Polaron effective mass

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(Received 5 January 1987; revised manuscript received 21 September 1987)

Adequacy of various definitions of polaron effective mass m^* is examined. The expression for m^* obtained by using the zero-temperature kernel is compared with the zero-temperature limit of the temperature-dependent effective mass obtained by employing the finite-temperature kernel. We find that consistent results are obtained when Saitoh's definition is employed. Our calculations are illustrated for a simple case of weak electron-phonon interaction.

The polaron problem[1-3] has continued to attract the attention of physicists[4-18] since the concept was first introduced by Landau[1] and subsequently developed by Fröhlich[2,3] Extensive reviews on the subject are now available.[19-22] Briefly, a polaron is an electron in a polar crystal moving together with the self-induced polarization of the lattice. As a consequence of the electron-phonon interaction (the Fröhlich interaction) the polaron tends to have a lower energy and higher effective mass compared to that of a bare electron. Several methods exist[20] for calculating these two important parameters of the polaron, viz., the self-energy and the effective mass. Perhaps the best among these is the famous path-integral theory of Feynman,[4] which is valid for arbitrary coupling strength α of the electron-phonon interaction.

The Lagrangian of the total system consists of a sum of the Lagrangian of the free phonons, the Lagrangian of the electron, and the interaction potential between the electron and phonons. The dynamics of this system is described by a path integral over electron and phonon coordinates.[4] Moreover, the Lagrangian being quadractic in phonon coordinates, the path integration over these coordinates can be performed exactly. Further, eliminating the phonon end points, the problem reduces to the path integration of a two-time (nonlocal) effective action functional S involving only the electron coordinates and the phonon kernel $G(t-s)$:

$$s=\frac{m}{2}\int_0^\beta dt\,\dot{\mathbf{x}}^2-\frac{\sqrt{2}\alpha\pi}{\sqrt{m}}\int_0^\beta dt\int_0^\beta ds\int\frac{d^3k}{(2\pi)^3}\frac{\exp\{i\mathbf{k}\cdot[\mathbf{x}(t)-\mathbf{x}(s)]\}G(t-s)}{k^2}\ . \tag{1}$$

The explicit form of the kernel $G(t-s)$ depends on how the phonon end points are eliminated from the joint electron-phonon density matrix. The so-called zero-temperature kernel results[23] if the phonon coordinates are eliminated by averaging the density matrix with respect to the ground state of the free phonons:

$$G(t-s)=\exp(-|t-s|)\ . \tag{2a}$$

On the other hand, if the averaging is done by taking trace of the total density matrix over the phonon coordinates, one gets[6] the finite-temperature kernel

$$G(t-s)=\cosh[(\beta/2)-|t-s|]/\sinh(\beta/2)\ . \tag{2b}$$

$G(t-s)$ is a function of $\tau\equiv|t-s|$. Since for a finite τ, kernel (2b) reduces to (2a) in the limit $\beta\to\infty$, it is expected on physical grounds that the expressions for all the physical quantities associated with the polaron obtained using kernel (2b) should go over to the corresponding expressions obtained by using kernel (2a) when the suitable limit is taken. However, such a claim cannot be rigorously justified. We have found a curious result regarding the polaron effective mass. We believe that this type of anomalous result is not so well known in the context of the polaron problem. Working with the Feynman definition of the effective mass and following Feynman's variational technique, we find that the expressions for the effective mass obtained by using kernels (2a) and (2b) turn out to be quite different even in the zero-temperature limit. One is led to similar conclusions if one follows the definition of the effective mass due to Krivoglaz and Pekar.[10] However, the definition given by Saitoh[12] and subsequently employed by Castrigiano *et al.*[18] is found to be free from the anomaly mentioned above. We shall illustrate these facts by considering the case of small coupling strength α.

It is well known that for small α the expression for Feynman effective mass of a polaron is given by

$$m^*/m=1+\alpha/6\ . \quad (3)$$

We find that the above result is obtained only when one employs the kernel (2a) (also employed by Feynman in his work). On the other hand if one employs the finite-temperature kernel (2b), then m^* diverges in the zero-temperature limit. The first *nondivergent* correction turns out to be $\alpha/12$, and consequently

$$m^*/m\approx 1+\alpha/12\ . \quad (4)$$

Since the zero temperature is always to be looked upon as the limit of finite temperature, one runs into an uncomfortable situation.

Based on the use of kernel (2a) in the action (1), Feynman conjectured[4] that for small polaron velocities (i.e., in the limit of $|\mathbf{x}''-\mathbf{x}'|\to 0$ and $\beta\to\infty$), the polaron density matrix (PDM) $K(\mathbf{x}'',\beta\,|\,\mathbf{x}',0)$ would have essentially the free-particle form

$$K(\mathbf{x}'',\beta\,|\,\mathbf{x}',0)\approx A\exp[-(m^*/2\beta)\,|\mathbf{x}''-\mathbf{x}'|^2]\ . \quad (5)$$

The coefficient of $=|\mathbf{x}''-\mathbf{x}'|^2/2\beta$, expected to be a finite constant in the limit $\beta\to\infty$, in the asymptotic expression for K is then identified as the effective mass of the polaron. Although Feynman did not employ this definition but resorted to somewhat intuitive considerations[4] to obtain m^*, he used kernel (2a) and obtained expression (3), which was in agreement with the then-available perturbation-theory estimate. Subsequently, Sa-yakanit[11] studied the problem using the polaron kernel (2b). He adopted the Feynman definition (5) of m^* and has derived an expression for it which is in complete agreement with the one derived by Feynman. In particular, his expression for m^* [with the use of kernel (2b)] for small α agrees with the expression (3). This gives the impression that the Feynman effective mass is *insensitive* to kernels (2a) and (2b) and apparently agrees with one's physical intuition. We demonstrate below that this is far from the truth.

Following Feynman we shall evaluate the PDM corresponding to the action (1) within the so-called first-cumulant approximation. Since we want to demonstrate the difference between the results for m^* for kernels (2a) and (2b) we shall restrict attention to the case of small α. For this case, a free-particle trial density matrix is adequate. Hence we shall approximate the PDM as

$$K(\mathbf{x}'',\beta\,|\,\mathbf{x}',0)=K_0(\mathbf{x}'',\beta\,|\,\mathbf{x}',0)\exp[-\langle(S-S_0)\rangle_{S_0}]\ , \quad (6)$$

where K_0 is the well-known free-particle density matrix

$$K_0(\mathbf{x}'',\beta\,|\,\mathbf{x}',0)=(m/2\pi\beta)^{3/2}\exp(-m\,|\mathbf{x}''-\mathbf{x}'|^2/2\beta) \quad (7)$$

corresponding to the trial action S_0 obtained from S of Eq. (1) by setting $\alpha=0$ and $\langle(S-S_0)\rangle_{S_0}$ has its usual meaning.[6] Thus the task of finding K within this approximation reduces to that of finding $\langle(S-S_0)\rangle_{S_0}$.

To obtain the polaron effective mass we need evaluate the asymptotic form ($\beta\to\infty$) of $\langle(S-S_0)\rangle_{S_0}$. Using the definition of $\langle\cdots\rangle$ and exploiting the symmetry of kernels (2a) and (2b) with respect to the interchange of t and s, a straightforward calculation leads to the following expression for $\langle(S-S_0)\rangle S_0$:

$$-\langle S-S_0\rangle_{S_0}=\frac{\sqrt{2}\alpha}{\sqrt{m}\,\pi}\int_0^\beta du(\beta-u)G(u)\times\int_0^\infty dk\frac{\sin(ka)}{ka}e^{-k^2b}\ , \quad (8)$$

where $a=|\mathbf{x}''-\mathbf{x}'|\,u/\beta$ and $b=u(\beta-u)/2m\beta$. The explicit form of G has thus far not been used. To express K in the form of (5) we write

$$-\langle S-S_0\rangle_{S_0}=(\alpha/\pi)(2/m)^{1/2}[Z_1+Z_2\,|\mathbf{x}''-\mathbf{x}'|^2+O(^2|\mathbf{x}''-\mathbf{x}'|^4)]\ , \quad (9)$$

where

$$Z_1=\frac{\sqrt{\pi}}{2}\int_0^\beta du\frac{(\beta-u)G(u)}{\sqrt{b}(u)} \quad (10)$$

and

$$Z_2=\frac{\sqrt{\pi}}{24\beta^2}\int_0^\beta du\frac{(\beta-u)u^2G(u)}{[b(u)]^{3/2}}\ . \quad (11)$$

The first term in the expression for $\langle S-S_0\rangle_{S_0}$, which is independent of $|\mathbf{x}''-\mathbf{x}'|$, contributes to the polaron ground state energy. The second term involving Z_2 contributes to the effective mass. Adopting the Feynman definition of m^* and using the explicit form of $b(u)$ we get

$$m^*/m=1+(\alpha/3)(\beta/\pi)^{1/2}\times\int_0^\beta[u/(\beta-u)]^{1/2}G(u)du\ . \quad (12)$$

With kernel (2a) we have $G(u)=\exp(-u)$ and we have the following closed-form expression for the integral in Eq. (12)

$$\int_0^\beta[u/(\beta-u)^{1/2}e^{-u}du=(\beta\pi/2)[I_0(\beta/2)-I_1(\beta/2)]e^{-\beta/2}\ , \quad (13)$$

where I_0 and I_1 are the modified Bessel functions. Employing the formulas for the asymptotic expansion for Bessel functions we find that the dominant contribution to the integral in expression (12) as $\beta\to\infty$ is $(\pi/4\beta)^{1/2}$. This shows that Feynman's conjecture regarding the asymptotic form of the PDM is valid for kernel (2a) and expression (3) for m^* results, in agreement with Feyman's estimate. Next consider kernel (2b). In this case the dominant contribution to the integral in Eq. (12) is no longer proportional to $1/\sqrt{\beta}$. In fact it is readily seen that

$$\int_0^\beta[u/(\beta-u)]^{1/2}\{\cosh[(\beta/2)-u]/\sinh(\beta/2\}du=\beta\pi I_0(\beta/2)/2\sinh(\beta/2)\ , \quad (14)$$

where I_0 is the modified Bessel function of order zero. Again from standard formulas for the asymptotic expansion for Bessel functions we see that the right-hand side of the above equation reduces to $(\pi\beta)^{1/2}+(\pi/16\beta)^{1/2}+O(\beta^{-3/2})$. Thus, in the case of kernel (2b), the PDM does not have the requisite asymptotic form conjectured by Feynman, because m^* diverges with β. If we retain the first nondivergent term we get the result (4). We may mention here that Sa-yakanit,[11] who also dealt with the polaron effective mass using the finite-temperature kernel (2b), inadvertently suppressed the above divergence by making a simplifying assumption. More specifically, the large-β approximation suggested by Eq. (16) of Ref. 11, viz.,

$$\int_0^\beta d\tau \int_0^\beta d\sigma\, g(|\tau-\sigma|) = 2\int_0^\beta dx(\beta-x)g(x) \approx 2\beta\int_0^\infty dx\, q(x)\ , \quad (15)$$

is valid only if $g(x)$ does not depend on β. It turns out that if one uses the correct dependence of $g(x)$ on β, Eq. (18) of Ref. 11 gets modified, indeed leading to a divergent m^*.

Apparently there seems to be no way of removing the divergent character and we may surmise that the definition of effective mass m^* portrayed by Eq. (5) is inadequate. In this context, it may be imperative to examine other definitions of m^* available in the literature.[10,12,16] Employing similar methodology as above, we find that the discrepancy between the two expressions for m^* persists for other definitions[10,16] as well, except the one given by Saitoh.[12] He considered the polaron under the influence of a vanishingly small force $\mathbf{f}$ and defined the effective mass in terms of the diagonal element of PDM as

$$K(\mathbf{0},\beta\,|\,\mathbf{0},0)=C\exp(-\beta^3\mathbf{f}\cdot\mathbf{f}/24m^*)\ . \quad (16)$$

To employ this definition one must modify the polaron action (1) and also the corresponding trial action to include a force term. A straightforward calculation leads to an expression for $\langle S-S_0\rangle_{S_0}$, which upon setting $\mathbf{x}''=\mathbf{x}'=0$ reads as

$$-\langle S-S_0\rangle_{S_0} = \frac{\sqrt{2}\alpha}{\sqrt{m}\,2\pi}\int_0^\beta dt\int_0^\beta ds\, G(t-s) \times\int_0^\infty dk\frac{\sin(k\,|A\,|f)}{k\,|A\,|f}e^{-k^2b}\ , \quad (17)$$

where $A=(t-s)(\beta-t-s)/2m$ and b is defined as before. We can write $\langle S-S_0\rangle_{S_0}$ in the form

$$-\langle S-S_0\rangle_{S_0}=(\alpha/\pi)(2/m)^{1/2}[Z_1+\mathbf{f}\cdot\mathbf{f}Z_2' +O((\mathbf{f}\cdot\mathbf{f})^2)]\ , \quad (18)$$

where after some simplification we get

$$Z_2'=-\frac{\sqrt{\pi}}{288\beta^2}\int_0^\beta du\frac{(\beta-u)^3u^2G(u)}{[b(u)]^{3/2}}\ . \quad (19)$$

This leads to an effective-mass formula

$$m/m^*=1-(\alpha/3\sqrt{\pi})(\beta)^{-3/2}\int_0^\beta\sqrt{u}\,(\beta-u)^{3/2}G(u)du\ . \quad (20)$$

The integral appearing in Eq. (20) can be evaluated in a closed form. It is equal to $(\pi\beta^2/4)e^{-\beta/2}[I_1(\beta/2)+I_2(\beta/2)]$ for kernel (2a) and $[\pi\beta^2/4\sinh(\beta/2)]I_1(\beta/2)$ for kernel (2b). Noting the asymptotic expansion of Bessel functions we see that the resulting expressions for m/m^* reduce to the correct limiting value $(1-\alpha/6)$ as $\beta\to\infty$.

Thus we see that the effective mass defined by Saitoh gives consistent results with regard to kernels (2a) and (2b). We may also add that the definition used by Peeters and Devreese[22] for the temperature-dependent effective mass is also adequate in the above sense. The reason why these two apparently different definitions[12,22] of the effective mass yield the correct value for m^* is probably due to the fact they are directly based on the response of the system under a small perturbative force. In contrast, the other definitions of the effective mass[4,10,16] are *ad hoc* and have no precise operational meaning.

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