Upper and Lower Bounds for the Intermediate-Coupling Polaron Ground-State Energy

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Using a variational ansatz in which pair correlations between wave vectors of virtually emitted phonons are taken into account, we have obtained better upper bounds to the polaron ground-state energy than have been available heretofore for $\alpha \leq 3.5$. The same variational trial functions are also used to obtain lower bounds for $\alpha \leq 2.5$. These lower bounds, although not completely rigorous, represent a considerable improvement over the Lieb-Yamazaki values, which are, to the author's knowledge, the only other lower bounds in the literature. The variational ansatz chosen is also suitable for practical calculations of the polaron effective mass.

INTRODUCTION

THE problem of finding the ground-state energy of the Fröhlich Hamiltonian has a fairly substantial literature,[1–4] mostly originating in the period 1950–1955. Aside from its intrinsic theoretical interest, there are two reasons why this problem again assumes significance.

First, effective masses have now been measured directly[5–7] by cyclotron-resonance techniques in a variety of materials in which the Fröhlich electron–LO-phonon coupling constants α lie in the intermediate coupling range $1<\alpha<4$. It is therefore of interest to obtain accurate theoretical values for the polaron contribution to the effective mass. Unfortunately, we have as yet no rigorous way of comparing the accuracy of the various published polaron effective-mass calculations. We can only assume that in comparing two approximate calculations the one giving the better ground-state energy will likely give the better effective mass. Thus we would like to have a highly accurate method of calculating the polaron ground-state energy in the region $0<\alpha<4$, particularly if this method could be readily extended to calculate effective masses.

Second, experiments on the ionization energy of bound polarons[8,9] require for their interpretation the theoretical difference in energy between the free-polaron ground state and the energy of the bound polaron. Since these energies are usually calculated separately, it is important to have good values for the free-polaron ground-state energy.

In this paper the theory of Lee, Low, and Pines[10] (LLP) is generalized to take into account correlations of the wave vectors of pairs of emitted virtual phonons. Our theory gives lower variational energies than have been obtained heretofore for $\alpha \lesssim 3.5$. Since the trial functions used are translationally invariant, our method also seems well suited for calculation of the polaron effective mass.

Surprisingly little attention has been paid to the problem of bounding the energies of low-lying polaron states from below; yet obtaining good lower bounds is a most reliable way of estimating the accuracy of a variational calculation. Using our optimized variational trial functions and the Temple lower-bound formula, we are able to obtain lower bounds for the polaron ground state for $\alpha \lesssim 2.5$. In this region we improve considerably upon the lower bounds obtained by the ingenious method of Lieb and Yamazaki.[3]

Finally, we discuss heuristically the relative accuracy of our upper and lower bounds.

VARIATIONAL UPPER BOUND

In dimensionless form the Fröhlich polaron Hamiltonian, whose ground-state wave function and eigenvalue we wish to approximate, is

$$H = p^2 + \sum n_{\mathbf{k}} + \sum \nu_k (e^{-i\mathbf{k}\cdot\mathbf{r}} b_{\mathbf{k}}^\dagger + \text{H.c.}), \qquad (1)$$

where energies are in units of the LO phonon energy, $\hbar\omega$, and length is in units of $r_0 = (\hbar/2m\omega)^{1/2}$, with m the bare mass or band mass of the electron. Momentum and wave vector are in units of $\hbar/r_0$ and $1/r_0$, respectively. The creation operator for an LO phonon of wave vector $\mathbf{k}$ is denoted by $b_{\mathbf{k}}^\dagger$, the number operator $b_{\mathbf{k}}^\dagger b_{\mathbf{k}}$ by $n_{\mathbf{k}}$, and

$$\nu_k = \left(\frac{4\pi\alpha}{\Omega/{r_0}^3}\right)^{1/2} \frac{1}{k},$$

$$\alpha = \tfrac{1}{2} \frac{e^2}{r_0} \frac{1}{\hbar\omega} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right),$$

Ω = crystal volume.

Following LLP, we take the exact ground-state wave

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function in the form

$$e^{-i\mathbf{r}\cdot\sum_{\mathbf{k}}n_{\mathbf{k}}}U\chi_0,$$
$$U=e^{\sum f_{\mathbf{k}}(b_{\mathbf{k}}^\dagger-b_{\mathbf{k}})}, \tag{2}$$

where χ_0 is a function of phonon coordinates only and f_k is a spherically symmetric function to be determined variationally. Substituting (2) into (1) gives the Schrödinger equation

$$\mathcal{H}(f)\chi_0=E_0\chi_0,$$
$$\mathcal{H}(f)=\mathcal{H}_0(f)+\mathcal{H}_1(f), \tag{3}$$

$$\mathcal{H}_0(f)=(\sum\mathbf{k}n_{\mathbf{k}})^2+\sum n_{\mathbf{k}}-\alpha',$$
$$\begin{aligned}\mathcal{H}_1(f)=&\sum[(1+k^2)f_k+\nu_k](b_{\mathbf{k}}^\dagger+b_{\mathbf{k}})\\&+2\sum(\mathbf{k}\cdot\mathbf{m})f_kf_mb_{\mathbf{k}}^\dagger b_{\mathbf{m}}\\&+\sum(\mathbf{k}\cdot\mathbf{m})f_kf_m(b_{\mathbf{k}}^\dagger b_{\mathbf{m}}^\dagger+b_{\mathbf{k}}b_{\mathbf{m}})\\&+2\sum(\mathbf{k}\cdot\mathbf{m})f_k(n_{\mathbf{m}}b_{\mathbf{k}}+b_{\mathbf{k}}^\dagger n_{\mathbf{m}}),\end{aligned} \tag{4}$$

where

$$-\alpha'=2\sum\nu_kf_k+\sum(1+k^2)f_k^2. \tag{5}$$

The LLP variational ansatz consists in approximating χ_0 by the phonon vacuum state $|0\rangle$ and minimizing $\langle0|\mathcal{H}|0\rangle$ with respect to f. This calculation gives

$$f_k=-\nu_k/(1+k^2) \tag{6}$$

and

$$\langle0|\mathcal{H}|0\rangle=-\alpha'=-\alpha.$$

One important limitation of the LLP wave function is that the probability amplitude $A_{\mathbf{kl}}$ of finding a pair of virtual phonons in the field with wave vectors $\mathbf{k}$ and $\mathbf{l}$ is

$$A_{\mathbf{kl}}=\langle\mathbf{kl}|U|0\rangle=f_kf_l\exp(-\tfrac{1}{2}\sum f_k^2), \tag{7}$$

where $|\mathbf{kl}\rangle=b_{\mathbf{k}}^\dagger b_{\mathbf{l}}^\dagger|0\rangle$ and is in our terminology a two-phonon state. Therefore, we can consider the phonons as being emitted into the single-particle state f independent of how many phonons are in the field. Intuitively we expect this approximation to be good when the electron has time to reabsorb an emitted virtual phonon before virtually emitting a second phonon, that is, when, say,

$$\bar{N}+[\langle0|U^{-1}(N-\bar{N})^2U|0\rangle]^{1/2}<1, \tag{8}$$

where

$$N=\sum n_{\mathbf{k}},\quad \bar{N}=\langle0|U^{-1}NU|0\rangle=\tfrac{1}{2}\alpha. \tag{9}$$

Evaluating the expectation value in (8), we obtain the condition

$$\tfrac{1}{2}\alpha+(\tfrac{1}{2}\alpha)^{1/2}<1 \text{ or } \alpha<\tfrac{1}{2}(\sqrt{5}-1)^2\sim0.76. \tag{10}$$

If condition (10) is seriously violated, we would expect that the electron would often emit a second phonon while still recoiling from the first emission. Under such circumstances we would anticipate significant correlation between the wave vectors of emitted phonons. Thus a proper description for somewhat larger α, satisfying, say,

$$\tfrac{1}{2}\alpha+(\tfrac{1}{2}\alpha)^{1/2}\gtrsim2 \qquad (\text{hence } \alpha\gtrsim2) \tag{11}$$

would require replacing the single-particle functions of (7) by an essentially two-particle function. To accomlish this we generalize the LLP ansatz by replacing $|0\rangle$ by $|\phi\rangle$, whose general form is given by

$$|\phi\rangle=d|0\rangle+\sum\tilde{d}_k|\mathbf{k}\rangle+\sum\tilde{d}_{\mathbf{kl}}|\mathbf{kl}\rangle. \tag{12}$$

We shall use the convention $\tilde{d}_{\mathbf{kl}}=0$ for $k>l$, and we assume $|\phi\rangle$ to be normalized.

It is obvious that (12) allows correlations between wave vectors of pairs of virtual phonons in the field. We obtain

$$\langle\mathbf{kl}|U|\phi\rangle=\exp(-\tfrac{1}{2}\sum f_m^2)[(\tilde{d}_{\mathbf{kl}}+\tilde{d}_{\mathbf{lk}})+f_kf_ld+\sigma_{kl}], \tag{13}$$

where

$$\begin{aligned}\sigma_{kl}=&f_k\tilde{d}_l+f_l\tilde{d}_k+f_kf_l(\sum f_rf_s\tilde{d}_{\mathbf{rs}}-\sum f_r\tilde{d}_r)\\&-f_k\sum f_s(\tilde{d}_{\mathbf{ls}}+\tilde{d}_{\mathbf{sl}})-f_l\sum f_s(\tilde{d}_{\mathbf{ks}}+\tilde{d}_{\mathbf{sk}}).\end{aligned}$$

Obviously any angular correlation between wave vectors of a pair of emitted phonons, if present, can only be contained in $\tilde{d}_{\mathbf{kl}}+\tilde{d}_{\mathbf{lk}}$. In deriving (13) we have made use of the identity

$$U=e^{\sum(f_mb_{\mathbf{m}}^\dagger-f_mb_{\mathbf{m}})}=e^{\sum f_mb_{\mathbf{m}}^\dagger}\,e^{-\sum f_mb_{\mathbf{m}}}\,e^{-\frac{1}{2}\sum f_m^2},$$

and in particular we have used

$$\langle0|Ub_{\mathbf{r}}^\dagger|0\rangle=-f_re^{-\frac{1}{2}\sum f_m^2},$$
$$\langle0|Ub_{\mathbf{r}}^\dagger b_{\mathbf{s}}^\dagger|0\rangle=f_rf_se^{-\frac{1}{2}\sum f_m^2}.$$

To investigate the properties of $|\phi\rangle$ further we minimize $\langle\phi|\mathcal{H}|\phi\rangle$ with respect to $\tilde{d}_k$, $\tilde{d}_{\mathbf{kl}}$, and f_k. It is easy to show that for given f the equations determining $\tilde{d}_k$, $\tilde{d}_{\mathbf{kl}}$, and $E_v(f)$, the variational energy, are given by

$$\begin{aligned}\langle0|\mathcal{H}(f)|\phi\rangle&=E_v(f)\langle0|\phi\rangle,\\\langle\mathbf{k}|\mathcal{H}(f)|\phi\rangle&=E_v(f)\langle\mathbf{k}|\phi\rangle,\\\langle\mathbf{kl}|\mathcal{H}(f)|\phi\rangle&=E_v(f)\langle\mathbf{kl}|\phi\rangle.\end{aligned} \tag{14}$$

Writing out (14) explicitly using (4) and (5), we obtain

$$E_v+\alpha'=\sum k^2f_k^2\eta(k)+\sum a_kf_kd_k, \tag{15a}$$

$$(E_v+\alpha'-1-k^2)d_k=[2k^2\eta(k)+Z(k)+a_k]f_k, \tag{15b}$$

$$\begin{aligned}[E_v+\alpha'-2-(\mathbf{k}+\mathbf{l})^2]d_{\mathbf{kl}}=&2\mathbf{k}\cdot\mathbf{l}(f_kf_l+f_ld_k+f_kd_l)\\&+2\mathbf{k}\cdot\mathbf{l}f_kf_l[\eta(l)+\eta(k)]\\&+a_kf_kd_l+a_lf_ld_k,\end{aligned} \tag{15c}$$

where $d_k=\tilde{d}_k/d$, $d_{\mathbf{kl}}=\tilde{d}_{\mathbf{kl}}/d$, (15c) is valid only for $k<l$, and

$$l^2f_l\eta(l)=\sum_{\mathbf{m}}\mathbf{l}\cdot\mathbf{m}f_m(d_{\mathbf{ml}}+d_{\mathbf{lm}}), \tag{15d}$$

$$f_lZ(l)=\sum_{\mathbf{m}}f_ma_m(d_{\mathbf{ml}}+d_{\mathbf{lm}}), \tag{15e}$$

$$f_la_l=\nu_l+(1+l^2)f_l. \tag{15f}$$

To complete the variational equations (15) we must minimize $E_v(f)$ with respect to f at fixed functions d_k and $d_{\mathbf{kl}}$ by taking the appropriate functional derivative

TABLE I. Comparison of variational energies E_v and E_f from Eqs. (18) and Feynman's calculation, respectively. Energies are in units of $\hbar\omega$. $\bar{N}_v$ is defined by $\langle\phi|U^{-1}\sum_k n_k U|\phi\rangle$ and d is defined in (12).

α	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
E_v	−0.5040	−1.0160	−1.5361	−2.0640	−2.5995	−3.1421	−3.6915	−4.2471
E_f	−0.5032	−1.0130	−1.5302	−2.0554	−2.5894	−3.1333	−3.6885	−4.2565
$\bar{N}_v$	0.258	0.532	0.822	1.126	1.442	1.768	2.100	2.436
d^2	0.9990	0.9957	0.9901	0.9817	0.9710	0.9581	0.9436	0.9280

in (15a). This gives us our final equation

$$2[\nu_k+(1+k^2)f_k]+2k^2\eta(k)f_k+(1+k^2)d_k=0. \quad (16)$$

Using definitions (15d) and (15e), Eqs. (15b) and (15c) can be easily transformed to a pair of coupled three-dimensional integral equations for η and Z. Because $d_{\mathbf{kl}}$ has the simple structure

$$d_{\mathbf{kl}}=\frac{-\mathbf{k}\cdot\mathbf{l}}{2+(\mathbf{k}+\mathbf{l})^2-E_v-\alpha'}\times\text{positive function independent of angles}, \quad (17)$$

all angular integrals are readily performed analytically, and the problem reduces to a pair of one-dimensional integral equations, which can be solved numerically by iteration. Taking an initial guess for E_v, f_k, and $d_{\mathbf{kl}}$, we iterate on η and Z until these functions become stable. We then adjust the values of E_v and f_k from (15a) and (16), respectively, and again solve for η and Z. The process is continued until self-consistency is obtained as evidenced by the stability of successive values of E_v.

Interestingly enough, we find that our optimum f_k is very close to the LLP value (6) and that the increase in variational energy due to the replacement of (16) by (6) is less than $\sim 0.1\%$ of the ground-state energy for the range $0\leq\alpha\leq 4$. If we do replace (16) by (6), our Eqs. (15) simplify considerably, for in that case $\alpha'=\alpha$ and $a_k=Z(k)=0$, giving

$$E_v=-\alpha+\sum k^2 f_k^2\eta(k), \quad (18a)$$

$$(E_v+\alpha-1-k^2)d_k=2k^2 f_k\eta(k), \quad (18b)$$

$$[E_v+\alpha-2-(\mathbf{k}+\mathbf{l})^2]d_{\mathbf{kl}}=2\mathbf{k}\cdot\mathbf{l}\{f_k f_l[1+\eta(k)+\eta(l)]+f_l d_k+f_k d_l\}. \quad (18c)$$

Because the marginal improvement afforded by Eqs. (15) and (16) seems hardly worth the additional complication, we shall consider $|\phi\rangle$ to be determined by Eqs. (18) in all subsequent discussion.

After performing the angular integrations analytically, we obtain from (18b), (18c), and (15d) the integral equation

$$\eta(l)=[l^2-h(l)]^{-1}\times\left[g(l)-\frac{\alpha}{4\pi l}\int_0^\infty dk\,\eta(k)G(k,l)\left(\frac{E_v+\alpha-1+k^2}{E_v+\alpha-1-k^2}\right)\right], \quad (19)$$

where

$$G(k,l)=[k(1+k^2)^2]^{-1}\left[-4klC+C^2\ln\left(\frac{C+2kl}{C-2kl}\right)\right],$$

$$C=2+k^2+l^2-E_v-\alpha,$$

$$g(l)=-\frac{\alpha}{4\pi l}\int_0^\infty dk\,G(k,l),$$

$$h(l)=\frac{E_v+\alpha-1+l^2}{E_v+\alpha-1-l^2}g(l).$$

The equation for E_v, (18a), becomes

$$E_v=-\alpha+\frac{2\alpha}{\pi}\int_0^\infty dk\frac{k^2\eta(k)}{(1+k^2)^2}. \quad (20)$$

As before, our procedure is to guess $\eta(l)$ and E_v, iterate (19) at fixed E_v, then recalculate E_v from (20) and repeat the process until E_v is stable. Convergence is sufficiently rapid to permit solution of (19) and (20) by hand calculation for $\alpha\lesssim 4$.

The weak-coupling limit of (19) and (20) is found by replacing C by $2+k^2+l^2$ and $k^2\eta(k)$ by $g(k)$, giving the result

$$\lim_{\alpha\to 0}E_v=-\alpha+\frac{2\alpha}{\pi}\int_0^\infty\frac{g(k)}{(1+k^2)^2}\cong-\alpha-0.015920\alpha^2. \quad (21)$$

In their paper, LLP[10] obtained essentially (21) by treating $\mathcal{H}_1(f)$ in (4) in second-order perturbation theory. However, the perturbation correction of Eq. (42) of LLP is too small by a factor of 2 and the numerical evaluation there is not accurate. Höhler and Mullensiefen[2] have also obtained result (21) by fourth-order perturbation theory in the representation of (1).

We remark that from (17) $d_{\mathbf{kl}}$ and $|d_{\mathbf{kl}}|$ both reach their maximum when $\mathbf{k}$ and $\mathbf{l}$ are antiparallel so that, at least if the coupling is not too strong, the two-phonon amplitude given by (13) is a maximum for given $|\mathbf{k}|$ and $|\mathbf{l}|$ when the magnitude of the total phonon wave vector, $|\mathbf{k}+\mathbf{l}|$, is a minimum. This result is undoubtedly a consequence of the presence of the recoil term, $(\sum \mathbf{k}n_{\mathbf{k}})^2$, in $\mathcal{H}_0$, which becomes very important when two or more virtual phonons are present in the field. We expect that for coupling strengths substantially violating (11) additional angular correlations involving three and more phonon wave vectors will assume im-

TABLE II. Comparison of lower bounds for the polaron ground-state energy from the present calculation, λ_v, with the Lieb-Yamazaki lower bounds λ_{LY}. Also compared are γ_v with the corresponding quantity from LLP, γ_{LLP}. All energies are in units of $\hbar\omega$.

α	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
λ_v	−0.5052	−1.027	−1.576	−2.172	−2.872			
λ_{LY}	−0.5227	−1.0998	−1.748	−2.487	−3.339	−4.322	−5.450	−6.730
γ_v	0.00121	0.0105	0.0381	0.0962	0.198	0.357	0.585	0.895
γ_{LLP}	0.0417	0.1667	0.375	0.667	1.042	1.500	2.042	2.667

portance in keeping the recoil term small. Whereas Eqs. (15) could readily be extended to include three and higher phonon states, the resulting integral equations to be solved become much less tractable numerically because of the difficulty of performing analytically the angular integrations.

In Table I we present a comparison of our variational upper-bound calculation and the Feynman theory[11] energies E_f for $0<\alpha\leq 4$. Note that the percentage difference between the Feynman energy and E_v decreases as α increases until E_f finally becomes lower than E_v at $3.5<\alpha<4.0$. For $\alpha>4$, E_v becomes worse and worse relative to E_f with increasing α but remains lower than the Lee-Pines energy[12] for $\alpha\lesssim 9$.

Finally, we note that Haga[13] has compared the exact results for the Gross model with a variational ansatz analogous to Eqs. (18) for that one-dimensional model. He finds substantial agreement between exact and variational answers for $\alpha\lesssim 3$ both for the ground state and low-momentum excited states.

LOWER BOUND

Our discussion of lower bounds for the polaron ground state is based upon the Temple formula, given by

$$E_0\gtrsim E_T=\langle\psi|\mathcal{H}|\psi\rangle-\gamma/(E_1-\langle\psi|\mathcal{H}|\psi\rangle)\,, \quad (22a)$$

$$\gamma=\langle\psi|\mathcal{H}^2|\psi\rangle-(\langle\psi|\mathcal{H}|\psi\rangle)^2\,, \quad (22b)$$

where E_0 is the exact ground-state energy and E_1 is the energy of the lowest lying of the exact excited states admixed in the normalized trial function $|\psi\rangle$. The inequality (22a) is valid only when $\langle\psi|\mathcal{H}|\psi\rangle<E_1$.[14]

Since we have admixed only states of zero total momentum in our trial function, we expect that $E_1\geq E_0+1$; the first excited state consists of a zero-momentum polaron with a free phonon of zero wave vector.[15] To optimize E_T we should not choose $|\psi\rangle=|\phi\rangle$, but rather we should vary our parameters d_k and d_{k1} to maximize the right-hand side of (22a). This, however, is a complicated procedure and it seems doubtful that a significant improvement could be obtained. By virtue of (14) it is a relatively simple matter to compute $\gamma_v=\langle\phi|\mathcal{H}^2|\phi\rangle-\langle\phi|\mathcal{H}|\phi\rangle^2$; moreover, γ_v, which would vanish if $|\phi\rangle$ were exact, is itself of interest since it gives a measure of how good our wave function $|\phi\rangle$ really is. Thus we obtain lower bounds λ_v from

$$E_T>\lambda_v=E_v-\gamma_v/(1+\lambda_v-E_v)\,, \quad (23)$$

where, to ensure that λ_v is in fact a lower bound, we have replaced E_1 in (22) by $1+\lambda_v$, which bounds E_1 from below.

Solving (23) gives

$$\lambda_v=\tfrac{1}{2}[-1+(1-4\gamma_v)^{1/2}]+E_v\,. \quad (24)$$

We notice from (24) that no real solutions exist for λ_v if $\gamma>0.25$. This is not a property of the general Temple formula (22a), but is rather a consequence of our lack of a sufficiently good lower bound for E_1 when $\gamma>0.25$. However, even if we had some independent lower bound β for E_0 satisfying $E_v-\beta<1$, inserting β for λ_v on the right-hand side of (23) would give a value of λ_v on the left-hand side which is lower than β when $\gamma_v>0.25$. Thus the Temple formula is useful in estimating lower bounds to the polaron ground-state energy only for α such that $\gamma\leq 0.25$.

The size of γ depends, of course, on the goodness of the wave function used to calculate it. If we use the LLP wave function in (22b), we obtain

$$\gamma_{LLP}=2\sum(\mathbf{m}\cdot\mathbf{n})^2 f_m{}^2 f_n{}^2=\tfrac{1}{6}\alpha^2\,, \quad (25)$$

which, as we shall see, is considerably larger than γ_v for $\alpha\lesssim 4$.

Equations (14) or, equivalently, the fact that $|\phi\rangle$ is the exact ground state of $\mathcal{H}$ in the subspace restricted to zero, one, and two phonon wave functions, implies

$$\gamma_v=\sum_i{}'\langle\phi_v|\mathcal{H}|i\rangle\langle i|\mathcal{H}|\phi_v\rangle\,, \quad (26)$$

where the sum $\sum_i{}'$ is restricted to intermediate states $|i\rangle$ containing three or more phonons (states of the type $|\mathbf{klm}\rangle$, $|\mathbf{klmn}\rangle$, etc.). We obtain explicitly

$$\begin{aligned}\gamma_v=\{&2\sum(\mathbf{m}\cdot\mathbf{n})^2 f_m{}^2 f_n{}^2[\textstyle\sum d_k{}^2+\frac{1}{2}\sum(d_{k1}{}^2+d_{1k}{}^2)]\\&+4\textstyle\sum(\mathbf{l}\cdot\mathbf{m})^2 f_m{}^2 f_l{}^2\eta^2(l)\\&+[\textstyle\sum l^2 f_l{}^2\eta(l)]^2\\&+\tfrac{2}{3}\alpha\textstyle\sum(k^2+\mathbf{k}\cdot\mathbf{l})(d_{k1}{}^2+d_{1k}{}^2)\\&+8\textstyle\sum(\mathbf{k}\cdot\mathbf{l})^2 f_l f_k\eta(l)(d_{k1}+d_{1k})\\&+4\textstyle\sum l^4 f_l{}^2\eta^2(l)\\&+4\textstyle\sum[2B^2(l)-2B(l)F(l)+F^2(l)]\}\\&\times(1+\textstyle\sum d_k{}^2+\sum d_{k1}{}^2)^{-1}\,,\end{aligned}$$

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[14] For a simple derivation, see, for example, T. Kinoshita, Phys. Rev. **105**, 1490 (1957).
[15] The assumption that the ground state is the only zero-momentum polaron state with energy less than E_0+1 can be proved rigorously to order α in the weak-coupling limit. For the range $0<\alpha\leq 2.5$, this assumption is at present only a conjecture which, however, the author regards as highly plausible.

where

$$B(l)=l^{-2}\sum(\mathbf{k}\cdot\mathbf{l})^2 f_k(d_{k1}+d_{1k}),$$
$$F(l)=\sum k^2 f_k(d_{k1}+d_{1k}). \quad (27)$$

In Table II we compare, where possible, λ_v and lower bounds λ_{LY} computed from the theory of Lieb and Yamazaki[3]; also compared are γ_v and γ_{LLP}. We note that λ_v becomes very close to E_v for small α, and represents, wherever calculable, a considerable improvement over λ_{LY}. Of course, the method of Lieb and Yamazaki has the advantage that it is applicable for all α.

Finally, we come to the question of fixing more precisely where in the range between E_v and λ_v the ground-state energy actually lies. Here we enter into the realm of conjecture. However, it seems clear that the true energy lies closer to E_v than to λ_v.

To justify this statement we consider the energy differences δ and ϵ defined by

$$\delta=E_0-\lambda_v,$$
$$\epsilon=E_v-E_0.$$

Defining the eigenfunctions of $\mathcal{H}$ by $\mathcal{H}\chi_i=E_i\chi_i$, we expand $|\phi\rangle$ as

$$|\phi\rangle=\sum c_i\chi_i. \quad (28)$$

Then

$$\epsilon=\sum(E_i-E_0)c_i^2. \quad (29)$$

Now consider E_T from Eqs. (22). It is not hard to see that Eqs. (22) can be rewritten

$$\langle\phi|(\mathcal{H}-E_1)(\mathcal{H}-E_T)|\phi\rangle=0=\sum(E_i-E_1)\times(E_i-E_0+\Delta)c_i^2, \quad (30)$$

where

$$\Delta=E_0-E_T.$$

Thus

$$-\Delta\sum(E_i-E_1)c_i^2=\sum(E_i-E_1)(E_i-E_0)c_i^2$$

or

$$\Delta(1-\epsilon)=\sum(E_i-E_0)^2c_i^2-\epsilon.$$

Defining

$$R_v=\sum(E_i-E_0)^2c_i^2/\sum(E_i-E_0)c_i^2$$

and

$$M_v=\sum(E_i-E_0)c_i^2/\sum_{i\neq 0}c_i^2, \quad (31)$$

it is easy to prove that $R_v>M_v$, and since from (23) we have $E_T>\lambda_v$ (and therefore $\delta>\Delta$), we can write

$$\delta/\epsilon>\Delta/\epsilon>R_v-1>M_v-1. \quad (32)$$

Presumably $|\phi\rangle$ accounts well for the admixture of one- and two-phonon eigenstates of $\mathcal{H}_0$ and χ_0. Thus we expect that, at least for $\alpha\lesssim 3$, the main contribution to $\sum_{i\neq 0}c_i\chi_i$ comes from three-phonon and higher-phonon states. Now comes the crucial assumption of our argument: The eigenstates of $\mathcal{H}$ are sufficiently similar to the eigenstates of $\mathcal{H}_0$ for $\alpha\lesssim 3$ that the main contribution to $\sum_{i\neq 0}c_i\chi_i$ comes from states χ_i corresponding to the three- and higher-phonon states of $\mathcal{H}_0$. These states χ_i, like their corresponding eigenstates of $\mathcal{H}_0$, have energies E_i-E_0 greater than ~ 3.

If this assumption is granted, we have to conclude from (31) that $M_v\lesssim 3$ and therefore from (32) that

$$\delta/\epsilon\lesssim 2. \quad (33)$$

Actually we think that (33) is conservative—we would not be surprised to find δ/ϵ greater than 3 or even 4, depending upon the value of α.

Computations of the effective mass are in progress.

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