Polaron density matrix and effective mass at finite temperature

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(Received 1 March 1999)

We calculate the density matrix elements of the polaron using Feynman's variational method. The density matrix is diagonalized, and the eigenvalues and eigenfunctions are derived. These results and the calculated density matrix are used to evaluate the root-mean-square (rms) displacements R_β and the effective mass (EM) m^* for various values of coupling strengths between electron and medium and of the temperature. We find that EM is related to the rms displacement. The temperature dependence of the EM is in qualitative agreement with experiment. [S0163-1829(99)08333-2]

I. INTRODUCTION

The concept of the polaron was first introduced by Landau[1] and subsequently developed by Fröhlich.[2,3] Extensive reviews on this subject are now available.[4–9] The polaron is an electron moving in a polar or ionic cystal together with the self-induced polarization of the lattice. Several methods exist for calculating the effective mass (EM) of the polaron. In the past, most works on polarons were devoted to calculating the ground-state energy and the effective mass of the polaron at zero temperature. Analytical results are available for these properties only for the limit of small and large values of electron-phonon coupling strengths.[10–16] The theory of Tyablikov[17] can prove results for both the weak-coupling as well as strong-coupling limits, but the method cannot resolve intermediate coupling behavior. Feynman's celebrated path integral[18,19] theory of the polaron[20] provides an excellent interpolation between the small and large electron-phonon coupling strengths. Recently,[21] the polaron spectrum $E(k)$ has been extracted using a diagrammatic Monte Carlo (MC) method from the asymptotic decay of the Green's function.

Different definitions and approximations lead to different dependences of the EM of the polaron on temperature. Some theories[7,22–24] predict that the EM of the polaron increases with increasing temperature, while other theories[10,25–27] lead to an EM that decreases with increasing temperature.

In the present paper we calculate the EM of the polaron from the density matrix at various temperatures which shows that the EM decreases with increasing temperature. In this work the qualitative behavior of the effective mass is in accordance with the experimental behavior.[28] To our knowledge this is the first evaluation of the temperature dependence of the EM for the polaron from the density matrix.

We have shown that the diagonalization of the density matrix yields eigenvalues and eigenvectors.[29] In this paper, we first calculate the density matrix of the polaron and then use this density matrix to calculate the eigenstates of the polaron. From the values of eigenfunctions and eigenvalues, we calculate various properties of the polaron including its EM and the root-mean-square (rms) displacement (correlation length). The EM found here obeys the definition

$$\frac{1}{m^*}=\left.\frac{\partial^2 E\mathbf{P}_t}{\partial \mathbf{P}_t^2}\right|_{P_t=0}, \tag{1.1}$$

where $\mathbf{P}_t$ is the total momentum of the electron plus the deformation created by it which moves along with it. This definition differs from the one used by Saitoh[25] in which a fictitious driving force acting on the electron was introduced in the action functional and the effective mass was calculated from the acceleration rate against the force.

The paper is organized as follows. We derive the expression for a density matrix of the polaron in Sec. II. We calculate the mean-square displacement in imaginary time and effective mass for various values of coupling constants (α) and β in Sec. III. This paper ends with a conclusion in Sec. IV.

II. POLARON DENSITY MATRIX

Let us begin with the Frölich Hamiltonian[2,3] for an electron in a polar crystal. We take all the optical phonons to have the same frequency and be equal to ω. The Frölich Hamiltonian is

$$H=\frac{\mathbf{P}^2}{2m}+\sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\frac{1}{\sqrt{V}}\sum_{\mathbf{k}}[c(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})a_{\mathbf{k}}+\text{H.c.}]. \tag{2.1}$$

Here $a_{\mathbf{k}}^{\dagger}$ and $a_{\mathbf{k}}$ are the operators which create and annihilate a phonon with wave vector $\mathbf{k}$ and energy $\hbar\omega_{\mathbf{k}}$, $\mathbf{P}$ and $\mathbf{r}$ are electron momentum and position operators, m is its band mass, and V is the volume of the system. The coupling strength between electron and phonon is expressed as

$$c(\mathbf{k})=\frac{c}{\mathbf{k}}, \tag{2.2}$$

where

$$c=-i\hbar\omega(\hbar/2m\omega)^{1/4}(4\pi\alpha)^{1/2},$$

and α is the coupling strength of the electron-phonon interaction. The dimensionless Frölich coupling constant is given by

$$\alpha=\frac{1}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\frac{e^2}{\hbar\omega}\left(\frac{2m\omega}{\hbar}\right)^{1/2},$$

where $-e$ is the electron charge, and ϵ_∞ and ϵ_0 are high frequency and static dielectric constants.

The action corresponding to the Frölich Hamiltonian [Eq. (2.1)] is

$$S=\frac{m}{2\hbar}\int_0^{\beta\hbar}dt|\dot{\mathbf{r}}(t)|^2-\frac{|c|^2}{4\pi\hbar^2}\int_0^{\beta\hbar}dt\int_0^{\beta\hbar}ds\,\frac{G(|t-s|)}{|\mathbf{r}(t)-\mathbf{r}(s)|}, \tag{2.3}$$

where

$$G(|t-s|)=\frac{\exp(|t-s|\omega)+\exp\{[\beta\hbar-|(t-s)|]\omega\}}{2\exp(\beta\hbar\omega-1)}. \tag{2.4}$$

For the above action [Eq. (2.3)] the path integral has not yet been evaluated exactly. Only approximate methods have been applied. The density matrix for the polaron can be written as

$$\rho(\mathbf{r},\mathbf{r}';\beta\hbar)=\int D\mathbf{r}(t)\exp\{-S[\mathbf{r}(t)]\}. \tag{2.5}$$

The density matrix also cannot be evaluated exactly; therefore, the first cumulant approximation is used to evaluate the density matrix.[30] To evaluate the density matrix by this approximation one has to choose a reference action S_0 for which the density matrix ρ_0 can be evaluated exactly. The exact expression for the density matrix can be written as

$$\rho(\mathbf{r},\mathbf{r}';\beta\hbar)=\rho_0(\mathbf{r},\mathbf{r}';\beta\hbar)\langle\exp(-[S-S_0])\rangle_{S_0}, \tag{2.6}$$

where

$$\rho_0(\mathbf{r},\mathbf{r}';\beta\hbar)=\int D\mathbf{r}(t)\exp\{-S_0(\mathbf{r}[t])\}. \tag{2.7}$$

The average on the right-hand side (RHS) of Eq. (2.6) can be expanded in cumulant, and if $S_0[\mathbf{r}(t)]$ is taken to be quadratic, only the first two cumulants are nonzero. Feynman's variational approach is confined to the first cumulant, and the density matrix is given by

$$\rho(\mathbf{r},\mathbf{r}';\beta\hbar)\cong\rho_0(\mathbf{r},\mathbf{r}';\beta\hbar)\exp[-\langle S-S_0\rangle_{S_0}]. \tag{2.8}$$

We choose the most general two-time quadratic action[31] in the present work. This action has parameters which are determined by minimizing the free energy. For the present work we take the trial action as

$$S_0=\frac{m}{2\hbar}\int_0^{\beta\hbar}dt|\dot{\mathbf{r}}(t)|^2+\frac{1}{2(\beta\hbar)^2}\int_0^{\beta\hbar}dt\int_0^{\beta\hbar}ds\;\gamma(t-s)\mathbf{r}(t)\cdot\mathbf{r}(s), \tag{2.9}$$

where γ has to fulfill the requirement

$$\int_0^{\beta\hbar}dt\;\gamma(t-s)=0\quad\text{for }0\leqslant t\leqslant\beta\hbar.$$

The action S is translationally invariant, i.e., $\gamma(t-\beta\hbar)=\gamma(t)$ for any t within $0\leqslant t\leqslant\beta\hbar$. The kernel ρ_0 is the sum of all possible paths which connect $\mathbf{r}$ and $\mathbf{r}'$ in time $\beta\hbar$. One can regard this as a straight line between $\mathbf{r}$ and $\mathbf{r}'$ plus all possible fluctuations around a straight line which vanishes at the end points. The fluctuations around the straight path are represented as a Fourier series. Therefore, the path can be written as

$$\mathbf{r}(t)=[\mathbf{r}+(\mathbf{r}'-\mathbf{r})t/\beta\hbar]+\mathbf{b}_0+\sum_{n=1}^{\infty}[\mathbf{b}_n\exp(i\Omega_n t)+\mathbf{b}_n^{\star}\exp(-i\Omega_n t)], \tag{2.10}$$

where $\Omega_n=2\pi n/\beta\hbar$, and b_n^* is complex conjugate of b_n. Thus the paths are labeled by the Fourier coefficients b_n and the sum over paths can be reduced to an integration over all coefficients b_n $(=b_n^r+ib_n^i)$ which satisfy the condition

$$\mathbf{r}(0)=\mathbf{r}\quad\text{and}\quad\mathbf{r}(\beta\hbar)=\mathbf{r}'.$$

By using Eq. (2.10) we have ρ_0 in the form

$$\rho_0(\mathbf{r}',\mathbf{r};\beta\hbar)=T\exp[-(\mathbf{r}-\mathbf{r}')^2Q]. \tag{2.11}$$

where

$$T=\left[\frac{1}{2\pi\lambda_e^2}\right]^{3/2}\prod_{n=1}^{\infty}\left[\frac{4\pi^2n^2}{\gamma_n\lambda_e^2+4\pi^2n^2}\right]^3, \tag{2.12}$$

$$\lambda_e^2=\frac{\beta\hbar^2}{m},$$

$$Q=\left[\frac{m}{2\beta\hbar^2}+\sum_{n=1}^{\infty}\frac{\gamma_n}{[4\pi^2n^2+\lambda_e^2\gamma_n]}\right], \tag{2.13}$$

$$\gamma_n=\frac{1}{\beta\hbar}\int_0^{\beta\hbar}dt\,\gamma(t)\exp(i\Omega_n t)=\gamma_{-n}. \tag{2.14}$$

We now calculate $\langle(S-S_0)\rangle_{S_0}$, where $\langle X\rangle_{S_0}$ is defined by

$$\langle X\rangle_{S_0}=\frac{\int X\exp(-S_0)d\mathbf{r}(t)}{\int\exp(-S_0)d\mathbf{r}(t)}.$$

From Eqs. (2.3) and (2.9) we get

$$-\langle(S-S_0)\rangle_{S_0}=\frac{|c|^2}{4\pi^2\hbar^2}\int_0^{\beta\hbar}dt\int_0^{\beta\hbar}ds\;G(|t-s|)\times\int\frac{d^3k}{2\pi^2k^2}\langle\exp\{i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(s)]\}\rangle_{S_0}+\left\langle\frac{1}{2(\beta\hbar)^2}\int_0^{\beta\hbar}dt\int_0^{\beta\hbar}ds\;\gamma(t-s)\times\mathbf{r}(t)\cdot\mathbf{r}(s)\right\rangle_{S_0}. \tag{2.15}$$

Finally, we obtain

$$-\langle (S-S_0)\rangle_{S_0} = \frac{2|c|^2}{4\pi^2\hbar^2}\int_0^{\beta\hbar} dt \int_0^{\beta\hbar} ds\, G(|t-s|) \times \int_0^{\infty} dk \frac{\sin[k(r'-r)E]}{k(r'-r)E}\exp(-k^2F) + (\mathbf{r}'-\mathbf{r})^2 G + 3H. \quad (2.16)$$

The propagator for polaron in the variational approximation therefore reduces to

$$\rho(\mathbf{r}',\mathbf{r};\beta\hbar) = T\exp[-Q(\mathbf{r}'-\mathbf{r})^2]\exp[-\langle (S-S_0)\rangle_{S_0}]. \quad (2.17)$$

E, F, G, and H in Eq. (2.16) are defined as

$$E = \frac{t-s}{\beta\hbar} + 2\lambda_e^2 \sum_{n=1}^{\infty} \frac{\gamma_n \cos[\Omega_n(t+s)/2]\sin[\Omega_n(t-s)/2]}{\pi n[4\pi^2 n^2 + \lambda_e^2\gamma_n]}, \quad (2.18a)$$

$$F = 2\lambda_e^2 \sum_{n=1}^{\infty} \frac{1-\cos[\Omega_n(t-s)]}{[4\pi^2 n^2 + \lambda_e^2\gamma_n]}, \quad (2.18b)$$

$$G = \sum_{n=1}^{\infty} \frac{4\pi^2 n^2 \gamma_n}{[4\pi^2 n^2 + \lambda_e^2\gamma_n]^2}, \quad (2.18c)$$

$$H = \sum_{n=1}^{\infty} \frac{\lambda_e^2\gamma_n}{4\pi^2 n^2 + \lambda_e^2\gamma_n}. \quad (2.18d)$$

Minimizing the free energy, one gets

$$\gamma_n = \frac{|c|^2}{12\pi^{3/2}\hbar^2}\int_0^{\beta\hbar} dt \int_0^{\beta\hbar} ds \times \frac{G(|t-s|)\{1-\cos[\Omega_n(t-s)]\}}{\left[2\lambda_e^2 \sum_{n=1}^{\infty} \frac{1-\cos[\Omega_n(t-s)]}{4\pi^2 n^2 + \lambda_e^2\gamma_n}\right]^{3/2}}. \quad (2.19)$$

We calculate γ_n numerically for various α and β values, and then calculate free energy and effective mass.

III. RESULTS AND DISCUSSIONS

A. Density matrix of the polaron

In this section we first calculate self-consistently the values of γ which represent the coupling between the electron and the medium. Figure 1(a) shows the natural logarithm of γ_n/n versus n for $\alpha=7$ and 3 at $\beta=0.25$, and Fig. 1(b) shows the same for $\beta=1$. We can write $\gamma_n = A_n n$, where A_n is smoothly decreasing function of n. From Figs. 1(a) and (1b) it is clear that as β increases, i.e., as the temperature decreases, the coupling between the electron and the medium decreases, while the coupling between the electron and the medium increases with increasing α.

Using these values of γ_n, we calculate the density matrix for the polaron for various α and β. In the numerical calculation we adopt units such that $\hbar=\omega=m=k_B=1$.

From Eqs. (2.16) and (2.17) it is clear that the polaron density matrix $\rho(\mathbf{r},\mathbf{r}';\beta\hbar)$ has the form

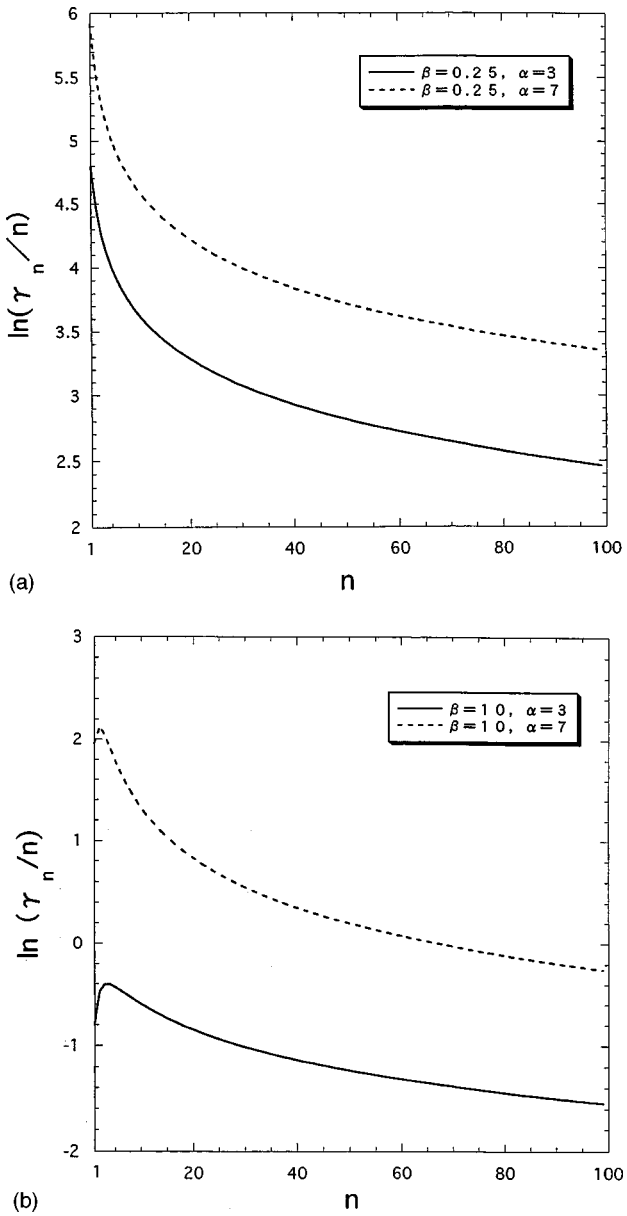

FIG. 1. Natural logarithm (base e) of the fully self-consistent variational constants $\ln(\gamma_n/n)$ for (a) $\alpha=3$ and $\alpha=7$ at $\beta=0.25$ and (b) $\alpha=3$ and $\alpha=7$ at $\beta=10.0$. γ_n is in units of the inverse length squared. It is an even function of n, and it is defined here only for integer n. It is zero at $n=0$.

$$\rho(\mathbf{r},\mathbf{r}';\beta\hbar) \propto \exp\left[-\frac{(\mathbf{r}-\mathbf{r}')^2}{\mu}\right]. \quad (3.1)$$

Here μ is a constant and is related to the EM. We expand the density matrix in terms of Legendre polynomials as

$$\rho(\mathbf{r},\mathbf{r}';\beta\hbar) = \sum_l \frac{(2l+1)\rho_l(r,r',\beta\hbar)}{4\pi rr'} P_l(\cos\theta). \quad (3.2)$$

From Eq. (3.2) we get

$$\rho_l(r.r';\beta\hbar) = 2\pi rr' \int_{-1}^{+1} \rho(\mathbf{r},\mathbf{r}';\beta\hbar) P_l(\cos\theta) d(\cos\theta). \quad (3.3)$$

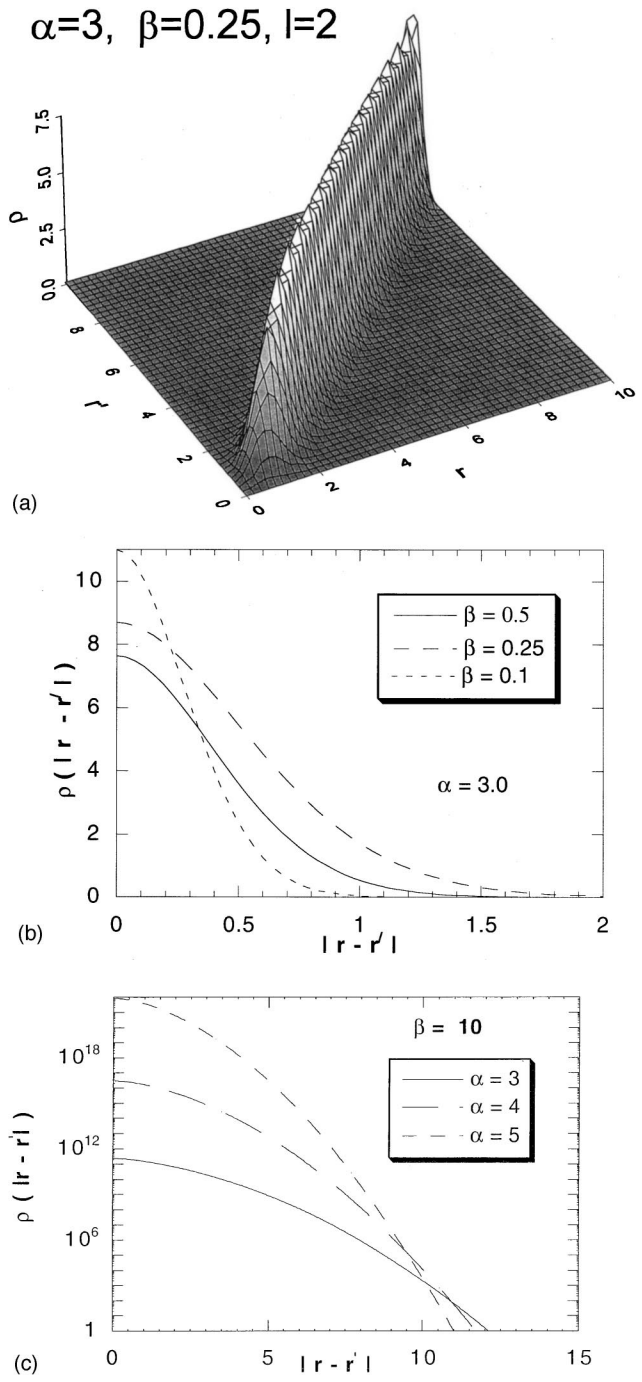

FIG. 2. (a) Density matrix plotted as a function of r and r' for $l=2$, $\alpha=3$, and $\beta=0.25$. (b) $\rho(\mathbf{r},\mathbf{r}';\beta\hbar)$ as a function of $|\mathbf{r}-\mathbf{r}'|$ for several values β at $\alpha=3.0$. (c) $\rho(\mathbf{r},\mathbf{r}';\beta\hbar)$ as a function of $|\mathbf{r}-\mathbf{r}'|$ for several values α at $\beta=10.0$.

$\rho_l(r,r';\beta\hbar)$ is calculated at various values of r and r' for a particular value of l. We plot the density matrix as a function of r and r' in Fig. 2(a). The diagonal part of Fig. 2(a) is the measure of partition function of the polaron. We observe from Fig. 2(a) that as r and r' increase the density matrix decreases very rapidly, which is evident from Eq. (3.2). In Figs. 2(b) and 2(c) we plot the density matrix as a function of $|\mathbf{r}-\mathbf{r}'|$ for various values of α and β. From Fig. 2(b) it is clear that as α increases (i.e., coupling between electron and the medium increases) the density matrix tends towards the δ function, and also from Fig. 2(c) it is evident as β tends to zero the density matrix tends towards the δ function.

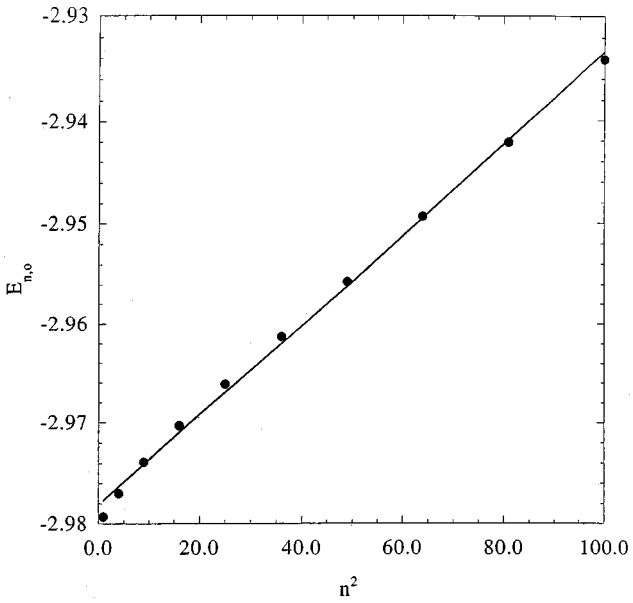

FIG. 3. Energy eigenvalues of the polaron as a function of square of level number at $l=0$.

B. Eigenenergies of the polaron

For a particular value of l, $\rho_l(r,r';\beta\hbar)$ is calculated at various values of r and r' in the form of a $(M+1)\times(M+1)$ square matrix, where M is the number of mesh with spacing Δ between 0 and L with $(4/3)\pi L^3=V$ being the size of the system. Sethia *et al.*[29] have shown earlier that the numerical accuracy of the energies and wave function calculated from $\rho_l(r,r';\beta\hbar)$ depends on the values of L and Δ. Since we use the complete density matrix, the parameter $\beta\hbar/P$ defined in Ref. 29 does not appear in the present calculation. In the calculation, one should take L large compared to λ_e and Δ should be as small as possible. After a few trials we choose $\Delta=0.075$ and $L=10.0$. The matrix is diagonalized using the house-holder method.[32]

The calculated energy levels $[E_{n,l}]$ are fitted well by the general equation

$$E_{n,0}=Dn^2+E_b\,. \tag{3.4}$$

This is shown in Fig. 3 in which we plot $E_{n,0}$ as a function of n^2 for $\alpha=3$ and $\beta=10.0$. Similar behavior is found for other values of α and β. The eigenstates found here are identical to those of a particle in a box moving in a constant attractive potential because of the translational invariance of the action [Eq. (2.3)]. The value E_b represents the strength of this potential and can be thought to represent the binding energy of the electron with the local disturbance it has created in the medium. The constant D in the above equation is related to the effective mass m^* of the polaron. This is in accordance with the definition given by Eq. (1.1).

C. Effective mass

The shape of the eigenvectors again supports the contention that the electron behaves as if it is a free particle in a box with effective mass $m^*\geqslant m$. This is due to the fact that the

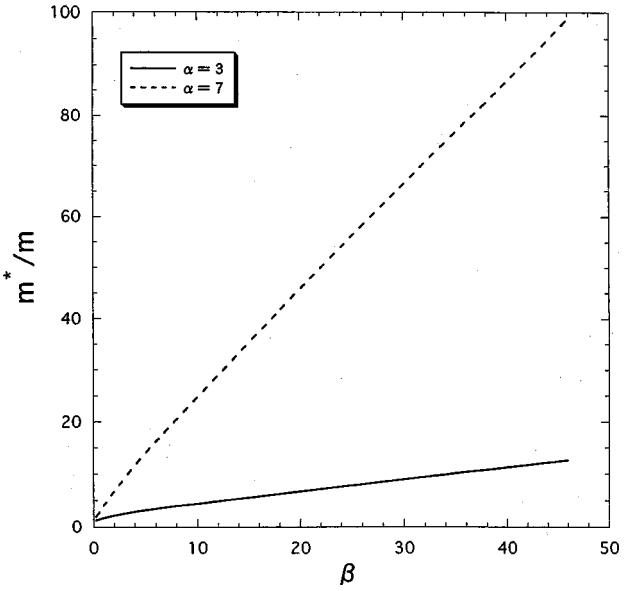

FIG. 4. Effective mass as a function of β for $\alpha=3$ (solid line) and $\alpha=7$ (dotted line).

electron drags along with it the disturbance it has created in the medium. Comparison of Eq. (3.4) with eigenvalues of a particle in a box leads to the relation

$$\frac{m^*}{m}=\frac{\lambda_e^2(\pi/L)^2}{2\beta D}, \tag{3.5}$$

where L is the radius of the sphere which we have used to truncate the elements of the density matrix. In principle, it is necessary to use a large size of the system. i.e., $L\gg\lambda_e$. We have used for all our calculations a value of $L=15.0$, which is much larger than any λ_e considered by us. The values of m^* and E_b reported here are independent of the values of L. Figure 4 shows the variation of the EM with β for $\alpha=3$ and 7. It is clear from Fig. 4 that the EM depends on the coupling α. As α increases, the electron has to drag more deformation and appears heavier.

To have a physical insight into the origin of E_b and m^*, let us consider a simple action

$$S_{nlho}=\frac{1}{2}\frac{m}{\hbar}\int_0^{\beta\hbar}dt|\dot{\mathbf{r}}(t)|^2+\frac{m\omega_{nl}^2}{4\beta\hbar^2}\times\int_0^{\beta\hbar}dt\int_0^{\beta\hbar}ds[\mathbf{r}(t)-\mathbf{r}(s)]^2, \tag{3.6}$$

characterizing a nonlocal harmonic oscillator. The density matrix for this action is well known,[33]

$$\rho_{nlho}(\mathbf{r},\mathbf{r}';\beta\hbar)=\left[\frac{m}{2\pi\beta\hbar^2}\right]^{3/2}\left(\frac{\omega_{nl}\beta\hbar}{2\sinh(\frac{1}{2}\omega_{nl}\beta\hbar)}\right)^3\times\exp\left\{-\frac{m\omega_{nl}}{4\hbar}(\mathbf{r}-\mathbf{r}')^2\coth(\omega_{nl}\beta\hbar/2)\right\}. \tag{3.7}$$

Diagonalization of ρ_{nlho} leads to the eigenspectrum of the form of Eq. (3.4). One can understand the origin of E_b and m^* by rewriting the Eq. (3.7) as

$$\rho_{\mathrm{nlho}}(\mathbf{r},\mathbf{r}';\beta\hbar)=\left[\frac{\hat{m}}{2\pi\beta\hbar^2}\right]^{3/2}\exp\left[-\beta\hat{E}_b-\frac{\hat{m}}{2\beta\hbar^2}(\mathbf{r}-\mathbf{r}')^2\right], \tag{3.8}$$

where

$$\frac{\hat{m}}{m}=\left[\frac{1}{2}\omega_{nl}\beta\hbar\coth\left(\frac{1}{2}\omega_{nl}\beta\hbar\right)\right]^3 \tag{3.9}$$

and

$$\hat{E}_b=-\frac{1}{\beta}\ln\left[\frac{\beta\hbar\omega_{nl}}{\sinh(\beta\hbar\omega_{nl})}\right]^{3/2} \tag{3.10}$$

for a nonlocal harmonic oscillator. Note that the action S given by Eq. (2.3) also characterizes a nonlocal harmonic oscillator with time (imaginary time) dependent spring constant. Because the system is translationally invariant, we do not find eigenvalues and eigenfunctions corresponding to the internal motion. The quantity $\hat{E}_b$ is in fact the contribution due to the internal motion of the polaron.

D. Mean-square displacement

Physically interesting quantities like the mobility and diffusion are intimately related to the mean-square displacement in real time. However, for imaginary time $\beta\hbar$, the mean-square displacement is defined as

$$R^2(\beta\hbar)\equiv R_\beta^2=\langle|\mathbf{r}(\beta\hbar)-\mathbf{r}(0)|^2\rangle. \tag{3.11}$$

The averaging in Eq. (3.11) is with respect to the density matrix $\rho(\mathbf{r},\mathbf{r}':\beta\hbar)$; i.e., we can write R_β^2 as

$$R_\beta^2=\frac{\int\rho(\mathbf{r},\mathbf{r}';\beta\hbar)(\mathbf{r}-\mathbf{r}')^2d\mathbf{r}\,d\mathbf{r}'}{\int\rho(\mathbf{r},\mathbf{r}';\beta\hbar)d\mathbf{r}\,d\mathbf{r}'}. \tag{3.12}$$

In Fig. 5 we plot R_β as a function of β and α. These trends are expected. As β increases (i.e., temperature decreases), the polaron will be more and more confined; i.e., R_β decreases, while as α increases again R_β decreases. Note that for a particular value of α, a larger β has a smaller R_β.

Since the nature of $E_{n,l}$ and $\psi_n(\mathbf{r})$ found from the density matrix suggests that the polaron behaves like a free particle with effective mass m^*, therefore the density matrix ρ should be Gaussian, i.e.,

$$\rho(\mathbf{r},\mathbf{r}';\beta\hbar)\propto\exp\left[-\frac{(\mathbf{r}-\mathbf{r}')^2}{2\lambda_e^2(m/m^*)}\right]. \tag{3.13}$$

Comparing Eq. (3.13) with Eq. (3.1) shows that μ is related to the EM as

$$\mu=2\lambda_e^2\frac{m}{m^*}.$$

Therefore, R_β must be related to the effective mass as

$$R_\beta=\lambda_e\left[\frac{m}{m^*}\right]^{1/2}. \tag{3.14}$$

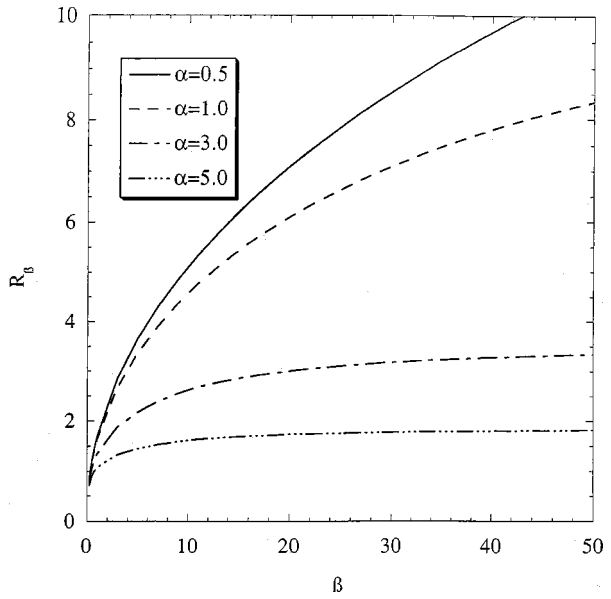

FIG. 5. Root-mean-square displacement as a function of β for various values of α.

The temperature dependence of the effective mass is in accordance qualitatively with the experimental behavior. However, quantitatively there is some discrepancy between theory and experiment. This is attributed to the following three reasons: (i) the acoustical phonon may play a role, (ii) Feynman's polaron model is a continuum model, and (iii) the structure of the medium has not been taken into account.

IV. CONCLUDING REMARKS

From the reported results it is clear that the polaron behaves almost like a free particle with effective mass m^* in a constant potential well. The potential well created by the electron in the medium leads to binding of the electron with the local disturbance. The wave functions have the symmetry of the translational invariance of the action of the system.[34] Because of this invariance we were not able to extract the eigenvalues and wave functions of the internal states themself, i.e., the states representing the binding of the electron with the local disturbance created by the electron itself. What we got are values of E_b and m^* which reflect the result of the internal states. It is, however, possible to explicitly break the symmetry by adding a potential energy term of the form $\frac{1}{2}\chi\mathbf{r}^2$ to the action of Eq. (2.3) and consider the behavior in the limit $\chi\rightarrow 0$.[35]

According to Sophn,[36] the EM defined by Eq. (1.1) is equivalent to

$$\frac{1}{m^*}=\frac{\langle|\mathbf{r}(\beta\hbar)-\mathbf{r}(0)|^2\rangle}{3\beta\hbar^2}. \tag{4.1}$$

Based on the calculation and discussion of the present work, we recommend that Eq. (4.1) should be used for the definition of the effective mass.

Saitoh[25] has calculated the EM by introducing a fictitious driving force $\mathbf{f}$ acting on the electron in the Hamiltonian or action and derived the effective mass from a term involving $\mathbf{f}^2$ in the expression of the free energy. This led to the following expression for the EM:

$$\frac{m}{m_s^*}=24\sum_{n\geqslant 1}\frac{1}{4\pi^2n^2+\gamma_n\lambda_e^2}. \tag{4.2}$$

The value m_s^* calculated from this equation is significantly smaller than that of the present work. This can be understood from the fact that the external field acts only on the electron and accelerates it. The associated medium deformation is not affected by the field. Therefore, the electron moves with lesser resistance offered by the medium than in the absence of an accelerating field.

ACKNOWLEDGMENTS

One of us (A.S.) thanks Professor B. L. Tembe for his critical comments, and one of us (Y.S.) acknowledges Department of Science and Technology (New Delhi), India for financial support.

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[1] L. Landau, Phys. Z. Sowjetunion **3**, 664 (1933).
[2] H. Frölich, H. Pelzer, and S. Zieman, Philos. Mag. **41**, 221 (1950).
[3] H. Frölich, Adv. Phys. **3**, 325 (1954).
[4] J. T. Devreese, in *Path Integrals and Their Application to Quantum Statistical and Solid State Physics*, edited by G. J. Papadopoulos and J. T. Devreese (Plenum, New York, 1978), pp. 315–343.
[5] J. T. Devreese, *Polarons in Ionic Crystals and Polar Seconductors* (North-Holland, Amsterdam, 1972); *Polarons and Excitons in Polar Semiconductors and Ionic Crystals*, edited by J. T. Devreese and F. M. Peeters (Plenum, New York, 1984).
[6] L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).
[7] F. M. Peeters and J. T. Devreese, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1984), Vol. 38, p. 81.
[8] T. K. Mitra, A. Chatterjee, and S. Mukhopadhyay, Phys. Rep. **153**, 91 (1987).
[9] *Polarons and Applications*, edited by V. D. Lakhno (Wiley, Chichester, 1994).
[10] K. Arisawa and M. Saitoh, Phys. Status Solidi B **120**, 361 (1983).
[11] G. Höhler and A. M. Mullensiefen, Z. Phys. **157**, 159 (1959).
[12] J. Röseler, Phys. Status Solidi **25**, 311 (1969).
[13] D. M. Larsen, Phys. Rev. **172**, 967 (1968).
[14] D. M. Larsen, Phys. Rev. B **29**, 3710 (1984).
[15] S. J. Miyake, J. Phys. Soc. Jpn. **38**, 181 (1975).
[16] A. L. Kholodenko and K. F. Freed, Phys. Rev. B **27**, 4586 (1983); **29**, 3711 (1984).
[17] S. V. Tyablikov, Zh. Eksp. Teor. Fiz. **25**, 688 (1953).
[18] R. P. Feynman, Rev. Mod. Phys. **20**, 367 (1948).
[19] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
[20] R. P. Feynman, Phys. Rev. **97**, 660 (1955).
[21] N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. Lett. **81**, 2514 (1998).

[22] V. K. Fedyanin and C. Rodriguez, Phys. Status Solidi B **110**, 105 (1982).
[23] F. M. Peeters and J. T. Devreese, Phys. Rev. B **25**, 7302 (1982).
[24] Y. Osaka, J. Phys. Soc. Jpn. **21**, 423 (1966); K. Okammoto and S. Takeda, *ibid.* **37**, 333 (1974).
[25] M. Saitoh, J. Phys. Soc. Jpn. **49**, 878 (1980); M. Saitoh and K. Arisawa, J. Phys. Soc. Jpn. Suppl. A **49**, 675 (1980).
[26] E. A. Kochetov and M. A. Smondyrev, Teor. Mat. Fiz. **47**, 375 (1981) [Theor. Math. Phys. **47**, 524 (1981)].
[27] M. Saitoh, J. Phys. Soc. Jpn. **49**, 886 (1980); K. Arisawa and M. Saitoh, Phys. Lett. **82A**, 462 (1981).
[28] A. Hirano and T. Masumi, Solid State Commun. **63**, 439 (1987).
[29] A. Sethia, S. Sanyal, and Y. Singh, J. Chem. Phys. **93**, 7268 (1990); **96**, 2428(E) (1992).
[30] R. P. Feynman, *Statistical Mechanics: A Set of Lectures* (Benjamin, Reading, MA, 1972).
[31] P. M. Platzman, in *Polarons and Excitons*, edited by C. G. Kuper and G. D. Whitfield (Oliver and Boyd, Edinburg, 1963); K. K. Thornber, Phys. Rev. B **3**, 1929 (1971).
[32] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in Fortran* (Cambridge University Press, New York, 1986).
[33] V. Bezak, Proc. R. Soc. London, Ser. A **315**, 339 (1970).
[34] V. Sa-yakanit, Phys. Rev. B **57**, 8739 (1998).
[35] M. P. A. Fisher and W. Zwerger, Phys. Rev. B **34**, 5912 (1986).
[36] H. Sophn, Ann. Phys. (N.Y.) **175**, 278 (1987).