Polaron and bipolaron dispersion curves in one dimension for intermediate coupling

D. M. Eagles,[1,2,*] R. M. Quick,[2] and B. Schauer[2]
[1]*Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Apartado Postal 70-360, 04510 México Distrito Federal, Mexico*
[2]*Department of Physics, University of Pretoria, Pretoria 0002, South Africa*
(Received 28 March 2006; revised manuscript received 31 October 2006; published 6 February 2007)

Bipolaron energies are calculated as a function of wave vector by a variational method of Gurari appropriate for weak or intermediate coupling strengths, for a model with electron-phonon interactions independent of phonon wave vector and a short-ranged Coulomb repulsion. It is assumed that the bare electrons have a constant effective mass. A two-parameter trial function is taken for the relative motion of the two electrons in the bipolaron. The energies of the bipolarons are compared with those of two single polarons as a function of wave vector for various parameter values. Results for the effective masses at the zone center are also obtained. Comparison is made with data of other authors for bipolarons in the Hubbard-Holstein model, which differs mainly from the present model in that it has a tight-binding band structure for the bare electrons.

DOI: 10.1103/PhysRevB.75.054305 PACS number(s): 71.38.Mx

I. INTRODUCTION

Many authors have studied the energies of large[1–15] and small[16–43]bipolarons in various numbers of dimensions, and some have made calculations of the bipolaron effective masses at the band minimum.[6,9,10,18,29,33,35–37] However, we are not aware of published calculations of bipolaron energies as a function of wave vector which extend to large wave vectors except in the case of small bipolarons when the electron-phonon coupling is strong.[26–28] In this paper we take up the study of this problem in a one-dimensional model with local interactions by use of a variational method used by Gurari for the single-polaron problem.[44] The method is appropriate for intermediate electron-phonon coupling strengths. It was discussed in some detail in a review article by Fröhlich,[45] and, for large polarons, gives the same results for binding energies and effective masses as those obtained by Lee *et al.*[46,47] using different approaches. The Hamiltonian we shall use for the bipolaron problem is similar but not identical to that of the Hubbard-Holstein model,[22,24,48,49] and will be formulated in terms of center-of-mass and relative coordinates of two electrons rather than in terms of electron creation and annihilation operators. This permits us to follow the variational method for the single-polaron problem with only minor modifications. The biggest difference of our model from the Hubbard-Holstein model is our assumption of a constant bare mass for the electron. We have not yet found a way to apply the Gurari method to the Hubbard-Holstein model itself.

The original motivation for this work was to help to find out whether large enhancements of electron-electron attractions mediated via phonons or other intermediate bosons predicted in the simplest perturbation approach to interactions[50–54] may still occur when complications due to intermediate coupling are included. For metals with Fermi energies large compared with the energy of any boson mediating electron-electron attractions, Eliashberg theory has been used to show that the net effect of enhancements of attractions is unlikely to lead to high-temperature superconductivity at high currents in either three-dimensional[54] or quasi-one-dimensional systems.[53] However, for small Fermi energies, infinite enhancements are predicted by the simplest perturbation approach at some drift velocities in one dimension.[52,53] A study of the bipolaron problem in one dimension should give some insight into how this conclusion is modified by effects beyond perturbation theory in the limit of low concentrations of electrons. Although we shall use the term "phonon" for the boson mediating the attraction, we have in mind that interactions mediated by plasmons may be of practical importance for understanding possible high-temperature superconductivity associated with bipolarons.

There have been many published studies of bipolarons in one dimension (including studies of two-site models),[10,18,19,22,24–28,30,32–37,39,41,42] but these mostly concentrate on finding the energies for the ground state as a function of coupling strength and Coulomb repulsion. Some calculate the bipolaron effective mass at the bottom of the band, but most do not discuss how energies vary with center-of-mass wave vector well away from the band minimum, except for strong electron-phonon coupling. Hohenadler *et al.*[41] give graphical results for the spectral function of bipolarons as a function of wave vector for various cases where the coupling is not very strong, and approximate $E(k)$ curves can be deduced from these. An easier comparison to make is with some unpublished calculations performed by El Shawish for the Holstein model for some parameters corresponding roughly to some of those we have used. These values correspond to high ratios of phonon energy to electronic transfer integral t.

In Sec. II we introduce the Hamiltonian and our variational method. Some numerical results are presented in Sec. III, and some discussion is given in Sec. IV.

II. HAMILTONIAN AND VARIATIONAL METHOD

With a notation somewhat similar to that of Ref. 5 but modified to apply to one dimension and for short-range interactions, we write the Hamiltonian H for the bipolaron problem with constant bare effective masses in the form

$$H = H_X + H_u + H_p + H_{\mathrm{e-p}}. \tag{1}$$

Here H_X is the center-of-mass kinetic energy given by

$$H_X = -\tfrac{1}{2}\nabla_X^2, \tag{2}$$

where the center-of-mass coordinate

$$X = \tfrac{1}{2}(x_1 + x_2), \tag{3}$$

and x_1, x_2 are the coordinates of the two electrons; H_u is the Hamiltonian for relative motion, with

$$H_u = -2\nabla_u^2 + W(u), \tag{4}$$

where

$$u = x_1 - x_2 \tag{5}$$

is the relative coordinate and

$$W(u) = \begin{cases} P & -\frac{1}{2}a < u < \frac{1}{2}a, \\ 0 & \text{otherwise}, \end{cases} \tag{6}$$

with a the lattice constant; the phonon Hamiltonian H_{p} and the electron-phonon interaction $H_{\mathrm{e-p}}$ are given by

$$H_{\mathrm{p}} = \sum_k a_k^\dagger a_k \tag{7}$$

and

$$H_{\mathrm{e-p}} = -iV(a/L)^{1/2}\sum_k \left[2\cos\left(\tfrac{1}{2}ku\right)e^{ikX}a_k\right] + \mathrm{H.c.}, \tag{8}$$

where $a_k^\dagger$ and a_k are creation and destruction operators for phonons of wave number k and L is the length of the crystal. We use the usual reduced units, with units of energy, length, and mass equal to $\hbar\omega$, $(\hbar/2m\omega)^{1/2}$, and $2m$, respectively, where ω is the phonon angular frequency and m is the bare electron mass. The form of the potential term in H_u is similar to but not the same as that in the Hubbard model because, with the form used, two electrons within a unit cell do not always interact, but this is compensated by interactions between electrons that are in neighboring cells but separated by less than a. We do not include any spin-dependent terms in the Hamiltonian, and in the following we shall not include any terms involving electron-spin wave functions. For bipolarons we implicitly assume that the two electrons in the pair have opposite spin by choosing a wave function for relative motion which is even in the relative coordinates.

For a given center-of-mass vector Q, we adopt a trial wave function Ψ of the form

$$\Psi = L^{-1/2}e^{\mathrm{i}QX}\phi_Q(u)\prod_k \psi(Q,k,u)\chi, \tag{9}$$

where χ is the phonon or other boson vacuum,

$$\psi(Q,k,u) = N(Q,k,u)\left[1 + L^{-1/2}c(Q,k)\cos\left(\tfrac{1}{2}ku\right)e^{-\mathrm{i}kX}a_k^\dagger\right], \tag{10}$$

where $c(Q,k)$ are variational parameters, $\phi_Q(u)$ is a normalized even function

$$\int |\phi_Q(u)|^2 du = 1 \tag{11}$$

depending on one or more parameters, and $N(Q,k,u)$ is a normalization constant given by

$$N(Q,k,u) = \left[1 + L^{-1}|c(Q,k)|^2\cos^2\left(\tfrac{1}{2}ku\right)\right]^{-1/2} \simeq 1. \tag{12}$$

With such a trial wave function, calculations similar to those in Sec. IV of Fröhlich's review article[45] for single polarons give the expectation values of the different terms in H. After replacing sums by integrals with use of the replacement

$$\sum_k \mapsto \frac{L}{2\pi}\int_{-\pi/a}^{\pi/a} dk, \tag{13}$$

we find

$$\langle H_{\mathrm{p}}\rangle = \frac{1}{2\pi}\int_{-\pi/a}^{\pi/a} |c(Q,k)|^2 h_k dk, \tag{14}$$

where

$$h_k = \int |\phi_Q(u)|^2\cos^2\left(\frac{1}{2}ku\right)du, \tag{15}$$

$$\langle H_{\mathrm{e-p}}\rangle = \frac{i}{\pi}Va^{1/2}\int_{-\pi/a}^{\pi/a}[c^*(Q,k) - c(Q,k)]h_k dk, \tag{16}$$

$$\begin{aligned}\langle H_X\rangle = {} & \frac{1}{2}Q^2 - \frac{1}{2\pi}\int_{-\pi/a}^{\pi/a} Qk|c(Q,k)|^2 h_k \\ & + \frac{1}{4\pi}\int_{-\pi/a}^{\pi/a}|c(Q,k)|^2 k^2 h_k dk \\ & + \frac{1}{8\pi^2}\int\int_{-\pi/a}^{\pi/a} kk'|c(Q,k)|^2|c(Q,k')|^2 h_{kk'}dk\,dk'.\end{aligned} \tag{17}$$

Here

$$h_{kk'} = \int |\phi_Q(u)|^2\cos^2\left(\frac{1}{2}ku\right)\cos^2\left(\frac{1}{2}k'u\right)du \tag{18}$$

and

$$\langle H_u\rangle = E_u + \frac{1}{4\pi}\int_{-\pi/a}^{\pi/a}|c(Q,k)|^2 k^2(1 - h_k)dk, \tag{19}$$

where the first term is independent of the variational coefficients $c(Q,k)$. Going back to sums over k in Eqs. (14), (16), (17), and (19), by minimization of $\langle H\rangle$ with respect to $c(Q,k)$ and $c^*(Q,k)$, we find

$$c(Q,k) = \frac{-2iVa^{1/2}}{1 - (Q - h_k^{-1}G_k)k + \frac{1}{2}h_k^{-1}k^2}, \tag{20}$$

where

$$G_k = \frac{1}{2\pi}\int_{-\pi/a}^{\pi/a} k' h_{kk'} |c(Q,k')|^2 dk'$$
$$= \frac{2V^2 a}{\pi}\int_{-\pi/a}^{\pi/a} \frac{k' h_{kk'}}{\left[1-(Q-h_{k'}^{-1}G_{k'})k' + \frac{1}{2}h_{k'}^{-1}k'^2\right]^2} dk'. \tag{21}$$

From Eqs. (15) and (18),

$$h_{kk'} = \tfrac{1}{2}h_k + \tfrac{1}{2}h_{k'} + \tfrac{1}{4}h_{k+k'} + \tfrac{1}{4}h_{k-k'} - \tfrac{1}{2}. \tag{22}$$

For the purpose of determining the coefficients we will make the following approximation:

$$h_{kk'} \simeq h_k h_{k'}. \tag{23}$$

This gives

$$c(Q,k) \simeq \frac{-2iVa^{1/2}}{1-(Q-g)k + \frac{1}{2}h_k^{-1}k^2}, \tag{24}$$

where

$$g = \frac{2V^2 a}{\pi}\int_{-\pi/a}^{\pi/a} \frac{k' h_{k'}}{\left[1 - Sk' + \frac{1}{2}h_{k'}^{-1}k'^2\right]^2} dk', \tag{25}$$

with

$$S = Q - g. \tag{26}$$

From Eqs. (1), (14), (16), (17), (19), and (24), we find that the expectation value of H, which we write as $E(Q)$, is given by

$$E(Q) = \frac{1}{2}(Q^2 - g^2) - \frac{2V^2 a}{\pi}\int_{-\pi/a}^{\pi/a} \frac{h_k}{1 - Sk + \frac{1}{2}h_k^{-1}k^2} dk + \frac{2V^4 a^2}{\pi^2}$$
$$\times \int_{-\pi/a}^{\pi/a}\int_{-\pi/a}^{\pi/a} \frac{kk'(h_{kk'} - h_k h_{k'})}{\left(1 - Sk + \frac{1}{2}h_k^{-1}k^2\right)^2\left(1 - Sk' + \frac{1}{2}h_{k'}^{-1}k'^2\right)^2}$$
$$\times dk\, dk' + E_u. \tag{27}$$

Although the variational coefficients determined in this approximation do not represent the optimal choice, nonetheless the expectation value of H, $E(Q)$, yields an upper bound to the exact energy.

The part E_u of the expectation value of H_u in Eq. (19) that is independent of $c(Q,k)$ can be written as

$$E_u = T_u + V_u. \tag{28}$$

Here the relative kinetic energy T_u is given by

$$T_u = \frac{2}{2\pi}\int |f_k|^2 k^2 dk, \tag{29}$$

where f_k is given by

$$f_k = \int \phi(u) e^{iku} du. \tag{30}$$

In Eq. (29) the integral over k is, in principle, unrestricted, i.e., it is an integral over k from $-\infty$ to ∞. However, we shall restrict our trial wave functions for relative electron motion to those that do not have Fourier components for $k > k_m = \pi/a$, and for such trial wave functions we use an integral from $-k_m$ to k_m.

Writing

$$\int_{-\infty}^{\infty} |\phi(u)|^2 e^{iku} du = d_k \tag{31}$$

we have, for a trial function for which $f_k = 0$ for $|k| > k_m$,

$$d_k = \frac{1}{2\pi}\int_{-(k_m - |k|/2)}^{k_m - |k|/2} f^*_{k'-k/2} f_{k'+k/2} dk'. \tag{32}$$

Using

$$\int_{-a/2}^{a/2} e^{-iku} du = \frac{2}{|k|}\sin\left(\frac{1}{2}|k|a\right), \tag{33}$$

from Eq. (6) we find that the potential term V_u in Eq. (28) is given by

$$V_u = \frac{2P}{2\pi}\int_{-2k_m}^{2k_m} d_k\left[\sin\left(\tfrac{1}{2}ka\right)/k\right] dk. \tag{34}$$

We restrict the integral to the limits shown in Eq. (34) because d_k vanishes for $|k| > 2k_m$. Remembering that

$$\cos^2\left(\tfrac{1}{2}ku\right) = \tfrac{1}{2}[\cos(ku) + 1], \tag{35}$$

Eqs. (15) and (31) enable us to write

$$h_k = \tfrac{1}{2} + \tfrac{1}{2}d_k; \tag{36}$$

$h_{kk'}$ is then determined from Eq. (22).

We now consider a two-parameter trial function for the relative motion, with an assumed function in real space modified by replacement of all Fourier components with wave vectors of magnitude greater than k_m replaced by zero.

Pseudo-real-space function for relative motion

We consider a function that has Fourier transforms up to $|k| = k_m$ of the same form, up to a proportionality factor, as the transforms of ϕ, where

$$\phi(u) = N_0(1 + b|u|)e^{-\lambda|u|}, \tag{37}$$

with b and λ adjustable parameters, and N_0 a normalization factor. If b in the trial function is small, then the maximum of ϕ is at $u = 0$, whereas if $b > \lambda$ there are two maxima at finite $|u|$. For $|k| > k_m$, we assume that the Fourier transform of ϕ is zero. Thus, using Eq. (37), f_k of Eq. (30) is given by

$$f_k = \begin{cases} N\left(\dfrac{2\lambda}{(\lambda^2+k^2)} + \dfrac{2b(\lambda^2-k^2)}{(\lambda^2+k^2)^2}\right) & \text{if } |k| < k_m, \\ 0 & \text{if } |k| > k_m, \end{cases} \tag{38}$$

where N is a normalization factor. From $(1/2\pi)\int_{-k_m}^{k_m}|f_k|^2=1$, we find that N is given by

$$N^2 = B^{-1}N_0^2, \tag{39}$$

where

$$N_0 = (1/\lambda + b/\lambda^2 + b^2/2\lambda^3)^{-1/2} \tag{40}$$

is the normalization factor of the wave function given by Eq. (37) before imposing a restriction on the Fourier components for $|k|>k_m$, and

$$B = \frac{1}{2\pi}\int_{-k_m}^{k_m}|f_{0k}|^2, \tag{41}$$

where f_{0k} is the same as f_k but with the normalization factor replaced by N_0. The departure from unity of the integral of Eq. (41) gives the fractional change of the square of the normalization factor due to putting the Fourier transforms of ϕ for $|k|>k_m$ as zero.

From Eqs. (15) and (37), if we were to suppose that the assumption of zero Fourier transforms of ϕ for $|k|>k_m$ only affected h_k for $|k|<k_m$ via the change of normalization factor, we would find

$$\frac{h_k}{N^2} = \frac{2\lambda}{4\lambda^2+k^2} + \frac{2b(4\lambda^2-k^2)}{(4\lambda^2+k^2)^2} + \frac{2b^2(8\lambda^3-6\lambda k^2)}{(4\lambda^2+k^2)^3} + \frac{1}{2} \tag{42}$$

for $|k|\leq k_m$. We have verified that, if the integral in Eq. (32) is extended to be from $-\infty$ to ∞ then Eq. (36) gives the result of Eq. (42).

The kinetic term T_u in Eq. (28) is given by Eq. (29). If ϕ were taken as in Eq. (37) without removal of the Fourier components for $|k|>k_m$, then using Eqs. (4), (6), and (37) the potential term V_u in Eq. (28) would be

$$V_u = P\int_{-a/2}^{a/2}|\phi|^2 du = PN_0^2[(1/\lambda + b/\lambda^2 + b^2/2\lambda^3)(1-e^{-\lambda a}) - (ab/\lambda + b^2a/2\lambda^2 - b^2a^2/4\lambda)e^{-\lambda a}]. \tag{43}$$

By comparison of numerical results obtained from Eqs. (34) and (36) with those from Eqs. (42) and (43), we can find the effect of putting the Fourier components of ϕ for $|k|>k_m$ on h_k and V_u for given values of the parameters.

III. NUMERICAL RESULTS

Marsiglio[25] states that the physical region of the Hubbard-Holstein model requires a condition $\alpha^2/K<U$, where α is a factor multiplying local vibrational coordinates x_i in the electron-phonon interaction, and K appears in the expression $\frac{1}{2}Kx_i^2$ for the vibrational potential energy. If we identify Pa in our model with U, although this correspondence is not exact, the same type of condition would require that

$$2V^2 \leq Pa. \tag{44}$$

However, in attractive Hubbard models ($U<0$), the negative U is usually thought to be brought about by effects of electron-phonon interactions overcoming a positive Hubbard U, and Marsiglio's condition would appear to imply that negative-U Hubbard models are unphysical. Therefore we shall not restrict our numerical work to the region defined by Eq. (44), although in cases in which we are using our model with short-range forces as a simple approximation for effects of long-range forces we shall need to take the condition more seriously.

For our numerical calculations we consider two types of cases. First we choose parameters which may be applicable to oxidized atactic polypropylene (OAPP),[55,56] and make use of some of the parameters used previously in the model for superconductivity in channels composed of arrays of quasi-one-dimensional filaments.[53] As in Ref. 53, we take the cross section of individual filaments to be 0.25 nm^2. However, because the periodic potential due to aligned dipoles near the strings of charges forming the filaments according to the model of Grigorov *et al.*[57–59] for individual filaments may not have very deep minima, we assume here that the bare electron mass is m_e and not $2m_e$ as in Ref. 53. We consider two variants of parameters which could be applicable to OAPP. One, as in Ref. 53, where the excitations mediating the electron-electron attraction are plasmons, and the other where optical phonons of average energy 0.36 eV mediate the attraction. For the plasmon-induced interaction, we should strictly have long-ranged forces, but we hope that the model used here with short-range forces will give a first approximation to the real situation. We choose 0.36 eV for a phonon energy because there are several branches of the phonon spectrum associated with C-H_2 and C-H_3 stretching vibrations whose energies at long wavelengths lie between 0.35 and 0.37 eV.[60]

For given values of V^2, a, Q, and P, we solve for g of Eq. (25) and then minimize the total energy with respect to λ and b, using our full expressions of Eqs. (32) and (36) for h_k, Eq. (34) for V_u, and the normalization factor of Eq. (39) for f_k. For computational purposes, we made use of programs or modifications of programs from a book.[61]

In the model for strings or nanofilaments of Refs. 57–59, if there is a periodic potential acting on the electrons in the string, it is due to groups of about three aligned dipoles surrounding each electron, and so the period of the potential, or lattice constant a, is equal to the inverse of the linear electron concentration $c=nd^2$, where n is the three-dimensional concentration in the filament and d^2 is its cross section. Thus we may not be free to choose the carrier concentration and lattice constant independently. However, we note that a recent theoretical study of channels through films of oxidized atactic polypropylene making use of Bose condensation of bosons in an array of nanofilaments with an $E(K)$ curve for bosons consisting of a combination of linear and quadratic terms,[62] as indicated to occur in studies of Cooper pair dispersion,[63] did not assume a periodic potential acting on the electrons in the nanofilaments. Another constraint was

imposed in Ref. 62 because it was thought that it was probably necessary for the Fermi energy to be smaller than a quarter of the energy of the excitation mediating the electron-electron attraction in order to have the possibility of large enhancements of interactions at high drift velocities.[53] However, in view of the results of the present paper, these enhancements may not occur when calculations of electron-electron interactions go beyond second-order perturbation theory.

Bearing in mind the possible constraints, and assuming $d^2=0.25$ nm^2 and $m_b=m_e$ as discussed above, we find two values of a and the related carrier concentrations corresponding to our two possible choices of phonons or plasmons to mediate the attraction. In both cases we use parameters such that the ratio of a to the polaron radius $r_p=(\hbar/2m\omega)^{1/2}$ satisfies $a/r_p=4$. Using a value for the high-frequency dielectric constant of 2.2,[64] we find, for plasmons mediating the attraction, that $a/r_p=4$ implies $a=0.53$ nm, the linear concentration $c=1/a=1.9\times10^7$ cm^{-1}, the three-dimensional carrier concentration n within a filament is $n=7.6\times10^{21}$ cm^{-3}, the plasmon energy $\hbar\omega_p$ calculated using a three-dimensional formula appropriate for not too long wavelengths is $\hbar\omega_p=2.2$ eV, the polaron radius $r_p=0.132$ nm, and, from a one-dimensional formula, the bare Fermi energy $\epsilon_F=0.34$ eV. The values of most of these quantities are only slightly different from those used in Ref. 53. For phonons of energy 0.36 eV, $a/r_p=4$ implies $a=1.3$ nm, $r_p=0.325$ nm, $n=3.1\times10^{21}$ cm^{-3}, and $\epsilon_F=0.056$ eV.

We also consider a different type of case appropriate for a quantum wire of a crystalline material. If, e.g., we assume that $m=2m_e$ and $\hbar\omega=0.05$ eV, then the polaron radius is 0.62 nm, and a ratio $a/r_p=0.5$ would then imply a plausible value of the lattice constant of 0.31 nm. We note that, for such a small value of a/r_p, there is no point in doing calculations for very large values of Q, since the type of variational method we are using will not be appropriate when the single-polaron energy lies more than $\hbar\omega$ above the bottom of the band.[45]

Note that, when the polaron or bipolaron energy above the bottom of the band becomes close to $\hbar\omega$, the discrepancy in energy from the types of states more generally discussed (see, e.g., Refs. 26–28 and 37) becomes large. This is because our method requires one or two electrons (for polarons or bipolarons) whose average wave vector or center-of-mass wave vector is equal to the center-of-mass wave vector of the polaron or bipolaron to be present whatever the energy of the state, whereas more commonly used methods find the lowest energy of the electron-phonon system for a given center-of-mass wave vector. Such wave functions have only a small electron component at the wave vector concerned when the threshold energy for emission of phonons is approached. We think that our method is concerned with states of more physical interest than the states usually discussed in this energy region. These states, with the wave vector provided by phonons and electrons at the bottom of the band, do not help in describing what happens when a polaron or bipolaron is accelerated rapidly past the threshold for emission of phonons.

Since we are using $a/r_p=4$ for both possible parameter choices for OAPP, the same computer calculations can be used for both plasmon- and phonon-induced interactions, with only the values of quantities obtained in real units being different. Figures 1 and 2 show values of the bipolaron energy $E(Q)$, the energy $2E_s$ of two widely separated polarons each with wave vector $0.5Q$, and the parameters λ and b in the bipolaron trial function, for two values of V^2 and two related values of P for each V as a function of Q/Q_m, where

$$Q_m = 2k_m = 2\pi/a. \tag{45}$$

For small b, $1/\lambda$ is the bipolaron radius in units of the polaron radius.

Figures 3(a) and 3(b) show results of similar calculations as a function of Q for a single value of V^2 for a more limited range of Q for the much smaller value of $a/r_p=0.5$ which may be appropriate for a quantum wire of crystalline material.

The figures also show the values of g of Eq. (25) and of the parameters λ and b which are found in the numerical work. We notice that in all cases shown in Figs. 1–3, there is a monotonic rise of energies with Q.

We have also considered two other types of trial functions for relative motion, a Gaussian type of function with a second parameter in the prefactor, and a wave function constant in k space for wave vectors with magnitudes between minimum and maximum values k_1 and k_2. Both these types of trial function gave poorer results for the bipolaron energies

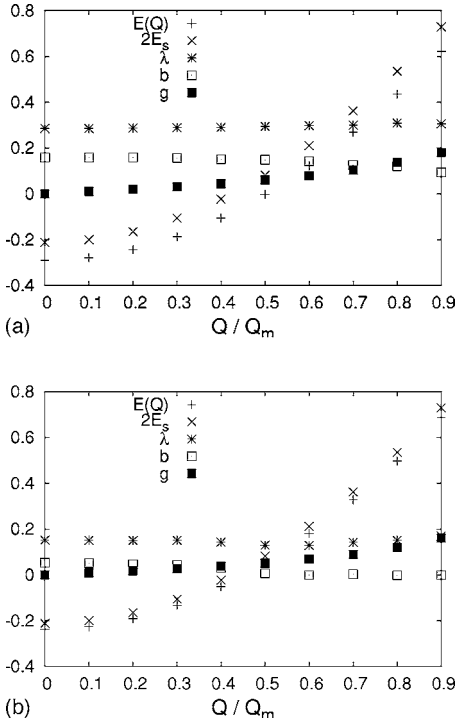

FIG. 1. Bipolaron energies $E(Q)$, the energy $2E_s$ of two widely separated single polarons, the parameters λ and b of the trial wave function for relative motion of Eq. (37), and the quantity g of Eq. (25) as a function of bipolaron wave vector Q, for $V^2=0.125$, $a=4$, and $P=$(a) 0, (b) 0.125. Energies are measured with respect to the bottom of the bare band, in units of the phonon energy. Q_m is defined by Eq. (45).

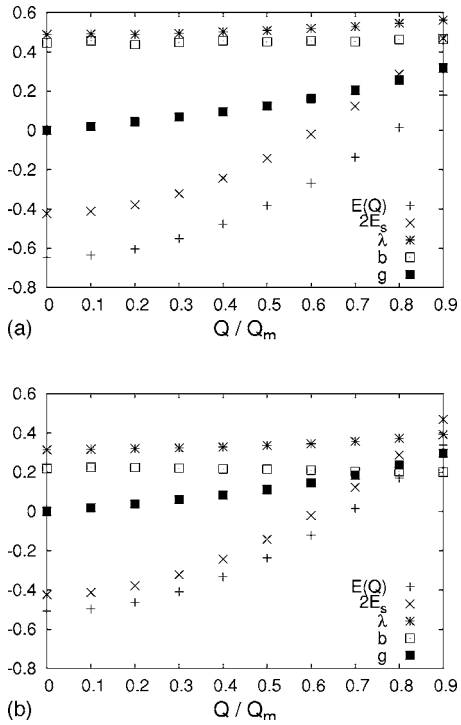

FIG. 2. As for Fig. 1, but with $V^2=0.25$, $a=4$ and $P=$(a) 0, (b) 0.25.

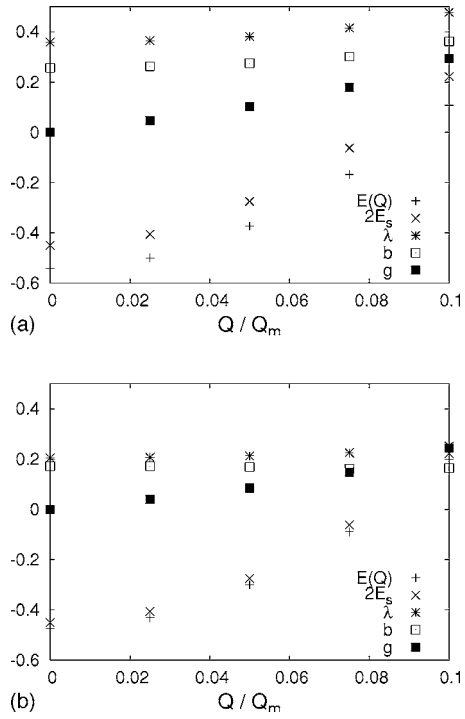

FIG. 3. As for Fig. 1, but with $V^2=1$, $a=0.5$, and $P=$(a) 0, (b) 1.

than the function used here. Also, in many cases k_1 turned out to be zero in the second type of function, and so our second parameter often did not improve matters.

IV. DISCUSSION

Bipolaron energies measured from the bottom of the bare bands for the Holstein model obtained from unpublished results of El Shawish for the case of $\hbar\omega/t=16$, $g^2=0.125$ and $\hbar\omega/t=4$, $g^2=0.5$, corresponding to $a=4$, $V^2=0.125$ and $a=2$, $V^2=0.5$ in our model, are equal to $-0.335\hbar\omega$ and $-1.22\hbar\omega$ compared with $-0.29\hbar\omega$ and $-0.92\hbar\omega$ obtained by us, and so our results are 13% and 25% smaller than those of El Shawish for the magnitudes of this quantity. The energies of two single polarons in our model for the same parameters are $-0.21\hbar\omega$ and $-0.64\hbar\omega$, and so our bipolaron binding energies are $0.08\hbar\omega$ and $0.28\hbar\omega$. Average effective masses (strictly the reciprocals of the average reciprocal masses) of bipolarons up to $Q=0.1Q_m$ in our model for the same pairs of parameters are $2.13m_b$ and $2.69m_b$, whereas the average masses over the same region of wave vectors inferred from the results of El Shawish are $2.88m_b$ and $3.05m_b$. Thus the departure of the mass from twice the single-particle mass is much larger in the results of El Shawish. For $a=4$, with $V^2=0.25$ and 0.375, bipolaron binding energies in our model are $0.22\hbar\omega$ and $0.38\hbar\omega$, respectively, while bipolaron masses for these two cases are $2.31m_b$ and $2.50m_b$. Thus we are able to get bipolaron binding energies of over a third of the phonon energy without very large effective masses.

In the limit that $a\to 0$ (with ta^2 constant), our method gives single-polaron binding energies $E_s=0.5V^2a\hbar\omega$ and effective masses m_s such that $m_s/m_b=1+0.25V^2a$. These results may be compared with those of Chen *et al.*[65] for a continuum model with short-range interactions with a single dispersionless phonon for values of V^2a up to 3 (corresponding to α up to 1.5 in their notation). For $V^2a=1$ ($\alpha=0.5$) and $V^2a=3$ ($\alpha=1.5$), from Figs. 5 and 8 of their paper we find $E_s\approx 0.52\hbar\omega$ and $E_s\approx 1.69\hbar\omega$, while their masses m_s satisfy $m_s/m_b\approx 1.2$ and 3.7 for the two values of coupling. Thus E_s for the two models differ by only 13% for $V^2a=3$, whereas masses for the two models are within 4% of each other for $V^2a=1$ (closer to 20% for the departure of m/m_b from unity), but for $V^2a=3$ the discrepancy in masses is large ($m_s/m_b=3.7$ in the model of Ref. 65, but 1.75 for our model). The larger discrepancy for masses between the two models than for the binding energies is related to the fact that intermediate-coupling methods are accurate for binding energies up to higher values of coupling constants α in the Fröhlich model than for masses.[47,66]

Another case for which we may make comparison with other authors is that of $a=1$, $V^2=1$, corresponding to $\omega/t=1$ and $g^2=1$ in the Hubbard-Holstein model. Here we find that the bipolaron energy measured from the bottom of the bare band is $-1.10\hbar\omega$, and the energy of two single polarons is $-0.80\hbar\omega$. Thus the bipolaron binding energy with respect to two single polarons is $0.30\hbar\omega$ in our model, compared with about $0.5\hbar\omega$ which can be inferred from the inset to Fig. 3 of a paper by Bonča *et al.*[35] For this case we have also found the value of Pa in our model for which the bipolaron binding energies for the above values of parameters vanish. We find the bipolaron energy vanishes for $Pa\approx 1.9$. The result of a vanishing of the binding energy at $Pa\approx 1.9$ may be compared with $U\approx 1.6$ for the binding en-

ergy to vanish which may be inferred from the inset to Fig. 3 of Ref. 35.

The smaller binding energies and masses, and larger partial bandwidths compared with what are probably accurate results for the Hubbard-Holstein model are thought to be due to a combination of (i) limitations of our variational method to quite weak couplings, (ii) the use of only a two-parameter model for the relative motion, and (iii) differences between a Holstein model and a model with constant bare mass. We do not know which of the three causes of discrepancy is most important at present.

A lower limit for the percentage change due to departure from weak coupling of the expectation value of the part of the Hamiltonian which does not depend on relative motion of the two electrons can be obtained by looking at the percentage change in single-polaron energies at the same value of coupling when this is known. An approximate upper limit to the percentage change in the same quantity can be obtained from the percentage change in the single-polaron binding energy when the coupling g^2 is twice as large, since, in the limit when the relative wave function is very small, the coupling to phonons is twice as large for a bipolaron as for a polaron. For example, for the case $g=1$, $t/\hbar\omega=1$, in the Holstein model, corresponding to $V^2=1$ and $a=1$ in our model, one can estimate from Fig. 1 of Ref. 67 that both the lower and upper limits in the errors in the bipolaron energy below the bottom of the bare band due to use of a weak-coupling method are very small.

A simple way to estimate errors due to the change from the constant-bare-mass model to the Holstein model is to compare the weak-coupling result for the single-polaron model in the Holstein model given in Eq. (8) of Ref. 67, which gives a polaron binding energy $E_{\rm bs}$ of $g^2\hbar\omega/(1+4J/\hbar\omega)^{1/2}$ in their notation.[68] In our notation, $J/\hbar\omega$ corresponds to $1/a^2$, and g to V. Thus their result in our notation is

$$E_{\rm bs} = V^2 a\,\hbar\,\omega/(4+a^2)^{1/2}. \tag{46}$$

Our method gives binding energies in units of $\hbar\omega$ for single polarons in the constant-bare-mass model of $0.21V^2a$, $0.32V^2a$, and $0.40V^2a$ for $a=4$, 2, and 1, which may be compared with $0.22V^2a$, $0.35V^2a$, and $0.45V^2a$ for the Holstein model for weak coupling from Eq. (46). Thus the fractional changes in binding energies at weak coupling due to use of the Holstein model appear to be approximately 0.05, 0.09, and 0.12 for the three values of a considered. The results presented above are for single-polaron theory, and what changes would be expected for bipolarons is not obvious. However, if we take the results based on single-polaron theory seriously for bipolarons, then we expect, e.g., for $a=4$, $V^2=0.125$, that the magnitude of the difference in the energy of the bottom of the bare and bipolaron bands will be increased from about $0.29\hbar\omega$ for the constant-bare-mass model to between 0.30 and $0.31\hbar\omega$ for the Holstein model, compared with $0.335\hbar\omega$ obtained by El Shawish. Thus in this case it appears probable that errors due to the restriction of our method to weak or intermediate coupling and due to use of a two-parameter trial function for relative motion may be of the order of 10% for bipolaron energies at $Q=0$.

In addition to differences from the Hubbard model, we also discuss briefly how far our method is likely to be fairly accurate within the framework of the constant-bare-mass model that we have used. We note the following points.

(1) From the results mentioned after Eq. (46) and the values of parameters used for the figures and other values mentioned in the first paragraph of this section, the single-polaron binding energy lies between about $0.105\hbar\omega$ (for $V^2=0.125$ and $a=4$) and $0.315\hbar\omega$ (for $V^2=0.375$ and $a=4$). The type of variational method we use is accurate to about 4% for single-polaron binding energies in the Fröhlich model and to within 20% for masses[66] up to polaron coupling constants $\alpha=3$, corresponding to polaron binding energies of about $3\hbar\omega$. Our binding energies are so far below this value that our method can be expected to be accurate for single polarons, and also for bipolarons if one assumes that the coupling constant for bipolarons to have the same percentage errors in masses as for single polarons is at least half as large as that for single polarons. (See point 3 below for further discussion of this.)

(2) There is also the question of whether we are anywhere near a transition between large and small polarons. Toyozawa[69] was the first to study such transitions, for the case of interactions between electrons and acoustical phonons, and found a sudden transition. However, since we are dealing with optical phonons here, his work does not have much relevance for our problem. For interactions with optical phonons such transitions (between large and nearly small polarons) were first discussed by one of the present authors.[70,71]

Emin[72] considers transitions between large and small polarons for a three-dimensional molecular-crystal model. For the case where the bare half bandwidth is ten times as large as the phonon energy, he finds a transition between types for the lowest-energy state as a function of the binding energy of a small polaron which would exist in the case of zero bare bandwidth. He calls this energy E_b. From his Fig. 2 one finds that the transition at $T=0$ for the above value of bare half bandwidth occurs when the polaron binding energy (not E_b) is about $2\hbar\omega$, although both types of solutions exist for weak-coupling polaron binding energies between about $\hbar\omega$ and $3\hbar\omega$. Even the lower bound on these values is considerably larger than the values of polaron binding energies of up to $0.315\hbar\omega$ which we have discussed in the present paper. Thus it is probable that our results are not influenced by any proximity to such a transition. However, Emin does not discuss in detail results in the opposite limit which we have considered when bare-band half bandwidths are small compared with phonon energies.

For a model with Fröhlich electron-phonon interactions, it appears that a large to small polaron transition occurs for coupling constants α near 3 to 5,[73,74] with details depending on the degree of adiabaticity. The transition is fairly sharp for bare half bandwidths greater than phonon energies, but more gradual for the opposite case. For the smallest bare half bandwidth of $\hbar\omega$ considered in Ref.73, their Fig. 3 indicates only a fairly small departure of masses from a linear dependence on coupling constant α up to 1. The cases we concentrate on are $a=4$ and $a=2$, corresponding to bare half bandwidths of $0.31\hbar\omega$ and $1.23\hbar\omega$ for a constant bare mass up to

the edge of the Brillouin zone at π/a, or to $0.125\hbar\omega$ and $0.5\ \hbar\omega$ if we convert masses to obtain transfer integrals t for a tight-binding model with the same bare mass at the bottom of the band. Thus, although our coupling constants correspond to polaron binding energies considerably smaller than $\hbar\omega$ in the Fröhlich model, we could not completely rule out a larger mass rise than we find by our method because of the beginning of a transition between polaron types if our band structure were similar to that of a tight-binding model as considered in Refs. 73 and 74. However, in our case we are assuming that any effect of the lattice periodicity on the bare electrons is small, and so in such a case any transitions between polaron types will correspond to transitions in the continuum model, i.e., to a change from the lattice following the instantaneous position of the electron for weak coupling to responding to some average position for stronger coupling, and the effects of such transitions are already included in calculations such as those reported in Ref. 66.

For our case where there is no significant effect of periodicity of the potential on the bare-electron wave function, there is no such thing as a small polaron in the sense of a state which is a linear combination of states with the electron on one lattice site and surrounded by the appropriate lattice polarization, since lattice sites are almost indistinguishable from positions in between them. In this case the fact that our single-polaron radius for $a=4$ is only a quarter of the lattice constant does not imply small polarons in the usual sense. The only way that the lattice constant comes into our model is by a cutoff in the phonon wave vector. Thus in this sense it is similar to the continuum-polarization model with a cutoff considered by Schultz.[66]

(3) Iadonisi *et al.*[38] also consider transitions between types for bipolarons. For the case shown in Fig. 1 of their paper, corresponding to a bare bandwidth equal to 20 times the phonon energy, the transition for bipolarons occurs at about an 8% smaller value of the coupling constant than for polarons. Thus our guess in point 1 above that a given percentage error of mass may occur at a value of coupling constant of about half that of polarons may be pessimistic.

We get no confirmation in this work of our conjectures based on perturbation theory of great enhancements of pair binding energies at certain large center-of-mass wave vectors.[52,53] Also, unpublished calculations of El Shawish up to bipolaron wave vectors of π/a do not give us much reason to expect that suggestions of a cusplike minimum at $2\pi/a$ (in an extended zone scheme), indicated by early attempts to extend results of our variational method to the Hubbard-Holstein model as reported in Ref. 75, are likely to occur in accurate calculations. However, we still cannot rule out the possibility that a dip in bipolaron energies would be obtained near certain wave vectors if we were to use a different type of variational wave function for relative motion which could take better advantage of the small denominators in the integrands in Eq. (27) for suitable values of Q and fairly weak coupling.

Our calculations indicate that there are parameter values where bipolarons do not have excessively high masses while having binding energies with respect to two single-polaron energies greater than a few tenths of the relevant boson energy. If the bosons are plasmons of energy of the order of 2 eV, then this permits bipolaron binding energies of the order of 0.5 eV without too great increases in masses, whereas for phonons of energies of about 0.36 eV, bipolaron binding energies of 0.1 eV can be obtained without too large mass increases. A binding energy of at least 0.1 eV is a minimum requirement for room-temperature superconductivity, assuming pair binding energies must be at least about $4k_BT$ for superconductivity at temperature T. The masses must not be too high in order to be able to have a high Bose-Einstein condensation temperature for bipolarons without excessively high bipolaron concentrations. Previous calculations of condensation temperatures for bosons with a quadratic $E(Q)$ curve[76] in arrays of nanofilaments have recently been extended[62] to cases with a dispersion approximated by a sum of linear and quadratic terms, as indicated to occur for Cooper pairs.[63] We hope to modify the calculations of Ref. 62 soon by use of a Bogoliubov-type of dispersion for pairs (see, e.g., Ref. 77), which we now think is more appropriate than that based on a Cooper pair model for the strongly coupled pairs at fairly low carrier concentrations in which we were interested in Ref. 62.

V. CONCLUSIONS

No support comes from our variational method for previous results based on perturbation theory that great enhancements of binding energies of pairs can be obtained at appropriate large center-of-mass velocities. However, parameters have been found such that bipolaron masses are smaller than about $3m_e$ while keeping binding energies with respect to energies of two single polarons greater than 0.1 eV. Thus bipolarons in one dimension may provide a basis for an explanation of probable room-temperature superconductivity in narrow channels through films of oxidized atactic polypropylene and other polymers, but for different reasons than conjectured in earlier papers.

ACKNOWLEDGMENTS

One of us (D.M.E.) would like to thank J. Robles-Dominguez for weekly discussions over a period of a few months on bipolarons and related subjects, S. El Shawish for sending results on bipolaron dispersion of the Holstein model for some parameters of interest, and M. Hohenadler for help in preparation of the manuscript.

*Corresponding author. Present address: 19 Holt Road, Harold Hill, Romford, Essex RM3 8PN, England. Electronic address: d.eagles@ic.ac.uk

[1] V. L. Vinetskii, Zh. Eksp. Teor. Fiz. **40**, 1459 (1961) [Sov. Phys. JETP, **13** (1961) 1023].
[2] H. Hiramoto and Y. Toyozawa, J. Phys. Soc. Jpn. **54**, 245 (1985).
[3] J. Adamowski, Phys. Rev. B **39**, 3649 (1989).
[4] G. Verbist, F. M. Peeters, and J. T. Devreese, Phys. Rev. B **43**, 2712 (1991).
[5] F. Bassani, M. Geddo, G. Iadonisi, and D. Ninno, Phys. Rev. B **43**, 5296 (1991).
[6] D. Emin and M. S. Hillery, Phys. Rev. B **39**, 6575 (1989).
[7] S. Dzhumanov, A. A. Baratov, and S. Abboudy, Phys. Rev. B **54**, 13121 (1996).
[8] P. Zh. Baĭmatov, D. Ch. Khuzhakulov, and Kh. T. Sharipov, Fiz. Tverd. Tela (S.-Peterburg) **39**, 284 (1997) [Phys. Solid State **39**, 248 (1997)].
[9] W. B. da Costa and F. M. Peeters, Phys. Rev. B **57**, 10569 (1998).
[10] E. P. Pokatilov, V. M. Fomin, J. T. Devreese, S. N. Balaban, and S. M. Klimin, Phys. Rev. B **61**, 2721 (2000), and references therein.
[11] A. E. Myasnikova, Phys. Lett. A **291**, 439 (2001).
[12] V. K. Mukhomorov, Fiz. Tverd. Tela (S.-Peterburg) **44**, 232 (2002) [Phys. Solid State **44**, 241 (2002)]; Fiz. Tverd. Tela (S.-Peterburg) **48**, 622 (2006) [Phys. Solid State **46**, 864 (2006)]. (Kashirina *et al.*, in Ref. 15 discuss what they report to be errors in several papers by Mukhomorov.)
[13] R. T. Senger and A. Erçelebi, Eur. Phys. J. B **26**, 253 (2002).
[14] B. S. Kandemir, Eur. Phys. J. B **37**, 527 (2004); Phys. Rev. B **74**, 075330 (2006).
[15] N. I. Kashirina, V. D. Lakhno, and V. V. Sychyov, Phys. Status Solidi B **239**, 174 (2003); Phys. Rev. B **71**, 134301 (2005).
[16] B. K. Chakraverty and C. Schlenker, J. Phys. Colloq. **37**, C4-353 (1976).
[17] A. Alexandrov and J. Ranninger, Phys. Rev. B **23**, 1796 (1981).
[18] M. H. Cohen, E. N. Economou, and C. M. Soukoulis, Phys. Rev. B **29**, 4496 (1984).
[19] J. Ranninger and U. Thibblin, Phys. Rev. B **45**, 7730 (1992).
[20] For further early references on small bipolarons see D. M. Eagles, Physica C **156**, 382 (1988); A. S. Alexandrov and N. F. Mott, *Polarons and Bipolarons* (World Scientific, Singapore, 1995).
[21] A. S. Alexandrov and N. F. Mott, Rep. Prog. Phys. **57**, 1197 (1994).
[22] A. S. Alexandrov, Phys. Rev. B **53**, 2863 (1996).
[23] A. S. Alexandrov and A. M. Bratkovsky, J. Phys.: Condens. Matter **11**, L531 (1999).
[24] A. S. Alexandrov and P. E. Kornilovitch, J. Phys.: Condens. Matter **14**, 5337 (2002); J. P. Hague, P. E. Kornilovitch, J. H. Samson, and A. S. Alexandrov, Phys. Rev. Lett. **98**, 037002 (2007).
[25] F. Marsiglio, Physica C **244**, 21 (1995).
[26] H. Fehske, H. Röder, G. Wellein, and A. Mistriotis, Phys. Rev. B **51**, 16 582 (1995).
[27] G. Wellein, H. Röder, and H. Fehske, Phys. Rev. B **53**, 9666 (1996).
[28] H. Fehske, J. Loos, and G. Wellein, Phys. Rev. B **61**, 8016 (2000).
[29] A. La Magna and R. Pucci, Phys. Rev. B **55**, 14886 (1997).
[30] Y. A. Firsov and E. K. Kudinov, Fiz. Tverd. Tela (S.-Peterburg) **39**, 2159 (1997) [Phys. Solid State **39**, 1930 (1997)].
[31] L. Proville and S. Aubry, Eur. Phys. J. B **11**, 41 (1999).
[32] Th. Frank and M. Wagner, Phys. Rev. B **60**, 3252 (1999).
[33] S. Sil, J. Phys.: Condens. Matter **11**, 8879 (1999).
[34] C. Zhang, E. Jeckelmann, and S. R. White, Phys. Rev. B **60**, 14092 (1999).
[35] J. Bonča, T. Katrašnik, and S. A. Trugman, Phys. Rev. Lett. **84**, 3153 (2000).
[36] J. Bonča and S. A. Trugman, Phys. Rev. B **64**, 094507 (2001).
[37] S. El Shawish, J. Bonča, L. C. Ku, and S. A. Trugman, Phys. Rev. B **67**, 014301 (2003).
[38] G. Iadonisi, C. A. Perroni, V. Cataudella, and G. de Filippis, J. Phys.: Condens. Matter **13**, 1499 (2001).
[39] G. De Filippis, V. Cataudella, G. Iadonisi, V. Marigliano Ramaglia, C. A. Perroni, and F. Ventriglia, Phys. Rev. B **64**, 155105 (2001).
[40] A. Macridin, G. A. Sawatzky, and M. Jarrell, Phys. Rev. B **69**, 245111 (2004).
[41] M. Hohenadler, M. Aichhorn, and W. von der Linden, Phys. Rev. B **71**, 014302 (2005).
[42] M. Hohenadler and W. von der Linden, Phys. Rev. B **71**, 184309 (2005).
[43] L. Y. Zheng, Y. N. Chiu, and S. T. Lai, J. Mol. Struct.: THEOCHEM **722**, 147 (2005).
[44] M. Gurari, Philos. Mag. **44**, 329 (1953).
[45] H. Fröhlich, Adv. Phys. **3**, 325 (1954).
[46] T. D. Lee and D. Pines, Phys. Rev. **88**, 960 (1952).
[47] T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. **90**, 297 (1953).
[48] J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963).
[49] T. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959); Ann. Phys. (N.Y.) **8**, 343 (1959).
[50] R. H. Parmenter, Phys. Rev. **116**, 1390 (1959); R. H. Parmenter, Phys. Rev. **140**, A1952 (1965).
[51] D. M. Eagles, Phys. Lett. **20**, 591 (1966).
[52] D. M. Eagles, in *Proceedings of the Conference on the Physics and Chemistry of Molecular and Oxide Superconductors* [J. Supercond. **7**, 679 (1994)].
[53] D. M. Eagles, Physica C **225**, 222 (1994), **280**, 335(E) (1997).
[54] D. Hone, Phys. Rev. **138**, A1421 (1965).
[55] Early references on superconductivity in narrow channels through films of OAPP are N. S. Enikolopyan, L. N. Grigorov, and S. G. Smirnova, Pis'ma Zh. Eksp. Teor. Fiz. **49**, 326 (1989) [JETP Lett. **49**, 371 (1989)]; V. M. Arkhangorodskiĭ, A. N. Ionov, V. M. Tuchkevich, and I. S. Shlimak, *ibid.* **51**, 56 (1990) [JETP Lett. **51**, 67 (1990)]; O. V. Demicheva, D. N. Rogachev, S. G. Smirnova, E. I. Shklyarova, M. Yu. Yablokov, V. M. Andreev, and L. N. Grigorov, *ibid.* **51**, 228 (1990) [JETP Lett. **51**, 258 (1990)]. See Ref. 53 and D. M. Eagles, J. Supercond. **15**, 243 (2002) for later references.
[56] The authors of Ref. 43 discuss results on superconductivity at room temperature in oxidized atactic polypropylene in terms of a model of two-site bipolarons on adjoining one-dimensional chains. However, we disagree with several results of these authors in this and previous papers of theirs.
[57] L. N. Grigorov, Makromol. Chem., Macromol. Symp. **37**, 159 (1990).
[58] L. N. Grigorov, V. M. Andreev, and S. G. Smirnova, Makromol. Chem., Macromol. Symp. **37**, 177 (1990).
[59] L. N. Grigorov, Pis'ma Zh. Tekh. Fiz. **17** (5), 45 (1991) [Sov. Phys. Tech. Phys. **17**, 368 (1991)].
[60] M. P. McDonald and I. M. Ward, Polymer **2**, 341 (1961).
[61] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling,

Numerical Recipes (Cambridge University Press, Cambridge, UK, 1986).
[62] D. M. Eagles, Philos. Mag. **85**, 1931 (2005).
[63] S. K. Adhikari, M. Casas, A. Puente, A. Rigo, M. Fortes, M. A. Solís, M. de Llano, A. A. Valladares, and O. Rojo, Phys. Rev. B **62**, 8671 (2000); Physica C **351**, 341 (2001).
[64] Obtained from the square of the refractive index $n=1.49$ given by J. Brandrup and E. H. Immergut, *Polymer Handbook* (Wiley, New York, 1989), Vol. V, p. 27.
[65] Q. H. Chen, Y. H. Ren, and Zh. K. Jiao, Eur. Phys. J. B **3**, 307 (1998).
[66] T. D. Schultz, Phys. Rev. **116**, 526 (1959).
[67] A. H. Romero, D. W. Brown, and K. Lindenberg, Phys. Rev. B **59**, 13728 (1999).
[68] We have been informed that an equivalent formula was obtained earlier by A. A. Gogolin, but we do not have the reference.
[69] Y. Toyozawa, Prog. Theor. Phys. **26**, 29 (1961).
[70] D. M. Eagles, Phys. Rev. **181**, 1278 (1969).
[71] Some errors in Ref. 70 are noted in D. M. Eagles and P. Lalousis, J. Phys. C **17**, 655 (1984), Sec. IV.
[72] D. Emin, Adv. Phys. **22**, 57 (1973).
[73] Y. Lépine and Y. Frongillo, Phys. Rev. B **46**, 14510 (1992).
[74] G. Iadonisi, V. Cataudella, G. de Filippis, and D. Ninno, Europhys. Lett. **41**, 309 (1998).
[75] D. M. Eagles, Rev. Mex. Fis., Suppl. 1 **45**, 118 (1999).
[76] D. M. Eagles, Physica C **301**, 165 (1998).
[77] P. Pieri, L. Pisani, and G. C. Strinati, Phys. Rev. B **70**, 094508 (2004).