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Asymptotic spectrum of momentum eigenstates of one-dimensional polarons

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We consider an electron interacting with acoustic phonons through the deformation potential in one dimension. By using a trial state that is an eigenfunction of momentum we show that at high momentum the velocity of the polaron approaches the speed of sound. Since the trial state that we are using is an upper bound for each momentum, the more usual quadratic energy-momentum relation is clearly eliminated.

I. INTRODUCTION

In a previous paper[1] we have studied the interaction of an electron with acoustic phonons through the deformation potential in one dimension. A major purpose of that work was to determine the energy-momentum relation for a polaron in a model which is soluble to a large degree. The energy-momentum relation in the strong-coupling regime was estimated variationally by using a trial-state vector which describes a lattice deformation centered about some arbitrary point and an electron bound in the potential well set up by that deformation. The electronic part of the trial-state vector contained a plane-wave phase factor in addition to a bound-state wave function. This phase factor then led to a nonzero expected value for the total momentum of the system. We refer to this variational theory as the moving Pekar theory, since it is an extension of the Pekar variational theory[2] which was devised originally to describe an electron self-trapped in a static-lattice deformation.

Variational energy estimates are generally useful because they are relatively insensitive to imprecise knowledge of the true energy eigenstate, and because they also provide an upper bound to the ground-state energy. Since the Hamiltonian and total momentum operator commute, the expected value of the Hamiltonian gives an upper bound to the lowest-energy eigenvalue for each value of momentum, provided the trial eigenstates are momentum eigenstates. Since the trial state in the moving Pekar theory is not a momentum eigenstate, the boundedness property at each momentum is not guaranteed in that theory.

This defect is remedied in the present work by constructing momentum eigenstates out of the moving Pekar trial states in a manner due originally to Höhler.[3] The expected value of the Hamiltonian in these momentum eigenstates is then expanded asymptotically for strong coupling. This asymptotic expansion takes a different form at small and large momentum. For $p \ll ms(4\pi\alpha)^2$, where m is the electron-band mass, s is the speed of sound, and α is the electron-phonon coupling constant, we make an effective-mass approximation to the polaron energy spectrum. The moving Pekar theory gives a self-energy and effective mass each of order α^2, while the Höhler theory gives a correction of order α to both the Pekar self-energy and Pekar effective mass. For $p \gg ms(4\pi\alpha)^2$, the polaron spectrum in the Pekar approximation is an asymptotic series in powers of $(p/ms)^{1/3}(4\pi\alpha)^{-2/3}$ with a leading term equal to sp. The Höhler theory gives an asymptotic series identical to the Pekar theory out to a term independent of p and of order α. Thus the Höhler theory verifies that the polaron energy is linear in p at large momentum.

In Sec. II we briefly review the moving Pekar theory, and in Sec. III we present the Höhler theory based on the moving Pekar theory, and construct the asymptotic expansion for strong coupling.

II. MOVING PEKAR THEORY

The system of an electron interacting with acoustic phonons in one dimension via the deformation potential is described by the Fröhlich Hamiltonian

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \sum_k a_k^\dagger a_k |k| + \left(\frac{4\pi\alpha}{l}\right)^{1/2} \sum_k (|k|)^{1/2}(a_k + a_{-k}^\dagger)e^{ikx}, \qquad (1)$$

where we use ms^2 as the unit of energy and $\hbar/ms$ as the unit of length. In Eq. (1) a_k is the boson destruction operator for a phonon of wave vector k, x is the electronic coordinate, and l is the length of the crystal lattice. The total momentum operator for the system is

$$P = -i\frac{\partial}{\partial x} + \sum_k a_k^\dagger a_k k, \qquad (2)$$

and generates translation of both the electron and lattice displacement.

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We now make a variational estimate of the system energy in a trial state:

$$|\psi_R(x)\rangle = e^{iw(x-R)}u(x-R)e^{S(R)}|0\rangle\,, \tag{3}$$

where $u(x-R)$ is an electronic wave function which describes an electron localized about a point R in the lattice. We assume that $u(x)=u(-x)$. In order for the electron momentum to then have a nonzero value, we must give the trial state a plane-wave phase factor $e^{iw(x-R)}$ which enables the electron to move through the lattice. The lattice part of the trial function is $e^{S(R)}|0\rangle$, where

$$S(R) = -S^\dagger(R) = \sum_k (d_k^* a_k e^{ikR} - d_k a_k^\dagger e^{-ikR})\,. \tag{4}$$

This lattice state describes a coherent lattice displacement (with Fourier components d_k) centered at R and thus correlated with the bound electron.

The parameters w and d_k and the functional form of $u(x)$ are now determined by minimizing the expected value of H subject to the constraints that the trial-state vector is normalized to unity and that the expected value of the momentum operator is p. We do this by introducing the Lagrange multipliers λ and v and then make

$$W = \int_{-\infty}^{\infty} dx\,\langle \psi_R(x)|(H-\lambda - vP)|\psi_R(x)\rangle \tag{5}$$

stationary. The results of the variational calculation are

$$w = v \tag{6}$$

and

$$d_k = d_k^* = \left(\frac{4\pi\alpha}{l}\right)^{1/2} \frac{(|k|)^{1/2}\rho_k}{(|k|-kv)}\,, \tag{7}$$

where

$$\rho_k = \rho_{-k} = \int_{-\infty}^{\infty} dx\, e^{ikx}u^2(x)\,. \tag{8}$$

In addition, a differential equation,

$$-\frac{1}{2}\frac{\partial^2}{\partial x^2}u(x-R) - \frac{4\pi\alpha}{l}\sum_k (|k|)^{1/2}(d_k + d_{-k}) \times e^{ik(x-R)}u(x-R) = \epsilon u(x-R)\,, \tag{9}$$

arises for the functional form of $u(x-R)$, and when d_k from Eq. (7) is introduced into this equation, we obtain

$$-\frac{1}{2}\frac{\partial^2}{\partial x^2}u(x-R) - 2\beta u^3(x-R) = \epsilon u(x-R)\,, \tag{10}$$

where

$$\beta = 4\pi\alpha/(1-v^2)\,. \tag{11}$$

Equation (10) has one bound-state solution for which

$$u(x-R) = (\tfrac{1}{2}\beta)^{1/2}\,\mathrm{sech}\,\beta(x-R)\,,\quad \epsilon = \tfrac{1}{2}\beta^2\,. \tag{12}$$

From these expressions we then calculate

$$\rho_k = (\pi k/2\beta)\,\mathrm{csch}(\pi k/2\beta)\,, \tag{13}$$

and then

$$E_p^0 \equiv \int_{-\infty}^{\infty} dx\,\langle\psi_R(x)|H|\psi_R(x)\rangle = \tfrac{1}{2}v^2 - \tfrac{1}{6}(4\pi\alpha)^2\,(1-5v^2)/(1-v^2)^3 \tag{14}$$

and

$$p = \int_{-\infty}^{\infty} dx\,\langle\psi_R(x)|P|\psi_R(x)\rangle = v + \sum_k k d_k^2 = v + \tfrac{2}{3}(4\pi\alpha)^2 v/(1-v^2)^3\,. \tag{15}$$

From these parametric equations for E_p^0 and p it follows that

$$\frac{dE_p^0}{dp} = v\,, \tag{16}$$

and v takes on the physical significance of the polaron velocity with a limiting value of 1 in velocity units of s.

III. HÖHLER THEORY

The trial-state vector in the moving Pekar theory is not a momentum eigenstate. Hence as noted above we cannot argue that E_p^0 is an upper bound at each momentum p. But consider the trial-state vector

$$|\psi_p(x)\rangle = N\int_{-\infty}^{\infty} dR\, e^{ipR}|\psi_R(x)\rangle\,, \tag{17}$$

where N is a normalization factor, so that

$$\int_{-\infty}^{\infty} dx\,\langle\psi_p(x)|\psi_p(x)\rangle = 1\,. \tag{18}$$

The state $|\psi_p(x)\rangle$ was first shown by Höhler[3] to be a momentum eigenstate. To see this we write

$$P|\psi_p(x)\rangle = N\int_{-\infty}^{\infty} dR\, e^{ipR}\left(-i\frac{\partial}{\partial x}\right)[u(x-R)e^{iv(x-R)}]e^{S(R)}|0\rangle + N\int_{-\infty}^{\infty} dR\, e^{ipR}u(x-R)e^{iv(x-R)}\sum_k a_k^\dagger a_k k e^{S(R)}|0\rangle\,. \tag{19}$$

From the general property

$$\frac{\partial}{\partial x} f(x-R) = -\frac{\partial}{\partial R} f(x-R) \tag{20}$$

and an integration by parts, we obtain

$$P\,|\psi_p(x)\rangle = p\,|\psi_p(x)\rangle + N\int_{-\infty}^{\infty} dR\, e^{ipR} u(x-R) e^{iv(x-R)} \left(\sum_k a_k^\dagger a_k k - i\frac{\partial}{\partial R}\right) e^{S(R)}\,|0\rangle \,. \tag{21}$$

It then follows from the identities

$$e^{-S(R)} a_k e^{S(R)} = a_k - d_k e^{ikR} \tag{22}$$

and

$$e^{-S(R)} i\frac{\partial}{\partial R} e^{S(R)} = i\frac{\partial}{\partial R} - \sum_k k d_k (a_k e^{ikR} + a_k^\dagger e^{-ikR}) + \sum_k k d_k^2 \tag{23}$$

that the integral term in Eq. (21) vanishes. Thus $|\psi_p(x)\rangle$ is an eigenstate of total momentum with eigenvalue p for *arbitrary* d_q, v, and $u(x)$. We then take these quantities as the ones given by the moving Pekar theory in Eqs. (7), (12), and (15). The parameter v retains its significance as the polaron velocity in the Höhler theory at high momentum to the order determined in this work.

We first determine the normalization factor N defined in Eq. (17). From Eq. (18) we obtain

$$N^{-2} = \int_{-\infty}^{\infty} dR \int_{-\infty}^{\infty} dR' \exp[i(p-v)(R-R')] \times f(R-R') g(R-R') \,, \tag{24}$$

where

$$g(R-R') = \int_{-\infty}^{\infty} dx\, u(x-R) u(x-R') = \beta r \operatorname{csch}(\beta r) \tag{25}$$

and

$$f(R-R') = \langle 0|\, e^{-S(R')} e^{S(R)}\,|0\rangle = \exp\left(-\sum_k d_k^2 (1-e^{-ikr})\right) , \tag{26}$$

with $r = R - R'$. By recalling from Eq. (15) that

$$p - v = \sum_k k d_k^2 \,,$$

we may write the normalization factor as

$$N^{-2} = \frac{2l}{\beta} \int_0^{\infty} du\, F_1(u) F_2(u) F_3(u) \,, \tag{27}$$

where the form factors $F_i(u)$ are given by

$$\begin{aligned} F_1(u) &= u \operatorname{csch}(u) \\ F_2(u) &= \exp\{-\beta[(1+v^2)/(1-v^2)] H_2(u)\} \,, \\ F_3(u) &= \cos\{\beta[2v/(1-v^2)] H_3(u)\} \,, \end{aligned} \tag{28}$$

with

$$\begin{aligned} H_2(u) &= \int_0^{\infty} \frac{dt}{\pi} \frac{1}{t} F_1^2\left(\frac{\pi t}{2}\right)[1-\cos(tu)] \,, \\ H_3(u) &= \int_0^{\infty} \frac{dt}{\pi} \frac{1}{t} F_1^2\left(\frac{\pi t}{2}\right)[tu - \sin(tu)] \,. \end{aligned} \tag{29}$$

In arriving at these expressions we have used the continuum correspondence

$$\frac{1}{l} \sum_k (\;) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} (\;)$$

and have introduced the changes of variable $u = \beta r$ and $t = k/\beta$.

In a similar way we calculate the Höhler energy

$$E_p \equiv \int_{-\infty}^{\infty} dx\, \langle \psi_p(x) | H | \psi_p(x) \rangle$$

$$= N^2 \int_{-\infty}^{\infty} dR \int_{-\infty}^{\infty} dR' \int_{-\infty}^{\infty} dx \exp[i(p-v)(R-R')] u(x-R') e^{-ivx} \langle 0 |\, e^{-S(R')} H e^{S(R)}\, | 0\rangle e^{ivx} u(x-R) \,. \tag{30}$$

This expression for the expected value of the Hamiltonian can then be cast in the form

$$E_p = E_p^0 + N^2 l \int_{-\infty}^{\infty} dr\, e^{i(p-v)r} f(r) \left[\sum_k |k|\, d_k^2 (e^{-irk} - 1) g(r) + iv\frac{d}{dr} g(r) - \left(\frac{4\pi\alpha}{l}\right)^{1/2} \sum_k (|k|)^{1/2} d_k (e^{-irk} - 1) h_k(r)\right] , \tag{31}$$

where

$$h_k(r) \equiv \int_{-\infty}^{\infty} dx\, u(x+r)u(x)e^{-ikx}$$

$$= \frac{\pi i}{2}(1-e^{ikr})\,\mathrm{csch}\left(\frac{\pi k}{2\beta}\right)\mathrm{csch}(\beta r)\,, \tag{32}$$

with $h_0(r) = g(r)$. By going to the continuum limit and changing the variables of integration as before, we obtain an expression for the deviation from the moving Pekar energy

$$\Delta E_p = E_p - E_p^0$$
$$= -\beta^2 \int_0^{\infty} du\, F_1(u)F_2(u)F_4(u) \Big/ \int_0^{\infty} du\, F_1(u)F_2(u)F_3(u)\,, \tag{33}$$

where $F_1(u)$, $F_2(u)$, and $F_3(u)$ are given in Eq. (28), and the additional form factor $F_4(u)$ is given by

$$F_4(u) = 2\left(\frac{1+v^2}{1-v^2}\right)\cos\left(\beta\frac{2v}{1-v^2}H_3(u)\right)\int_0^{\infty}\frac{dt}{\pi}F_1^2\left(\frac{\pi t}{2}\right)\sin^2\left(\frac{tu}{2}\right)$$
$$+ v\sin\left(\beta\frac{2v}{1-v^2}H_3(u)\right)\left[\int_0^{\infty}\frac{dt}{\pi}F_1^2\left(\frac{\pi t}{2}\right)\left(\frac{4\sin^2(tu/2)}{tu} - \frac{2\sin(tu)}{1-v^2}\right) + \frac{1}{\beta}\frac{d}{du}\ln F_1(u)\right]. \tag{34}$$

We are interested in corrections to E_p^0 in the limit $\beta \to \infty$ for which we require $4\pi\alpha \gg 1 - v^2$. When β is large the important contribution to the integrals in ΔE_p comes from small u. From the expansions

$$H_2(u) = c_2u^2 + \cdots, \quad H_3(u) = c_3u^3 + \cdots, \tag{35}$$

with

$$c_2 = 3\zeta(3)/\pi^3, \quad c_3 = 4\zeta(4)/\pi^4, \tag{36}$$

where $\zeta(n)$ is the Riemann ζ function, it is evident that the most rapidly varying form factor is $F_2(u)$. Since we are interested in the leading term in an asymptotic expansion for ΔE_p, we use the approximation

$$F_1(u) \simeq 1,$$
$$F_2(u) \simeq \exp[-\beta[(1+v^2)/(1-v^2)]c_2u^2], \tag{37}$$
$$F_3(u) \simeq 1,$$
$$F_4(u) \simeq 3\left(\frac{1+v^2}{1-v^2}\right)c_3u^2 - \frac{4v^2(1+v^2)}{(1-v^2)^2}\beta c_2c_3u^4,$$

from which we compute

$$\Delta E_p = -8\alpha\,\zeta(4)/\zeta(3)(1+v^2). \tag{38}$$

Finally, to determine E_p as an explicit function of p we must eliminate v between E_p and p through Eqs. (14), (15), and (16). At small momentum this elimination leads to

$$E_p = E_0 + p^2/2m^*, \tag{39}$$

where in dimensional units we have

$$E_0 = (4\pi\alpha)^2ms^2[-\tfrac{1}{6} - 0.5732(4\pi\alpha)^{-1} + \cdots],$$
$$m^* = m(4\pi\alpha)^2[\tfrac{2}{3} - 1.1464(4\pi\alpha)^{-1} + \cdots]. \tag{40}$$

In both of these expressions the second term in the brackets arises from the use of the Höhler state rather than the Pekar state. At large momentum the elimination of v between E_p and p leads to[4]

$$E_p^0 = (4\pi\alpha)^2ms^2(y - 0.655y^{2/3} - 0.0954y^{1/3}$$
$$- 0.0278 - 0.00927y^{-1/3} - \cdots)$$
$$- ms^2(0.5 - 0.0728y^{-1/3} + \cdots) \tag{41}$$

and

$$\Delta E_p = -4\pi\alpha ms^2(0.2866 + \cdots)\,, \tag{42}$$

where

$$y = p[ms(4\pi\alpha)^2]^{-1}. \tag{43}$$

It is evident that for

$$p/ms \gtrsim (4\pi\alpha)^2 \gg 1, \tag{44}$$

the corrections due to using a Höhler variational state are small in comparison with the moving Pekar theory, and in particular,

$$\lim_{p\to\infty}\frac{dE_p}{dp} = s$$

persists. The polaron is trapped below the speed of sound.

[1]G. Whitfield and P. B. Shaw, Phys. Rev. B 14, 3346 (1976).
[2]S. Pekar, J. Phys. USSR 10, 341 (1946).
[3]G. Höhler, *Lectures on Field Theory and Many Body Theory*, edited by E. F. Caianiello (Academic, New York, 1961).
[4]In Ref. 1 the coefficient of $y^{2/3}$ is incorrectly given as $\frac{1}{3}$ that of Eq. (41).