Polaron effective mass from Monte Carlo simulations

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(7 January 1997)

A new Monte Carlo algorithm for calculating polaron effective mass is proposed. It is based on the path-integral representation of a partial partition function with fixed total quasi-momentum. Phonon degrees of freedom are integrated out analytically resulting in a single-electron system with retarded self-interaction and open boundary conditions in imaginary time. The effective mass is inversely proportional to the covariance of total energy calculated on an electron trajectory and the square distance between ends of the trajectory. The method has no limitations on values of model parameters and on the size and dimensionality of the system although large statistics is required for stable numerical results. The method is tested on the one-dimensional Holstein model for which simulation results are presented.

PACS numbers: 63.20.Kr, 71.38.+i

The polaron problem is a classic problem of condensed-matter physics \cite{1,2}. In recent years it has attracted additional attention in relation to high-temperature superconductivity \cite{3}. Currently active theoretical research is being conducted by various methods on models with strong electron-phonon phonon interaction as well as on models with both electron-phonon and electron-electron interaction such as Hubbard-Holstein and $t-J$-Holstein models. The Monte Carlo simulation method is widely used in these studies \cite{4} because it provides unbiased information about thermodynamic and dynamic properties of the system even in regions of model parameters hardly accessible by standard theoretical tools.

The polaron problem was among the first applications of the Quantum Monte Carlo method after its introduction in condensed-matter physics in the Seventies. In simulations of many-polaron systems either both the positions of the electrons and the ions are simulated \cite{5,6} or the electrons are integrated out analytically and only the phonon subsystem is simulated \cite{7}. For the single-polaron problem, De Raedt and Lagendijk \cite{8} developed an effective algorithm in which phonon degrees of freedom are integrated out analytically by the Feynman technique \cite{9}. This results in a single-electron problem with retarded self-interaction along the imaginary-time direction. Since a system with only one degree of freedom can be easily simulated by the Metropolis Monte Carlo algorithm \cite{10} this method provides accurate results for thermodynamic polaron properties such as internal energy and specific heat and on other static quantities of interest, for instance the electron-phonon correlation function. Unfortunately, the estimation of dynamic properties with this method, such as the polaron spectrum, is much more difficult, the reason being that this would require an analytic continuation of simulation results from the imaginary-time to the real-time domain. This procedure is mathematically ill-posed and is thus very sensitive to the statistical noise in the input data. In previous work \cite{11} we have applied the singular-value decomposition technique to carry out such a continuation. However, due to the narrowing effect \cite{12} the polaron band is expected to be very narrow, especially in the strong-coupling regime, and the bandwidth smaller than the accuracy with which the polaron spectrum could be obtained by analytic continuation.

In this paper we show that despite these difficulties the polaron effective mass, which is defined as an inverse second derivative of internal energy with respect to quasi-momentum in the limit of zero temperature, can be obtained directly from Monte Carlo simulations without going to real time. This possibility is based on a special kind of fluctuation-dissipation relation and resembles Feynman’s calculation of the Fröhlich polaron effective mass \cite{13} and the method of calculation of the superfluid fraction in liquid helium \cite{14}.

Our starting point is the fact that total quasi-momentum $P$ is a conserved quantity in an electron-phonon system. Since states with different $P$ do not mix during the evolution it is meaningful to calculate a partial partition function $Z_P$ which is a sum over states with fixed $P$:

$$Z_P = \sum_n \langle n | e^{-\beta H} | n \rangle \delta_{P,P_n}. \quad (1)$$

Here $H$ is the Hamiltonian, $\beta = 1/k_B T$, $n$ numbers states of a complete basis in the Hilbert space and $P_n$ is the total quasi-momentum of state $| n \rangle$. The total partition function is obviously $Z = \sum_P Z_P$. The total Hilbert space is a direct product of the one-electron $\{ k \}$ and the phonon Hilbert spaces. The latter in turn can be divided into subspaces $\{ n_{ph}^Q \}$ with fixed total phonon quasi-momentum $Q$. We rewrite (1) as follows

$$Z_P = \sum_k \sum_Q \sum_{n_{ph}^Q} \langle k, n_{ph}^Q | e^{-\beta H} | n_{ph}^Q, k \rangle \delta_{P, k+Q}. \quad (2)$$

We have used a momentum-space basis because the conservation of quasi-momentum is conveniently written in
momentum space. However, matrix elements of the evolution operator $\exp(-\beta H)$ are easily calculated in real space [3]. Therefore, our first goal is to transform Eq.(3) to a real-space basis. We do this in two steps. Firstly, introducing the Wannier basis for the electron $|r\rangle = N^{-1/2} \sum_k e^{i k r} |k\rangle$ and exercising the delta-function one gets

$$Z_P = \frac{1}{N} \sum_{r,r'} \sum_Q e^{i(P-Q)(r'-r)} \sum_{n_{ph}^Q} \langle n_{ph}^Q | e^{-\beta H} | n_{ph}^Q, r \rangle$$

where $N$ is the total number of sites in the lattice. Secondly, we introduce a new basis for the phonon states in terms of ion configurations $|\xi_i\rangle$, $i = 1, \ldots, N$. Such a configuration represents a state where $i$-th ion is displaced from its equilibrium position by distance $\xi_i$. (For simplicity we assume only one phonon degree of freedom per lattice site). These states are normalised as follows

$$\langle \xi_i | \xi_i' \rangle = \left\{ \begin{array}{ll}
1 & |\xi_i' - \xi_i| < \frac{\Delta r}{2} \\
0 & \text{otherwise}
\end{array} \right.$$}

Insertion of the identity twice into $Z_P$ yields

$$Z_P = \frac{1}{N} \sum_{r,r'} e^{i P(r'-r)} \int_{-\infty}^{\infty} D\xi \langle \xi_i' | e^{-\beta H} | \xi_i \rangle \cdot W$$

$$W = \sum_Q e^{-i Q(r'-r)} \sum_{n_{ph}^Q} \langle \xi_i | n_{ph}^Q | n_{ph}^Q \rangle \langle \xi_i' | n_{ph}^Q \rangle.$$

The quantity $W$ can now be simplified by the following argument. Let us expand configuration $|\xi_i\rangle$ in a Fourier series over states with definite wave vectors $q$: $|\xi_i\rangle = N^{-1/2} \sum_q a_q e^{i q R_i} |q\rangle$. By $|q\rangle$ we mean a state in which the $i$-th ion is displaced from its equilibrium position by distance $\xi_i$. That is, if we write $q$ as a wave of classical displacement of the $i$-th ion, we mean a wave with wave vector $q$ and the unit amplitude. Now comes an important observation which is crucial for the whole method. The only component of the latter expansion which survives projection onto $|n_{ph}^Q\rangle$ is the one with $q = Q$. Although $|q\rangle$ is a wave of classical displacements with no definite phonon occupation numbers its expansion in quantum states $|n_{ph}\rangle$ would contain only those with total quasi-momentum $Q = q$ (this is simply because both the classical and the quantum states must belong to the same irreducible representation of the translation group). It is convenient to take care of this property by introducing an extra summation over the lattice $\delta_{Q,q} = N^{-1} \sum_m e^{im(Q+q)}$. Now configurations $|\xi_i\rangle$ and $|\xi_i'\rangle$ are automatically projected on the subspace with total quasi-momentum $Q = q$ and the sum $\sum_{n_{ph}^Q} \langle n_{ph}^Q | n_{ph}^Q \rangle$ in Eq.(3) may be replaced by the unity operator. With these transformations $W$ takes the form

$$W = \frac{1}{N^3} \sum_Q e^{-i Q(r'-r)} \sum_{m,m'} e^{i Q(m'-m)} \times$$

$$\sum_{q,q'} a_q^* a_{q'} e^{-i q (R_i-m)} e^{i q' (R_i-m')} \langle q | q' \rangle =$$

$$= \frac{1}{N^2} \sum_{m,q,q'} a_q^* a_{q'} e^{-i q (R_i-m)} e^{i q' (R_i-m+r'-r)} \langle q | q' \rangle =$$

$$= \frac{1}{N} \sum_m \langle \xi_i-m | \xi_i-m+r'-r \rangle = \prod_{i=1}^N \delta(\xi_i - \xi_i') \delta(r_i-r'_{i}).$$

Deriving this result we have first summed over $Q$, then transformed from $|q\rangle$ states back to $|\xi_i\rangle$ states and finally used normalization of the latter. Substitution of Eq.(3) into Eq.(5) and integration over $\xi_i'$ leads now to the final result

$$Z_P = \frac{1}{N} \sum_{r,r'} e^{i P(r'-r)} \int_{-\infty}^{\infty} D\xi \langle \xi_i' | e^{-\beta H} | \xi_i \rangle \cdot W$$

Thus, unlike the total partition function, the partial partition function with fixed $P$ is a sum over all imaginary-time trajectories with open boundary conditions. Moreover, the boundary conditions for the electron and the phonons are correlated. If the final position of the electron (i.e. at imaginary time $\tau = 0$) is shifted from the initial one (at $\tau = \beta$) by $\Delta r = r' - r$ then the final phonon configuration should be obtained from the initial one by shifting the latter by the same $\Delta r$ along the lattice. Each $Z_P$ receives contributions from trajectories with all possible $\Delta r$. Obviously, Eq.(5) satisfies the condition $\sum P Z_P = Z$.

The importance of the conservation of total quasi-momentum in the polaron problem was first recognized by Lee, Low and Pines [3] who used a canonical transformation to eliminate electron coordinates from the problem. Here we follow a different strategy, namely to eliminate phonon degrees of freedom in the spirit of the De Raedt and Lagendijk's method. The resulting single-electron problem can be simulated by Monte Carlo. Unfortunately, the complex factor $e^{i P(r'-r)}$ appearing in Eq.(5) makes it impossible to simulate the system at arbitrary $P$ due to the complex trajectory weight. However, there is no sign-problem at $P = 0$. This fact may be used, for instance, for more accurate estimation of polaron ground state energy from the Monte Carlo method.

In this paper we would like to point out the possibility of calculating polaron effective mass, which arises from equation (1). One can define the partial internal energy in the usual manner as $U_P = -Z_P^{-1} \partial Z_P / \partial \beta$. In the limit of zero temperature $U_P$ is reduced to the lowest eigenvalue with quasi-momentum $P$. Then the inverse effective mass is (up to factor $h^2$) a second derivative of $U_P$ with respect to a chosen component of $P$: $1/m_a^\ast = \partial^2 U_P / \partial P_a^2 |_{P=0}$. From Eq.(5) we have

$$\frac{1}{m_a^\ast} \propto - \langle (r_a' - r_a)^2 E \rangle - \langle (r_a - r_a') (E) \rangle |_{P=0} \quad (6)$$
where $E$ is the value of the energy estimator calculated on the trajectory which begins at $r$ and ends at $r'$ and $\langle \ldots \rangle$ means the Monte Carlo average over an ensemble of such trajectories, e.g. $\langle E \rangle |_P = U_P$. Thus, the polaron effective mass is inversely proportional to the covariance of energy of the trajectory and the square distance between ends of the trajectory. Its value can be obtained directly from Monte Carlo simulations of the equilibrium system with open boundary conditions at $P = 0$.

We point out that, on the semi-intuitive level, the relation between the width of the electron trajectory and the polaron effective mass was used previously to demonstrate the increase of the latter [3]. In the present paper, however, such a relation, Eq. (6), is derived rigorously.

In order to test this method we now consider the one-dimensional Holstein polaron problem [14]. In this model the phonon subsystem is a chain of non-interacting oscillators with frequency $\omega$ and the electron interacts linearly only with the oscillator it currently occupies. The model Hamiltonian reads

$$H = H_1 + H_2 + H_3$$

$$H_1 = -t \sum_i \left( c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1} \right); \quad H_2 = \sum_i \frac{\tilde{p}_i^2}{2m}$$

$$H_3 = \sum_i \frac{m\omega^2}{2} \xi_i^2 - \tilde{g} \sum_i c_i^\dagger c_i \xi_i.$$

Here $H_1$ represents electron kinetic energy, $t$ being the nearest-neighbour hopping amplitude, $m$ is the oscillator reduced mass, $\xi_i$ is the displacement of $i$-th oscillator, $\tilde{p}_i = -i\hbar \partial / \partial \xi_i$, and $\tilde{g}$ is the electron-phonon coupling constant. The rest of the notation is standard. In what follows periodic boundary conditions in real space are assumed.

To be able to use the Monte Carlo method one needs a path-integral representation of the matrix element $G$ which appears in Eq. (6). Following the standard procedure [5] we divide the imaginary-time dimension (whose extent is $\beta$) into $M \gg 1$ intervals, insert the resolution of the identity $M-1$ times, then use the Trotter decomposition and evaluate all the matrix elements of the operator $e^{-\beta/M}H$ to get

$$G = c_1 \sum_{\{x_j\}} \int_0^\infty \prod_{i=1}^N \prod_{j=0}^{M-1} d\xi_{ij} \int_0^\infty \prod_{j=0}^{M-1} I(x_{j+1} - x_j) e^{-S_{ph}} e^{-\sum_{j=0}^{M-1} I(x_{j+1} - x_j)}$$

$$I(x_{j+1} - x_j) = \frac{1}{N} \sum_{k_n} \cos \left[ k_n (x_{j+1} - x_j) \right] e^{2\pi \tau \cos k_n}. \quad (8)$$

Here $\{x_j\}$ is an electron trajectory in imaginary time with boundary conditions $x_0 = x, x_M = x'$; $k_n$ are single-particle momenta allowed in a chain of $N$ sites: $k_n = 2\pi n/N$, $n = 0, \ldots, N-1$; $\tau \equiv \beta t/M$ and $S_{ph}$ is the phonon action [5].

$$S_{ph} = \sum_{i=1}^N \sum_{j=0}^{M-1} \left[ \frac{m}{2\tau \hbar^2} (\xi_{i,j+1} - \xi_{ij})^2 + \tau \hbar \omega^2 \xi_{ij}^2 - \tilde{g} \xi_{ij} \delta_{ij,x_j} \right]$$

(9)

In Ref. [8] polaron thermodynamics were studied. There the following result was obtained for the integral over $\xi$s with periodic boundary conditions $\xi_M = \xi_0$

$$\int_{-\infty}^\infty D\xi \ldots = Z_{ph} \exp \left[ \sum_{j=0}^{M-1} \sum_{j'=0}^{M-1} F(j-j') \delta_{x_j,x_{j'}} \right]$$

(10)

where $Z_{ph}$ is the partition function of free phonons and $F(j - j')$ is the memory function

$$F(j-j') = \frac{\hbar^2 g^2}{4M} \sum_{l=0}^{M-1} \frac{\cos \frac{2\pi l}{M}(j-j')}{1 - \cos \frac{2\pi l}{M} + \frac{\hbar\omega^2}{2}}$$

(11)

with $g^2 \equiv \hbar^2 \tilde{g}^2 / m^4$ and $\tilde{\omega} \equiv \hbar \omega / t$. In our case one has to perform the integration over $\xi$s with twisted boundary conditions $\xi_{i+x'-x,M} = \xi_{i,0}$. Having done this, however, we found that, as long as the condition $\beta\hbar\omega \gg 1$ is satisfied, the final result for $x' - x \neq 0$ acquires only exponentially small corrections relative to Eqs. (10)-(11). The details of the calculation are cumbersome and will be published elsewhere [13].

Thus, in the low-temperature limit the path-integral representation of the partial partition function for the model (7) has the form

$$Z_P = \frac{1}{N} \sum_{\{x_j\}} e^{i P(x' - x)} \rho(\{x_j\})$$

(12)

$$\rho(\{x_j\}) = \prod_{j=0}^{M-1} I(x_{j+1} - x_j) e^{\sum_{j,j'=0}^{M-1} F(j-j') \delta_{x_j,x_{j'}}}.$$
of the simulation results. We observed such a dependence in the small-polaron regime \( g \geq 2.5 \). For these values of \( g \) a \( 1/M^2 \)-scaling was used to extrapolate to \( M = \infty \). In the beginning of each series of measurements we used 50,000 \( \cdot M \) single-particle steps to warm up the system. After that consecutive measurements were taken every \( M \) steps. For each set of parameters from six to nine series of \( 2 \cdot 10^6 \) and \( 3 \cdot 10^6 \) measurements were made.

Results of the simulations averaged over the different series are shown in Fig.1. The effective mass increases exponentially with the coupling constant, reaching \( m^* \sim 100 m_0 \) in the small polaron regime \( g > 2.5 \). In spite of the large number of measurements statistical errors are not small but decrease with \( g \). This reflects the nature of the object simulated. In the absence of electron-phonon coupling the electron trajectory is very flexible and its ends fluctuate strongly. As the interaction is turned on the trajectory becomes more and more rigid. This is because trajectories with straight segments acquire exponentially large weights (see Eq.(12)) and dominate the sampling. Also shown in Fig.1 is the result of Ref. [10] (see also [11,14]) for the inverse effective mass (or the polaron bandwidth) \( m_0/m^* = \exp(-g^2/2\omega^3) \). In the intermediate-coupling regime \((1.0 < g < 2.5)\) at \( \omega = 1.0 \) the Monte-Carlo polaron mass is lighter than \( \exp(g^2/2) \), which is in agreement with exact diagonalization of finite clusters [1].

In conclusion, we have developed a Monte Carlo algorithm for calculating polaron effective mass. It is based on the representation of the partition function with fixed quasi-momentum as a path-integral with open boundary conditions in imaginary time. The boundary conditions for the electron and phonon subsystem are correlated. After analytical elimination of phonon degrees of freedom the resulting single-electron system with retarded self-interaction can be simulated by Monte Carlo at zero total quasi-momentum. The polaron effective mass turns out to be inversely proportional to the covariance of the energy of the electron trajectory and the square distance between ends of the trajectory. The method does not impose any particular limitations on the size and dimensionality of the system and on values of the model parameters provided a low enough temperature can be reached to satisfy the condition \( \beta \hbar \omega \gg 1 \). We have tested the method on the one-dimensional Holstein model and obtained physically reasonable results. Statistical errors do not appear to be small and large statistics might be required to get stable numerical results.

We are thankful to Prof. A. S. Alexandrov for attracting our attention to this problem and to V. Kabanov and E. Klepfish for numerous and helpful discussions.

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