]^{-1}$ is the full partition of free phonons. It is a multiplicative constant that does not influence polaron dynamics and drops out of the configuration weight in Monte Carlo simulations. $T$ is the action piece originating from the kinetic energy of the particle. On the lattice and in continuous imaginary time treatment of the kinetic energy is non-trivial as has been described elsewhere\(^{36}\). The periodic action $A_0$ is given by the formula \(^{33}\) which is valid for any temperature. This action can be used to calculate equilibrium polaron thermodynamics: free energy, specific heat, static correlation functions, and so on. The action correction $\Delta A$ is due to shifted boundary conditions (non-zero $\Delta r$) and is given by equations (35) and (31)-(32). The formulae are valid in the low temperature limit, i.e. the difference between eq. (35) and the exact formula is $O(e^{-\hbar \omega_{k\lambda} \beta})$. Equation (35) can be used to calculate the polaron mass, spectrum, and density of states. If for some reason the full $\Delta r \neq 0$ action is needed at a finite temperature, then the exact expression (33) should be used.

V. SPECIAL CASES

The formulae derived in the preceding section are general but can be difficult to evaluate. In this section, simplified expressions for several special cases are obtained that can be used in practical calculations.
A. Independent oscillators

The independence of oscillators implies that the force constants are diagonal in the unit cell index and in the degree of freedom index: \( v_{ns,n's'} = v_n \delta_{nn'} \delta_{s's'} \). Then the matrix elements \( w_{s's'}(k) = (v_s/m_s) \delta_{ss'} \) are real and independent of the momentum, see eq. 13. The eigenvalue problem 15 becomes diagonal with eigenvectors \( u_{s\lambda} = \delta_{s\lambda} \) and eigenvalues \( \omega^2_s = v_s/m_s \), where \( 1 \leq \lambda \leq p \). Neither \( n \) nor \( \omega \) depend on \( k \). Substitution into the periodic action leads to the following simplifications: (i) Summation over \( k \) yields \( N \delta_{mm'} \); (ii) The emerged delta function removes the summation over \( n' \); (iii) Summations over \( s \) and \( s' \) are performed using the explicit form of the eigenvectors \( u \); (iv) The summation index \( \lambda \) is changed back to index \( s \) to unify the notation. As a result, the periodic function takes the form:

\[
A_0[f_{ns}(\tau)] = \sum_{s=1}^{p} \sum_{n} \frac{h}{4m_s \omega_s} \int_{0}^{B} d\tau \int_{0}^{\tau} d\tau' \frac{\cosh h \omega_s (\frac{\beta}{2} - |\tau - \tau'|)}{\sinh h \omega_s \frac{\beta}{2}} f_{ns}(\tau)f_{ns}(\tau') ,
\]

where \( \omega_s = \sqrt{v_s/m_s} \). After the same transformations, the action correction becomes

\[
\Delta A[f_{ns}(\tau)] = \sum_{s=1}^{p} \sum_{n} \frac{h}{2m_s \omega_s} B_{ns} (C_{n+\Delta r,s} - C_{ns}) ,
\]

\[
B_{ns} = \int_{0}^{\beta} d\tau' \frac{\sinh h \omega_s (\beta - \tau')}{\sinh h \omega_s \beta} f_{ns}(\tau') ,
\]

\[
C_{ns} = \int_{0}^{\beta} d\tau' \frac{\sinh h \omega_s \tau'}{\sinh h \omega_s \beta} f_{ns}(\tau') .
\]

These expressions can be used in analysis of isotropic and anisotropic spherical oscillators in two, three, and higher dimensions.

B. One phonon branch

Substantial simplifications take place in the case of only one phonon degree of freedom per unit cell with mass \( m \) and force function \( v(n - n') \). It should be emphasized that this does not restrict the dimensionality of the lattice in any way. Rather, the electron interacts predominantly with one type of ion displacement. Mathematically, the indices \( s \) and \( \lambda \) accept only one value 1, and therefore can be omitted hereafter. The eigenvalue matrix equation 15 reduces to one linear equation with the solution \( u^k = 1 \) and

\[
\omega^2_k = w(k) = \frac{1}{m} \sum_n v(n) e^{ikn} .
\]

Thus, the phonon frequency is explicitly known. Note that \( \omega^2_k \) is automatically real because \( v(-n) = v(n) \). These results transform the action as follows

\[
A_0[f_{ns}(\tau)] = \frac{1}{N} \sum_{k} \frac{h}{4m_\omega_k} \int_{0}^{\beta} d\tau \int_{0}^{\tau} d\tau' \frac{\cosh h \omega_k (\frac{\beta}{2} - |\tau - \tau'|)}{\sinh h \omega_k \frac{\beta}{2}} \sum_{n'n'} \cos[k(n - n')] f_{n}(\tau)f_{n'}(\tau') ,
\]

\[
\Delta A[f_{ns}(\tau)] = \frac{1}{N} \sum_{k} \frac{h}{2m_\omega_k} \sum_{n'n'} \{ \cos[k(n - n' + \Delta r)] - \cos[k(n - n')] \} B_{kn} C_{kn'} ,
\]

where \( B \) and \( C \) are given by 11-12 with indices \( s \) and \( \lambda \) removed. The derived action should be used, e.g., in analysis of the polaron on a linear chain of one-dimensional coupled oscillators.18.
C. Holstein interaction

The Holstein local interaction is one of the most popular polaron models\textsuperscript{11}. At the same time, it is usually studies in combination with an Einstein set of decoupled one-dimensional oscillators. Here we will derive the action for the Holstein polaron interacting with an arbitrary phonon subsystem. We assume only one electron Wannier state per unit cell, leaving the multi-orbital case for future work. In the spirit of the Holstein model, we further assume that the electron interacts only with the ion degrees of freedom of the unit cell it currently occupies, i.e.

\begin{equation}
    f_{ns}(\tau) = \kappa_s \delta_{nn(\tau)},
\end{equation}

where \(r(\tau)\) is the electron coordinate at imaginary time \(\tau\). Note that the local force constants \(\kappa_s\) are different for different displacements. The locality of the interaction eliminates the summations over \(n\) and \(n'\) in equations (34)–(35). As a result, the Holstein polaron action becomes

\begin{equation}
    A_0[r(\tau)] = \frac{1}{N} \sum_{k \lambda} \frac{\hbar}{4 \omega_{k \lambda}} \int_0^\beta \int_0^\beta \mathrm{d}\tau \mathrm{d}\tau' \frac{\cosh \hbar \omega_{k \lambda} (\frac{\beta}{2} - |\tau - \tau'|)}{\sinh \hbar \omega_{k \lambda} \frac{\beta}{2}} \sum_{ss'} \frac{\kappa_s \kappa_{s'}}{\sqrt{m_s m_{s'}}} \Re \left[ u_{s \lambda} u_{s' \lambda}^* e^{i \mathbf{k}[r(\tau) - r(\tau')]} \right],
\end{equation}

\begin{equation}
    \Delta A_{\Delta r}[r(\tau)] = \frac{1}{N} \sum_{k \lambda} \frac{\hbar}{2 \omega_{k \lambda}} \int_0^\beta \int_0^\beta \mathrm{d}\tau \mathrm{d}\tau' \frac{\sinh \hbar \omega_{k \lambda} (\beta - \tau) \sinh \hbar \omega_{k \lambda} \tau'}{\sinh^2 \hbar \omega_{k \lambda} \beta} \times \sum_{ss'} \frac{\kappa_s \kappa_{s'}}{\sqrt{m_s m_{s'}}} \Re \left[ u_{s \lambda} u_{s' \lambda}^* e^{i \mathbf{k}[r(\tau) - r(\tau')]} e^{i \mathbf{k}[r(\tau) - r(\tau') + \Delta \mathbf{r}]} - e^{i \mathbf{k}[r(\tau) - r(\tau')]} \right].
\end{equation}

The three cases considered in this section are important on their own right, but they also serve as examples of how particular models are derived from the general polaron action. Many more models can be developed. In particular, one can envision combinations of the above cases: Holstein interaction with one dispersive phonon branch, Holstein interaction with uncoupled three-dimensional oscillators, and so on.

VI. DISCUSSION

In this paper, the polaron action for the general dispersive phonon system has been derived. It is important to list the conditions under which these results have been obtained. First of all, the crystal lattice is treated in the quadratic approximation, i.e. the phonons do not interact with each other. Secondly, the electron-phonon interaction is limited to the electron density - ion displacement type. There are other important classes of electron-phonon interactions – most notably the Jahn-Teller and Su-Schrieffer-Heeger ones – which require separate analysis. Finally, the complexity of the electron kinetic energy has not been fully addressed. This generalization is yet to be addressed in the polaron literature.

The motivation for the present work was the extension of the capabilities of the path-integral polaron Monte Carlo method. However, the practical usefulness of the developed formalism entirely depends on the efficient calculation of the action. Consider the general formulas (44) and (45). Not only they involve double integration over the imaginary time, but also summation over all phonon momenta and branches, and a double sum over the unit cells and ion degrees of freedom. Thus direct calculation of the full action at every Monte Carlo update may be prohibitively expensive. Development of the practical ways to apply the present formalism to specific polaron models will be the subject of future investigations.

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1. J. E. Hirsch and E. Fradkin, Phys. Rev. Lett. 49, 402 (1982); Phys. Rev. B 27, 4302 (1983).
2. J. E. Hirsch and E. Fradkin, Phys. Rev. B 27, 1680 (1983).
3. H. de Raedt and A. Lagendijk, Phys. Rev. Lett. 49, 1522 (1982); Phys. Rev. B 27, 6097 (1983); Phys. Rep. 127, 234 (1985).
4. H. de Raedt and A. Lagendijk, Z. Phys. B: Condens. Matter 65, 43 (1986).
5. C. Alexandrou and R. Rosenfelder, Phys. Rep. 215, 1 (1992).
6. P. E. Kornilovitch, Phys. Rev. Lett. 81, 5382 (1998); Phys. Rev. B 60, 3237 (1999).
7. N. V. Prokof’ev and B. V. Svistunov, Phys. Rev. Lett. 81, 2514 (1998); A. S. Mishchenko, N. V. Prokof’ev, A. Sakamoto, and B. V. Svistunov, Phys. Rev. B 62, 6317 (2000).
8. A. Macridin, G. A. Sawatzky, and M. Jarrell, Phys. Rev. B 69, 245111 (2004).
9. M. Hohenadler, H. G. Evertz, and W. von der Linden, Phys. Rev. B 69, 024301 (2004).
10. H. Fröhlich, H. Pelzer, and S. Zienau, Philos. Mag. 41, 221 (1950); H. Fröhlich, in Polaron and Excitons, editors C. G. Kuper and G. D. Whitfield (Plenum Press, New York, 1963), p. 1, and references therein.
11. T. Holstein, Ann. Phys. 8, 325 (1959); Ann. Phys. 8, 343 (1959).
12. P. E. Kornilovitch, Phys. Rev. Lett. 84, 1551 (2000).
13. A. S. Mishchenko and N. Nagaosa, Phys. Rev. Lett. 93, 036402 (2004).
14. A. S. Alexandrov and P. E. Kornilovitch, Phys. Rev. Lett. 82, 807 (1999); P. E. Kornilovitch, Phys. Rev. B 59, 13531 (1999); P. E. Spencer, J. H. Samson, P. E. Kornilovitch, and A. S. Alexandrov, Phys. Rev. B 71, 184310 (2005).
15. J. P. Hague, P. E. Kornilovitch, A. S. Alexandrov, and J. H. Samson. [cond-mat/0509059] (to be published).
16. R. P. Feynman, Phys. Rev. 97, 660 (1955).
17. R. P. Feynman, Statistical mechanics (Benjamin, Reading, 1972), chapter 8.
18. H. de Raedt and A. Lagendijk, Phys. Rev. B 30, 1671 (1984).
19. M. Zoli, Phys. Rev. B 71, 184308 (2005).
20. M. Born and K. Huang, Dynamical theory of crystal lattices (Oxford, Clarendon Press, 1954).