Polarons in quasi-one-dimensional systems

D. K. Campbell, A. R. Bishop, and K. Fesser

Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory,
Los Alamos, New Mexico 87545
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We discuss the nature of polaron excitations in two models of current interest in the study of quasi-one-dimensional materials: the coupled electron-phonon and molecular-crystal models. Using for definiteness parameters appropriate to $trans$-$(CH)_x$, we show that, although qualitatively very similar, the two polarons differ quantitatively in many respects. We then consider the very weakly bound polaron limit and show that here the two polarons become identical. We indicate that this limit, although not applicable to $trans$-$(CH)_x$, may be relevant to other interesting quasi-one-dimensional materials.

I. INTRODUCTION

The past few years have witnessed an enormous growth of interest in nonlinear excitations corresponding to intrinsic defects in quasi-one-dimensional condensed-matter systems.[1] One of the most celebrated examples has been the linear conjugated polymer $trans$-polyacetylene $[(CH)_x]$.[2] Here both microscopic coupled electron-phonon[3-7] and phenomenological[8-10] models have shown that the double degeneracy of the ground state allows kink-like solitons to exist. Apart from their possible direct experimental implications[1,2,7,9,11-13] for transport properties, doping mechanisms, and the observed metal-insulator transition in $(CH)_x$, these kink solitons, with their unconventional spin and charge assignments,[3] have stimulated theoretical work on the existence and role of "fractional charge"[14-17] in both solid-state systems and field-theory models.

More recently it has been recognized that the *same* theoretical models that predict kink solitons in $trans$-$(CH)_x$ also predict nonlinear "polaron" solitons.[18-20] This result is important because polarons, although more familiar and conventional in their properties than kinks, are also more generic, in the sense that they do *not* require the (atypical) ground-state degeneracy for their existence. Thus in the more typical case of polymers with a *non*degenerate ground state—cis-$(CH)_x$ and polyparaphenylene are examples—polarons (but *not* kinks) are expected. Indeed, polarons in cis-$(CH)_x$ have been explicitly studied[10,19,21] in a variant[19] of the coupled electron-phonon model, and the optical-absorption effects of polarons have been calculated for both isomers of polyacetylene.[22] Further, recent

experiments provide some indications that polarons are observed in both cis- (Ref. 23) and $trans$-$(CH)_x$.[24]

Given the rapidly developing interest in the polarons that emerge from the coupled electron-phonon model of conjugated polymers, it is natural to consider how these excitations are related to the more standard models of polarons[25] in quasi-one-dimensional systems. To understand this relation is of more than academic interest, in view of the recent studies[26,27] of the conventional polaron of the molecular-crystal model[26,27] in the context of the *dynamics* of self-localized charge carriers in quasi-one-dimensional solids.[26,27] In particular, the extensive calculations[27] of polaron dynamics and possible implications for transport that are currently being made in the molecular-crystal model have not yet been carried out in the coupled electron-phonon model.

Thus in this paper we study the relation between the polarons described by the molecular-crystal and coupled electron-phonon models. To permit analytic calculations, we work in the continuum limit of these models, an approximation validated by the large spatial extension of the polarons.[18-21] For definiteness, we present our results in the specific context of $trans$-$(CH)_x$. However, as we have stressed above, similar polarons are expected to occur in a much wider class of quasi-one-dimensional materials. Hence our conclusions concerning the relations between these two polarons are of applicability and relevance beyond $trans$-$(CH)_x$.

In Sec. II we review the lattice versions of the coupled electron-phonon[3] and molecular-crystal models.[26,27] We indicate a set of relations among the parameters of these two models that makes

them as similar as possible in the continuum limit. In Sec. III we discuss in detail this continuum limit and show that, for the parameters appropriate to trans-$(CH)_x$, the polarons in the two models are qualitatively similar but differ quantitatively. In particular, the polaron in the coupled electron-phonon model is somewhat less extended and substantially more bound than its counterpart in the molecular-crystal model. In Sec. IV we establish that, in the very weakly bound limit, the static polarons of the two models become *precisely* equivalent. We indicate that, although *not* appropriate to trans-$(CH)_x$, this limit may apply to other members of the class of interesting quasi-one-dimensional materials. In Sec. V we compare the effective polaron masses, finding that for the parameters appropriate to trans-$(CH)_x$, the coupled electron-phonon polaron, although light, is much more massive than that in the molecular-crystal model. In Sec. VI we summarize and discuss our results. Finally, in the Appendix we present the technical details necessary for one of our calculations.

II. THE LATTICE MODELS

To understand the similarities (and differences) of the polarons in the *continuum* versions of the coupled electron-phonon and molecular-crystal models, it is illuminating to start from the *lattice* form of the models. In the case of the electron-phonon model, the lattice version is the Su-Schrieffer-Heeger (SSH) Hamiltonian, which has the form[3]

$$H_{SSH} = \tfrac{1}{2}M \sum_n \dot{u}_n^2 + \tfrac{1}{2}K \sum_n (u_{n+1} - u_n)^2$$
$$- t_0 \sum_{n,s} (c_{n+1,s}^\dagger c_{n,s} + c_{n,s}^\dagger c_{n+1,s})$$
$$+ \alpha \sum_{n,s} (u_{n+1} - u_n)(c_{n+1,s}^\dagger c_{n,s}$$
$$+ c_{n,s}^\dagger c_{n+1,s}) .$$

(2.1)

Here u_n represents the deviation from its equilibrium position of the nth molecular unit on the chain and $c_{n,s}^\dagger$ ($c_{n,s}$) creates (annihilates) an electron at the nth site. The physical interpretation of the four terms in (2.1) is clear. The first represents the lattice kinetic energy, the second the bond strain energy between adjacent molecules, the third the constant part of the electron hopping integral between adjacent sites, and the fourth the "phonon-

mediated" hopping term, which couples the electron and lattice motions and is responsible for the interesting physics of the model. In its application to trans-$(CH)_x$, H_{SSH} is supplemented by the requirement that there is precisely one electron per site: that is, the (π-electron) band is half-filled.[28] Thus H_{SSH} considers *all* the electrons in the relevant band and includes their interactions as mediated by the phonons.[29]

The values of the parameter in (2.1) in the case of trans-$(CH)_x$ are taken to be (Ref. 3) $M = 13$ a.u. $= 2.18 \times 10^{-23}$ g, $K = 21$ eV/$\AA^2$, $t_0 = 2.5$ eV, and $\alpha = 4.1$ eV/$\AA$.[30] In addition, the lattice spacing along the chain, which is necessary to relate (2.1) to its continuum limit, is $a = 1.22$ $\AA$.

In contrast to the SSH model, which although of wider applicability was developed specifically in the context of trans-$(CH)_x$, the molecular-crystal model was developed[26,27,31,32] as a generic model of polarons: that is, electrons that are "self-trapped" due to their interactions with the vibrations of a molecular lattice. In one spatial dimension, the lattice form of the molecular-crystal Hamiltonian (denoted by H_H, where the subscript stands for Holstein[31,32]) is[33]

$$H_H = \tfrac{1}{2}M \sum_n \dot{y}_n^2 + \frac{M}{2}\omega_E^2 \sum_n y_n^2$$
$$- J \sum_{n,s} (a_{n,s}^\dagger a_{n+1,s} + a_{n+1,s}^\dagger a_{n,s})$$
$$- A \sum_{n,s} y_{n,s} a_{n,s}^\dagger a_{n,s} .$$

(2.2)

Here y_n is conventionally interpreted as the vibrational displacement of the individual diatomic nuclear coordinate from its equilibrium value and $a_n^\dagger$ (a_n) creates (annihilates) an electron on the nth molecule. In (2.2) the four terms represent, respectively, the lattice kinetic energy, the (vibrational potential) energy of the molecular lattice, the hopping energy associated with moving an electron between adjacent sites, and, finally, the coupling of the electron and lattice motions. In its application to a single polaron on the molecular chain, H_H is considered as acting on a one-electron state, the wave function of which is (in general) spread over the lattice sites.

Apart from the clear differences in the underlying physical motivations and assumptions, the detailed structures of the two lattice Hamiltonians differ substantially; for example, both the lattice strain energy and the electron-lattice interaction are bond diagonal in H_{SSH} and are site diagonal in H_H. Further, the explicit ground states of the two

models are quite different. For the continuum electron-phonon model, the ground state contains the dimerized lattice and a filled valence band separated by a gap from an empty conduction band. For the molecular-crystal model, the ground state is the (unexcited) molecular lattice and an empty conduction band. Nonetheless, in both models, the result of adding a single additional electron to the ground state is a polaron excitation. In addition, in both models, for the parameter values appropriate to $trans$-$(CH)_x$, these polarons are extended over many lattice sites. This (correctly) suggests that the continuum limits of H_{SSH} and H_H can usefully be studied. This is particularly fortunate, since analytic solutions exist in the continuum limit for polarons in both models. These solutions will allow us to establish that the two polarons are always quali-tatively similar and, in a particular limit,[34] become identical. Thus, although the underlying physics and the lattice models do differ strikingly, their polaron excitations are closely related.[35]

To relate the electron-phonon and molecular-crystal models in the context of $trans$-$(CH)_x$ it is of course necessary to choose the coupling constants appropriately. Introducing in (2.1) the staggered displacement $\omega_n = (-1)^n u_n$ and noting that the leading term in the continuum limit will have $\omega_{n+1} = \omega_n + O(a)$, we see that the models in (2.1) and (2.2) can be made to correspond in the continuum limit by the identifications

$$M \leftrightarrow M , \tag{2.3a}$$

$$4K \leftrightarrow M\omega_E^2 , \tag{2.3b}$$

and

$$4\alpha \leftrightarrow A . \tag{2.3c}$$

In addition, one requires a relation between the constant hopping terms in the molecular-crystal model (J) and in the electron-phonon model (t_0). Here a slight subtlety arises, since the SSH model includes all the electrons in the half-filled band, whereas the molecular-crystal model focuses on the single- (localized-) electron state just below the conduction band. The single-electron energy spectra for the two cases are sketched in Figs. 1 and 2. For the molecular-crystal model, as shown in Fig. 1, the energy levels are given by the standard form

$$\epsilon(k) = -2J\cos ka , \tag{2.4a}$$

which, for the states (near the bottom of the band) relevant to the limit of a single electron, become

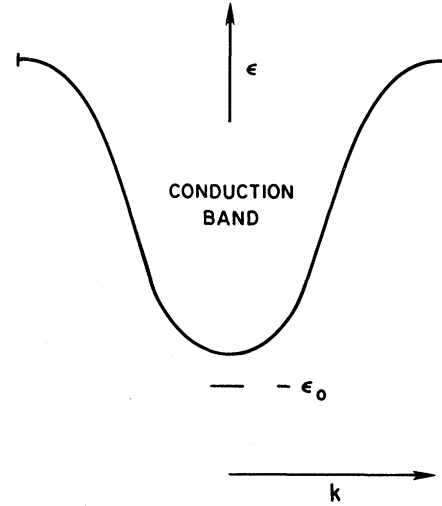$$\epsilon(k) = -2J + 2J\frac{1}{2}k^2 a^2 + \cdots . \tag{2.4b}$$

FIG. 1. Generic single-electron spectrum of the molecular-crystal model illustrating the conduction band and the localized electron state with energy $\epsilon = -\epsilon_0$ with respect to the bottom of the band.

For the electron-phonon model, as indicated in Figs. 2(a) and 2(b) the (initially) relevant limit is that of a half-filled band, in which case for excitations near $k_F = \pi/2a$, with $k' = k_F + k$,

$$\epsilon(k') = -2t_0\cos(k_F + k)a \tag{2.5a}$$

$$\simeq +2t_0\sin ka \simeq 2t_0 ak \equiv v_F k , \tag{2.5b}$$

as shown in Ref. 36.

As discussed in detail elsewhere,[5−7,19,20] this apparently linear Luttinger-type spectrum is altered by the familiar Peierls instability of coupled electron-phonon systems. This results in the formation of a gap, of full width $2\Delta_0$ [$\simeq 1.6$ eV in $trans$-$(CH)_x$], in the electron spectrum. In the continuum limit [see Figs. 2(c) and 2(d)] the resulting single-electron energy spectrum is[5−7,19,20]

$$\epsilon(k) = \pm(k^2 v_F^2 + \Delta_0^2)^{1/2} , \tag{2.6a}$$

or, for states near the bottom of the conduction band,

$$\epsilon(k) = \Delta_0 + \frac{k^2 v_F^2}{2\Delta_0} + \cdots . \tag{2.6b}$$

Hence to identify the two models correctly we expect that

$$2Ja^2 \leftrightarrow v_F^2/\Delta_0 , \tag{2.7a}$$

or, using[36] $v_F = 2t_0 a$,

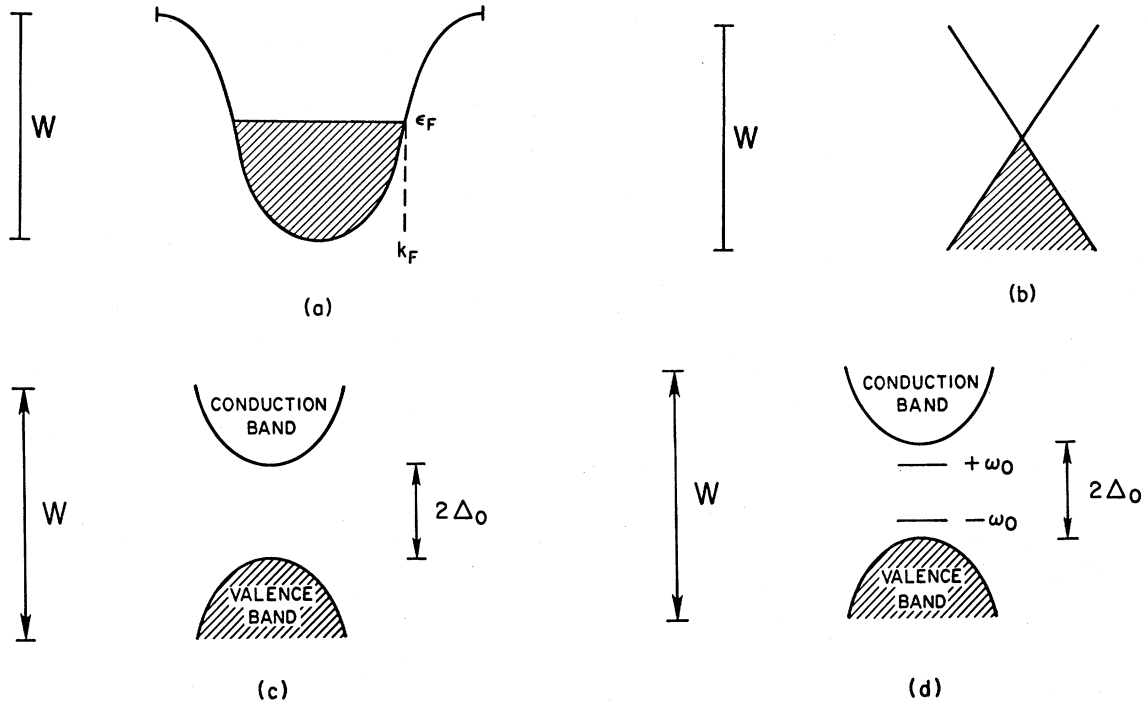$$J \leftrightarrow 2t_0^2/\Delta_0 . \tag{2.7b}$$

FIG. 2. Single-electron spectrum in the coupled electron-phonon Hamiltonian: (a) the lattice spectrum before the Peierls's instability, (b) the Luttinger-type spectrum obtained by expanding (a) around $\epsilon = \epsilon_F$, $k = k_F$, (c) the continuum spectrum after the Peierls's instability for constant gap parameter $\Delta = \Delta_0$; $\epsilon(k) = [(k^2 v_F^2 + \Delta_0^2)]^{1/2}$, and (d) the spectrum for the polaron solution. For the electron polaron the state at $(-\omega_0)$ is doubly occupied and that at $(+\omega_0)$ is singly occupied. For the hole polaron, the state at $(-\omega_0)$ is singly occupied. Possible bipolaron states are described in Refs. 21—23.

III. THE CONTINUUM LIMIT

The adiabatic continuum limit of the molecular-crystal model has been derived and discussed elsewhere[26,27,31] in considerable detail, and thus we shall here only briefly motivate the results. One introduces an adiabatic electron wave function $a_n^{(0)}$, and treats the lattice displacements as c numbers, $y_n^{(0)}$. Varying the expectation value of H_H in this one-electron state with respect to $y_n^{(0)}$ determines the minimal energy displacements to be

$$y_n^{(0)} = \frac{A}{M\omega_E^2} |a_n^{(0)}|^2 , \qquad (3.1)$$

whereas varying with respect to the $a_n^{(0)}$ leads to Schrödinger-type equation,[37]

$$\epsilon a_n^{(0)} = -Ay_n^{(0)} a_n^{(0)} - J(a_{n+1}^{(0)} + a_{n-1}^{(0)} - 2a_n^{(0)}) . \qquad (3.2)$$

Assuming $a_n^{(0)}$ is a smooth function of its lattice-site "argument" n one can approximate[38]

$$a_{n+1}^{(0)} + a_{n-1}^{(0)} - 2a_n^{(0)} \simeq \frac{d^2 a_n^{(0)}}{dn^2} . \qquad (3.3)$$

Thus substituting (3.1), one obtains the equation for the continuum polaron in the molecular-crystal model as

$$-J\frac{d^2 a_n^{(0)}}{dn^2} - \frac{A^2}{M\omega_E^2} |a_n^{(0)}|^2 a_n^{(0)} = \epsilon a_n^{(0)} . \qquad (3.4)$$

This is (a time-independent version of) the well-known "nonlinear Schrödinger equation,"[25,39] and the polaron is just the familiar (envelope) soliton solution[39]

$$a_n^{(0)} = \left[\frac{\gamma}{2}\right]^{1/2} \mathrm{sech}\gamma(n - n_0) , \qquad (3.5)$$

with n_0 being the (lattice-site) location of the polaron and γ [$= A^2/(4M\omega_E^2 J)$] being the inverse polaron width. The normalization condition on (3.5) is

$$\sum |a_n^{(0)}|^2 = 1 . \qquad (3.6)$$

The energy eigenvalue in (3.4) is

$$\epsilon \equiv -\epsilon_0 = -J\gamma^2 , \qquad (3.7)$$

and the total polaron *binding* energy[40] is

$$\mathscr{E}_p = -\left[-\epsilon_0 + \tfrac{1}{2}M\omega_E \sum_n (y_n^{(0)})^2\right]$$

$$= \tfrac{1}{3}\epsilon_0 = \tfrac{1}{3}J\gamma^2 . \tag{3.8}$$

For later comparative purposes, note that if we use the correspondences indicated by Eqs. (2.3) and (2.7) to determine the parameters appropriate for *trans*-$(CH)_x$, we find that the polaron is about 22 lattice sites wide ($\gamma = 0.045$), the localized electron energy level lies 0.036 eV below the conduction band ($\epsilon_0 = 0.036$ eV), and the polaron binding energy is 0.012 eV.

The adiabatic continuum limit of the SSH model has also been extensively discussed,[5-7,19-21] and thus we shall again merely sketch the results. The continuum Hamiltonian corresponding to (2.1) is

$$H = \frac{M}{2}\left[\frac{1}{16\alpha^2 a}\right]\int dx \left|\frac{d\Delta}{dt}\right|^2 + \frac{\omega_Q^2}{2g^2}\int dx\,\Delta^2(x)$$

$$-iv_F \int dx \left[u(x)\frac{\partial u(x)}{\partial x} - v(x)\frac{\partial v(x)}{\partial x}\right]$$

$$+ \int dx\,\Delta(x)[u^*(x)v(x) + v^*(x)u(x)] . \tag{3.9}$$

Here Δ is the (real) band-gap parameter and u and v are the two components of the electron field. For $\Delta = 0$, u and v correspond (respectively) to right- and left-going electrons [see Fig. 2(b)]. In terms of the lattice parameters,

$$\omega_Q^2 = 4K/M , \tag{3.10a}$$

$$g = 4\alpha(1/M)^{1/2} , \tag{3.10b}$$

and[36]

$$v_F = 2t_0 a . \tag{3.10c}$$

The continuum equations following from (3.9) are for the single-electron wave function (u_n, v_n)

$$\epsilon_n u_n(x) = -iv_F\frac{\partial}{\partial x}u_n(x) + \Delta(x)v_n(x) , \tag{3.11a}$$

$$\epsilon_n v_n(x) = +iv_F\frac{\partial}{\partial x}v_n(x) + \Delta(x)u_n(x) , \tag{3.11b}$$

and for the (self-consistent) gap parameter

$$\Delta(x) = -\frac{g^2}{\omega_Q^2}\sum_{n,s}{}'[v_n^*(x)u_n(x) + u_n^*(x)v_n(x)] . \tag{3.11c}$$

In (3.11c) the summation is over the full valence band plus, for the polaron, the appropriate states in the gap[19,20] [see Fig. 2(d)].

The analytic form of the gap parameter for the polaron solution to (3.11) is

$$\Delta_p(x) = \Delta_0 - \kappa_0 v_F[\tanh\kappa_0(x + x_0)$$

$$-\tanh\kappa_0(x - x_0)]$$

$$= \Delta_0 - (\kappa_0 v_F)^2\omega_0^{-1}\mathrm{sech}\kappa_0(x + x_0)$$

$$\times\mathrm{sech}\kappa_0(x - x_0) , \tag{3.12a}$$

with

$$\omega_0^2 + (\kappa_0 v_F)^2 = \Delta_0^2 \tag{3.12b}$$

and

$$\tanh2\kappa_0 x_0 = \kappa_0 v_F/\Delta_0 . \tag{3.12c}$$

The electron wave functions for the positive-energy localized state are

$$u_0(x) = N_0[(1-i)\mathrm{sech}\kappa_0(x + x_0)$$

$$+(1+i)\mathrm{sech}\kappa_0(x - x_0)] \tag{3.13a}$$

and

$$v_0(x) = N_0[(1+i)\mathrm{sech}\kappa_0(x + x_0)$$

$$+(1-i)\mathrm{sech}\kappa_0(x - x_0)] , \tag{3.13b}$$

with $N_0 = (\sqrt{\kappa_0})/4$ so that

$$\int dx(|u_0|^2 + |v_0|^2) = 1 . \tag{3.14}$$

Since we do not need the explicit forms of the wave functions in the conduction and valence bands, we shall not quote them here.[20] It is important to recall, however, that the electron wave functions satisfy (3.11a) and (3.11b) with $\Delta(x) = \Delta_p(x)$ for *any* $\kappa_0 v_F$ in the allowed range $0 \le \kappa_0 v_F \le \Delta_0$. The self-consistency condition (3.11c) determines the specific value of $\kappa_0 v_F$ for a solution to the full-coupled equation. For *trans*-$(CH)_x$, $\kappa_0 v_F = \Delta_0/\sqrt{2} = \omega_0$. In this case the characteristic width of the polaron, which we take as $2x_0$, is[20,41]

$$2x_0 = (W/2\Delta_0)\sqrt{2}\ln(1 + \sqrt{2})a \simeq 8.9a , \tag{3.15}$$

using $W = 4t_0 = 10$ eV and $2\Delta_0 = 1.4$ eV. The amount by which the localized electron state lies below the conduction band is

$$\Delta\epsilon = \Delta_0 - \omega_0 = \Delta_0\left[\frac{\sqrt{2}-1}{\sqrt{2}}\right] = 0.21 , \tag{3.16}$$

and the binding energy of the polaron is[19,20]

$$\mathscr{E}_p = -\left[\frac{2\sqrt{2}}{\pi}-1\right]\Delta_0 \simeq 0.1\Delta_0 \simeq 0.07 , \tag{3.17}$$

both values being expressed in units of eV. These numbers all indicate that the continuum polaron in the electron-phonon model is, for corresponding values of the parameters, less extended and more deeply bound than that in the molecular-crystal model.

IV. EQUIVALENCE IN THE WEAKLY BOUND LIMIT

Deeper insight into the relation between the polarons in the two models can be obtained by considering a formal limit[34] of Eq. (3.11), in which the polarons of the continuum electron-phonon model become precisely equivalent to those of the continuum molecular-crystal model. This limit is that of a very weakly bound polaron, in which[42]

$$\kappa_0 v_F / \Delta_0 \ll 1 . \tag{4.1}$$

To see how the equivalence appears when (4.1) holds, let us start with the electron wave-function equations. We first transform from the right- and left-going components $\{u_n, v_n\}$ to components $\{\psi_n^{(1)}, \psi_n^{(2)}\}$ which satisfy

$$\psi_n^{(1)} = \frac{1}{\sqrt{2}}(u_n + v_n) , \tag{4.2a}$$

$$\psi_n^{(2)} = \frac{-i}{\sqrt{2}}(u_n - v_n) , \tag{4.2b}$$

so that Eqs. (3.11) read

$$\epsilon_n \psi_n^{(1)} = +v_F \frac{\partial \psi_n^{(2)}}{\partial x} + \Delta \psi_n^{(1)} , \tag{4.3a}$$

$$\epsilon_n \psi_n^{(2)} = -v_F \frac{\partial \psi_n^{(1)}}{\partial x} - \Delta \psi_n^{(2)} , \tag{4.3b}$$

and the gap equation (3.11c) becomes

$$\Delta(x) = -\frac{g^2}{\omega_Q^2} \sum_n{}' (|\psi_n^{(1)}|^2 - |\psi_n^{(2)}|^2) . \tag{4.3c}$$

For a weakly bound polaron we expect Δ to differ only slightly from its ground-state value [viz., (3.12a) in the limit (4.1)]. Thus we write $\Delta = \Delta_0 - \widetilde{\Delta}$ and study Eqs. (4.3) in powers of $1/\Delta_0$. For electron states near the bottom of the conduction band,

from (2.6b), $\epsilon_n \simeq \Delta_0 + O(k^2)$. Thus, since $\epsilon_n + \Delta \simeq 2\Delta_0$, we see that (4.3b) implies

$$\psi_n^{(2)} \simeq \frac{1}{2\Delta_0}\left[-v_F \frac{\partial \psi_n^{(1)}}{\partial x}\right] , \tag{4.4}$$

so that $\psi^{(2)}$ is of order $(1/\Delta_0)$ relative to $\psi^{(1)}$ and, further, that this leading term in $\psi_n^{(2)}$ can be calculated directly from $\psi_n^{(1)}$. Hence to leading order in $1/\Delta_0$, only the $\psi_n^{(1)}$ equation (4.3a) remains.[43] Focusing on a weakly bound state with

$$\epsilon_0 = (\Delta_0^2 - \kappa_0^2 v_F^2)^{1/2} \simeq \Delta_0 - \kappa_0^2 v_F^2 / 2\Delta_0 ,$$

and substituting for $\partial \psi_0^{(2)}/\partial x$ by differentiating (4.4)—valid to leading order in (κ_0/Δ_0) (Ref. 43)—yields

$$\epsilon_0 \psi_0^{(1)} = v_F \frac{(-v_F)}{2\Delta_0}\left[\frac{\partial^2 \psi_0^{(1)}}{\partial x^2}\right] + (\Delta_0 - \widetilde{\Delta})\psi_0^{(1)} \tag{4.5a}$$

or

$$\left[-\frac{\kappa_0^2 v_F^2}{2\Delta_0}\right]\psi_0^{(1)} = -\frac{v_F^2}{2\Delta_0}\frac{\partial^2 \psi_0^{(1)}}{\partial x^2} - \widetilde{\Delta}\psi_0^{(1)} . \tag{4.5b}$$

This clearly has the form of a Schrödinger equation [cf. (3.4)] with potential $\widetilde{\Delta} \equiv \Delta_0 - \Delta$. From (3.12a) we see that

$$\widetilde{\Delta} = (\kappa_0 v_F)^2 \omega_0^{-1} \mathrm{sech}\kappa_0(x + x_0)\mathrm{sech}\kappa_0(x - x_0) , \tag{4.6a}$$

so that for $\kappa_0 v_F / \Delta_0 \ll 1$, to leading order,

$$\widetilde{\Delta} \simeq (\kappa_0 v_F)^2 \Delta_0^{-1} \mathrm{sech}^2\kappa_0 x + \cdots , \tag{4.6b}$$

where the ellipsis represents higher orders. Similarly, from (3.13) and (4.2a), we see that $\psi_0^{(1)}$, which, in general, is given by

$$\psi_0^{(1)} = \frac{1}{\sqrt{2}}(u_0 + v_0)$$

$$= \sqrt{2}N_0[\mathrm{sech}\kappa_0(x + x_0) + \mathrm{sech}\kappa_0(x - x_0)] , \tag{4.7}$$

with $N_0 = \sqrt{\kappa_0}/4$, becomes, to leading order for $\kappa_0 v_F / \Delta_0 \ll 1$,

$$\psi_0^{(1)} \simeq \left[\frac{\kappa_0}{2}\right]^{1/2} \text{sech}\kappa_0 x \ ,$$

with   (4.8)

$$\int dx \ |\psi_0^{(1)}(x)|^2 = 1 \ .$$

By inspection, we see that (4.6b) and (4.8) imply

$$\widetilde{\Delta} = \frac{2\kappa_0 v_F^2}{\Delta_0} \ |\psi_0^{(1)}|^2 \ ,$$ (4.9)

and hence (4.5b) can be rewritten as

$$-\frac{v_F^2}{2\Delta_0}\frac{\partial^2 \psi_0^{(1)}}{\partial x^2} - \frac{2\kappa_0 v_F^2}{\Delta_0}\ |\psi_0^{(1)}|^2 \psi_0^{(1)} = -\frac{\kappa_0^2 v_F^2}{2\Delta_0}\psi_0^{(1)} \ ,$$

(4.10)

with the solution as above in (4.8). Clearly, Eqs. (3.4) and (4.8) are identical in structure. Before showing that they are precisely equivalent—constants and all—let us discuss briefly the consistency of the limiting result (4.9) with the general form of the self-consistency equation for Δ, (3.11c) or (3.4c). In particular, in (4.9), what has happened to all the states in the valence band and to the negative-energy bound state (at $\epsilon = -\omega_0$)? From Fig. 2(d), one sees that for small $\kappa_0 v_F/\Delta_0$, these states are all separated by a "large" energy ($\sim 2\Delta_0$) from the state at $\epsilon = +\omega_0$. Further, these states are all fully occupied in the polaron configuration[44] just as they are in the ground state. This motivates the "frozen-valence-band approximation," in which one argues that, since $\Delta(x)$ differs only slightly from its ground-state value, the shifts in the states in *and* near the valence band are small, and one can ap-

proximate the sum over all states with energies less than zero by its value in the ground state. This approximation is indicated graphically in Fig. 3. In the Appendix we show that, to leading order in $(\kappa_0 v_F/\Delta_0)$, this frozen-valence-band approximation is valid.

To see what this implies, let us rewrite (3.11c) as

$$\Delta_p(x) = \Delta_0 - \widetilde{\Delta} = -\frac{g^2}{\omega_Q^2}\left[\sum_{n,s}' v_n^* u_n + u_n^* v_n\right]_p$$

$$= -\frac{g^2}{\omega_Q^2}(\ |\psi_0^{(1)}|^2 - |\psi_0^{(2)}|^2)$$

$$-\frac{g^2}{\omega_Q^2}\left[\sum_{\epsilon_n<0,s}' v_n^* u_n + u_n^* v_n\right]_p \ .$$

(4.11)

The last term—the sum over all states with energy less than zero—is, in the frozen-valence-band approximation, replaced by its ground-state value, which is just Δ_0.[5-7,19,20] Thus, recalling that $\psi_0^{(2)}$ is $O\ (\kappa_0 v_F/\Delta_0)$ smaller than $\psi_0^{(1)}$, we see that we can approximate (4.11) as

$$\Delta_0 - \widetilde{\Delta} = -\frac{g^2}{\omega_Q^2}\ |\psi_0^{(1)}|^2 + \Delta_0 + \cdots$$ (4.12a)

or

$$\widetilde{\Delta} = \frac{g^2}{\omega_Q^2}\ |\psi_0^{(1)}|^2 \ \cdots \ .$$ (4.12b)

The comparison of this result to (4.9) shows that $\kappa_0 v_F$ for the weakly bound polaron is determined in terms of known parameters to be
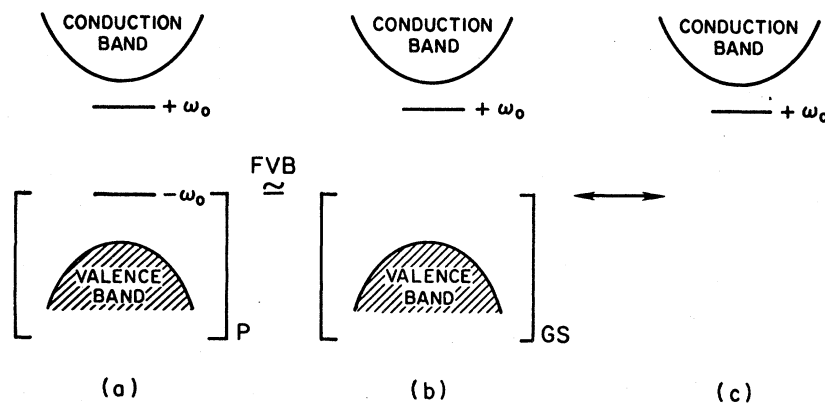

FIG. 3. Graphic illustration of the frozen-valence-band (FVB) approximation. The actual full one-electron spectrum for the polaron configuration (a) is approximated (FVB) by replacing the states below the Fermi energy by their values in the ground state (b) so that the spectrum corresponds directly to that considered in the molecular-crystal model (c).

$$\kappa_0 v_F = \frac{g^2 \Delta_0}{2\omega_Q^2 v_F} . \tag{4.13}$$

It is now a matter of straightforward algebra to establish the exact equivalence of the two polaron solutions in the weakly bound limit. Starting from the form of the two wave functions $a_n^{(0)}$ [Eq. (3.5)] and $\psi_0^{(1)}$ [Eq. (4.8)], we see that, recalling the relation $na \leftrightarrow x$, these solutions are identical provided $\kappa_0 a \leftrightarrow \gamma$. From (4.13) and the definition of γ, using the correspondences in (2.3) and (2.7), we find

$$\kappa_0 a = \frac{ag^2}{2\omega_Q^2}\frac{\Delta_0}{v_F^2} = \frac{1}{2}\frac{16\alpha}{4K}a^2\frac{\Delta_0}{v_F^2} \leftrightarrow \frac{1}{2}\frac{A^2}{M\omega_0^2}\frac{1}{2J} \equiv \gamma , \tag{4.14}$$

which proves the relation. Similarly, again recalling $x \leftrightarrow na$, one can see that each term in (4.10) corresponds precisely to a term in (3.4). In particular, from (3.7) the energy of the occupied electron state is

$$-\frac{\kappa_0^2 v_F^2}{2\Delta_0} = -(k_0 a)^2\frac{v_F^2}{2\Delta_0^2} \leftrightarrow -\gamma^2 J , \tag{4.15}$$

as expected.

The comparison of the full energy of the two polarons proves quite interesting. For the continuum version of the molecular-crystal model, by direct calculation the binding energy is, as given in (3.8), $J\gamma^2/3$. One could similarly calculate directly the total energy for the polaron of the continuum electron-phonon model, and by the equivalence of the solutions, would find the same result. It is more instructive, however, to start from the general expression[19,20] in the electron-phonon model of *trans*-(CH)$_x$ for the energy of the polaron configuration as a function of $\kappa_0 v_F$,

$$E(\kappa_0 v_F) = \omega_0 + \frac{4}{\pi}\kappa_0 v_F - \frac{4}{\pi}\omega_0\tan^{-1}\frac{\kappa_0 v_F}{\omega_0} . \tag{4.16}$$

Minimizing this expression yields the actual values of $\kappa_0 v_F$ and binding energy appropriate to the polaron in *trans*-(CH)$_x$. In the limit $\kappa_0 v_F \ll \Delta_0$, expanding (4.16) gives

$$E(\kappa_0 v_F) \simeq \Delta_0 - \frac{\kappa_0^2 v_F^2}{2\Delta_0} + \frac{4}{\pi}\frac{\kappa_0^3 v_F^3}{3\Delta_0^2} + \cdots . \tag{4.17}$$

This expression has a minimum at

$$\kappa_0 v_F = \left[\frac{\pi}{4}\right]\Delta_0 , \tag{4.18}$$

at which point $\mathscr{E}_p \equiv +\Delta_0 - E_p(\kappa_0 v_F)$,

$$\mathscr{E}_p = \frac{1}{6}\frac{(\kappa_0 v_F)^2}{\Delta_0} , \tag{4.19}$$

which, by comparison with (4.15), can be seen to correspond exactly to (3.8).

Note that (4.18), which gives $\kappa_0 v_F/\Delta_0 = \pi/4 \simeq O(1)$, directly contradicts the assumption that $\kappa_0 v_F \ll \Delta_0$—under which it was derived. This is an explicit illustration of our earlier remarks that, although one can *formally* study the weakly bound polaron limit, this limit is *not* applicable to *trans*-(CH)$_x$. However, there are expected to be physically interesting systems to which the weakly bound limit *does* apply. In particular, for *cis*-(CH)$_x$ and related systems with nondegenerate ground states, if the ratio of the extrinsic gap to the intrinsic gap is large and the electron-phonon coupling is small,[19-21] single-polaron states *will* have $\kappa_0 v_F \ll \Delta_0$.[45] To see this explicitly, we recall that the expression analogous to (4.16) giving the energy of a polaron configuration in *cis*-(CH)$_x$ is[19,20]

$$E_p^c(\kappa_0 v_F) = \omega_0 + \frac{1}{\pi}\kappa_0 v_F - \frac{4}{\pi}\omega_0\tan^{-1}(\kappa_0 v_F/\omega_0)$$

$$+ \frac{4}{\pi}\overline{\Delta}_0\Gamma\left[\tanh^{-1}\left[\frac{\kappa_0 v_F}{\overline{\Delta}_0}\right]\right.$$

$$\left. - \kappa_0 v_F/\overline{\Delta}_0\right] . \tag{4.20}$$

Here the full gap $\overline{\Delta}_0 = \Delta_e + \Delta_i^0$, where Δ_e is a constant extrinsic gap, and only Δ_i^0 is sensitive to electron feedback. The existence of an extrinsic gap breaks the ground-state degeneracy and leads to a unique ground state for *cis*-(CH)$_x$. The parameter $\Gamma \equiv \Delta_e/\lambda_c\overline{\Delta}_0$, where λ_c is the dimensionless electron-phonon coupling appropriate to *cis*-(CH)$_x$. Since $(\kappa_0 v_F)^2 + \omega_0^2 = \overline{\Delta}_0^2$, we can express $E_p^c(\kappa_0 v_F)$ in terms of θ where $\kappa_0 v_F = \overline{\Delta}_0\sin\theta$ and $\omega_0 = \overline{\Delta}_0\cos\theta$. Minimizing with respect to θ then yields

$$\theta + \Gamma\tan\theta = \pi/4 . \tag{4.21}$$

For $\Gamma = 0$—no extrinsic gap and a degenerate ground state—the solution to (4.21) gives $\kappa_0 v_F = \overline{\Delta}_0/\sqrt{2}$, which is the *trans*-(CH)$_x$ result and is clearly *not* in the weakly bound limit. For large Γ, however, the solution to (4.21) yields a small value for θ, and this implies that $\kappa_0 v_F/\overline{\Delta}_0$ is much less than 1.

For our final direct comparison of the two polarons we study the respective polaron masses. To some extent, these masses, which influence polaron dynamics, go beyond the static properties we have thus far considered. It is worth emphasizing that this dynamical information is limited in that the masses are calculated in the adiabatic approximation.

In the molecular-crystal model the effective mass of the polaron is given by[26,27]

$$M_p \equiv M \sum_n \left[\frac{\partial y_n^{(0)}(n - \xi/a)}{\partial \xi} \right]^2 , \qquad (4.22)$$

where $\xi(=n_0 a)$ is the (physical) location of the polaron on the lattice. Using the form of $u_n^{(0)}$ from (3.1) and (3.5) and changing the sum to an integral, one readily obtains

$$\frac{M_p}{M} = \frac{4\gamma^3}{15a^2} \left[\frac{A^2}{M\omega_E^4} \right] , \qquad (4.23)$$

which, for the parameters relevant to trans-$(CH)_x$, gives $M_p/M = 0.62 \times 10^{-6}$, or

$$M_p = 0.015 m_e \qquad (4.24)$$

(where m_e is the electron mass), indicative of the very small distortion which this polaron represents.

For the continuum electron-phonon model, the expression analogous to (4.22) is[21]

$$\frac{M_p}{M} = \frac{1}{16\alpha^2} \int \frac{dx}{a} \left[\frac{\partial \Delta_p}{\partial x_0} \right]^2 , \qquad (4.25)$$

which can be evalutated as a function of $X = \kappa_0 v_F/\Delta_0$,

$$\frac{M_p}{M} = \frac{1}{16\alpha^2} \frac{\Delta_0^3}{a v_F}$$
$$\times \left\{ \frac{8}{3} X^3 - 4(1 - X^2) \left[\ln \left[\frac{1+X}{1-X} \right] - 2X \right] \right\} . \qquad (4.26)$$

For arbitrary X (in the physical interval $0 \leq X \leq 1$) this function is plotted in Fig. 4. For $X = 1/\sqrt{2}$, the value for the polaron in trans-$(CH)_x$, one finds, inserting the appropriate parameters, $M_p/M \simeq 4.21 \times 10^{-5}$, so that

$$M_p \simeq 1.0 m_e , \qquad (4.27)$$
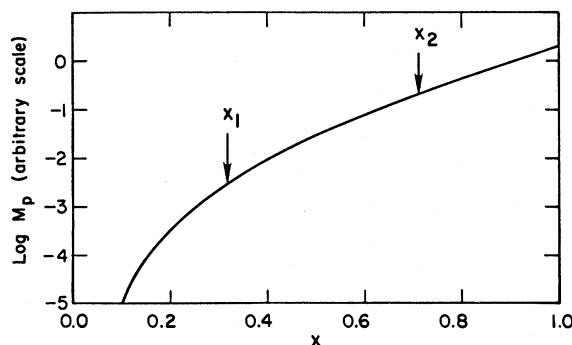
which, although light, is substantially "heavier"

FIG. 4. Logarithm of the effective mass (in arbitrary units) of the polaron in the continuum electron-phonon model vs $X \equiv \kappa_0 v_F/\Delta_0$. The value at the point labeled X_1 corresponds to the value expected in the molecular-crystal model for the parameters appropriate to trans-$(CH)_x$. The value of X_2 is the prediction of the coupled electron-phonon model for trans-$(CH)_x$. Note that, as calculated in the text, these differ by nearly a factor of 70.

than the polaron in the molecular-crystal model. In the weakly bound limit, $X \ll 1$ [Eq. (4.26)] reduces to

$$\frac{M_p}{M} = \frac{1}{16\alpha^2} \left[\frac{\Delta_0^3}{a v_F} \right] \frac{16}{15} \left[\frac{\kappa_0 v_F}{\Delta_0} \right]^5 + \cdots . \qquad (4.28)$$

Using the correspondences in (2.3) and (2.7) and recalling $\kappa_0 a \leftrightarrow \gamma$, one can easily see that (4.28) is precisely the same as (4.23) and hence the masses of the polarons in the two models become the same.

Although for the parameters appropriate to trans-$(CH)_x$ the polaron masses predicted by the two models differ by a factor of nearly 70, in both cases the polaron mass is surprisingly small. This small mass should be quite significant in the dynamics involving polarons, including recombination of polaron pairs to soliton pairs and charge transport, both intra- and interchain. More precise, quantitative statements on either of these effects will require a more detailed understanding of the overall dynamics of the models. Some analytic progress has been made for the molecular-crystal model,[27] but for the coupled electron-phonon model, one must so far rely on numerical simulations for guidance.[18] Another aspect of the smallness of the polaron's mass is the potential importance of quantum fluctuation effects[46]; for example, for polarons which are bound to charged dopant molecules or defects by Coulomb attraction, the small mass will mean larger zero-point motion.

V. DISCUSSION AND CONCLUSIONS

The results of the previous sections have clearly established that the polarons of the coupled electron-phonon and molecular-crystal models are qualitatively similar and, in the weakly bound limit, become identical. Outside this limit, there are quantitative differences, in that for corresponding values of the parameters the polaron of the coupled electron-phonon model is less spatially extended, more bound, and more massive than its molecular-crystal counterpart.

The implications of these differences depend strongly on the physical system being modeled. For trans-$(CH)_x$, for example, one is *not* in the weakly bound limit, and the actual polaron excitation is therefore presumably closer to that described by the coupled electron-phonon model, since this model is nearer to the microphysics of the material. More importantly, in trans-$(CH)_x$ the possibility of kink solitons radically changes the conventional picture of polaron dynamics and transport. To see this, we recall that the energy of a kink (S) or antikink $(\bar{S})$ is $E_S = E_{\bar{S}} = 2\Delta_0/\pi$ and that, by topological constraints, kinks *must* be produced in $S\bar{S}$ pairs from the ground state. The implications of this are that polarons are the lowest state available to a single electron,

$$E_p = (2\sqrt{2}/\pi)\Delta_0 < E_S + E_{\bar{S}} \ ,$$

and hence will be important at light levels of doping by *single* carriers. At heavier doping levels, however, since

$$2E_p = 2\left[\frac{2\sqrt{2}}{\pi}\Delta_0\right] > E_S + E_{\bar{S}} = \frac{4}{\pi}\Delta_0 \ ,$$

rather than forming additional polaron states, the excess carriers will be accommodated on $S\bar{S}$ pairs. Hence, in this case, to understand properly the transport and dynamical properties in trans-$(CH)_x$, it is *essential* to have a model which incorporates both kink and polaron excitations.

In contrast, in cis-$(CH)_x$ and related systems with nondegenerate ground states, the absence of kink solitons removes the striking qualitative effects of $PP \rightarrow S\bar{S}$. Further, depending on parameters, the weakly bound limit may apply, so that the two static polarons are quantitatively essentially identical. Since the molecular-crystal model considers only the single localized electron state, whereas the continuum electron-phonon model incorporates all oc-

cupied electronic states, dynamical calculations are *much* simpler in the framework of the molecular-crystal model. This simplicity offers the potential for qualitatively accurate, analytic insights into effects that, in the more complicated model, are probably accessible only through numerical studies.

Finally, we should comment on the optical absorption from polarons, particularly in view of its importance as a potential signature of these excitations.[23,24] In the continuum electron-phonon model, the underlying electron-hole symmetry automatically means that when a localized state is formed below the conduction band at $+\omega_0$, a similar state is formed at $-\omega_0$, just above the valence band. Thus, although the polaron involves the addition of only a single electron to the dimerized ground state, the self-consistency reflected in the gap equation (3.11c) leads to changes in the electronic spectrum in the valence band as well as in the conduction band. For an electron polaron, the localized state at $-\omega_0$ is doubly occupied, whereas that at $+\omega_0$ is singly occupied. Hence, apart from interband transitions, for the electron polaron there are three (independent) transitions involving localized levels [see Fig. 2(d)]: $-\omega_0 \rightarrow +\omega_0 (\equiv \alpha_1)$, $+\omega_0 \rightarrow$ conduction band $(\equiv \alpha_2)$, and $-\omega_0 \rightarrow$ conduction band[47] $(+ \equiv \alpha_3)$. A striking prediction[22] of the continuum electron phonon is that $\alpha_2 \gg \alpha_3$, even though both involve a transition from an extended to a localized state.

In the molecular-crystal model (or any related single electronic state, i.e., "frozen-band" model), the absence of a dynamic valence band means that one would not automatically have the doubly occupied state at $-\omega_0$ in the presence of a singly occupied localized level at $+\omega_0$. It would be rather natural, though, to consider a state just above the valence band, and hence to predict a "hole" polaron at $-\omega_0$. One could also calculate the phase-shift effects of the polaron-lattice configuration on plane-wave states in the valence and conduction bands and, with these, work out the appropriate optical-absorption matrix elements. In this manner one could effectively produce in the molecular-crystal model the optical transitions predicted by the continuum electron-phonon model. However, it is hard to see how, with further *ad hoc* assumptions, one could obtain the surprising result $\alpha_2 \gg \alpha_3$.

calculations of polaron dynamics, and David Emin for useful comments on the general features of polarons in one dimension.

APPENDIX

In this appendix we establish the validity of the frozen-valence-band approximation (see Sec. IV and Fig. 3) in the weakly bound polaron limit, $\kappa_0 v_F < \Delta_0$. The general form of the self-consistency relation for the polaron gap parameter is[20]

$$\Delta_p(x) = -\frac{g^2}{\omega_Q^2} [1(u_0^* v_0^* + v_0 u_0)$$

$$+ 2(u_{-0}^* v_{-0} + v_{-0}^* u_{-0})$$

$$+ 2\int_{-K}^{K} dk (u_-^* v_- + v_-^* u_-)] , \tag{A1}$$

where we have explicitly displayed the contributions of the positive- (u_0, v_0) and negative- (u_{-0}, v_{-0}) energy localized-state wave functions. Using the explicit forms of the wave functions[20] (A1) can be written as

$$\Delta_p(x) = \frac{g^2}{\omega_Q^2} \left[1 \frac{\omega_0}{2v_F}(t_+ - t_-) - 2\frac{\omega_0}{2v_F}(t_+ - t_-) - \frac{2}{2\pi}\int_{-K}^{K} \frac{dk}{(k^2 v_F^2 + \Delta_0^2)^{1/2}} \left[\Delta_p(x) - \frac{\omega_0^2 \kappa_0 v_F}{k^2 v_F^2 + \kappa_0^2 v_F^2}(t_+ - t_-) \right] \right] , \tag{A2}$$

where $t_\pm \equiv \tanh \kappa_0(x \pm x_0)$ and K is a momentum cutoff. To study the limit $\kappa_0 v_F \ll \Delta_0$, we write $\Delta_p(x)$ in the form shown in (3.12) and collect terms as

$$\Delta_0 - \kappa_0 v_F(t_+ - t_-) = + \frac{2g^2}{\pi \omega_Q^2} \int_0^K \frac{dk}{(k^2 v_F^2 + \Delta_0^2)^{1/2}} \left[\Delta_0 - \frac{g^2}{\omega_Q^2}\frac{\omega_0}{2v_F}(t_+ - t_-) \right]$$

$$- \frac{2g^2}{\omega^2}(t_+ - t_-)\left[\frac{1}{\pi}\int_0^K \frac{dk}{(k^2 v_F^2 + \Delta_0^2)^{1/2}}\left[\kappa_0 v_F + \frac{\kappa_0 v_F \omega_0^2}{k^2 v_F^2 + \kappa_0^2 v_F^2} \right] - \frac{\omega_0}{2v_F} \right] . \tag{A3}$$

From the definition[20] $\Delta_0 \equiv We^{-1/\lambda}$ of Δ_0 in terms of the full bandwidth $W \simeq 2K$ and coupling constant $\lambda = 2g^2/(\pi v_F \omega_Q^2)$, the first term on the right-hand side of (A3) reduces to

$$\frac{2g^2}{\pi \omega_Q^2}\int_0^K \frac{dk}{(k^2 v_F^2 + \Delta_0^2)^{1/2}}\Delta_0 = \Delta_0 , \tag{A4}$$

so that Δ_0 can be canceled from both sides of (A3). Using (A4) a second time together with the result[20]

$$\frac{1}{\pi}\int_0^K \frac{dk}{(k^2 v_F^2 + \Delta_0^2)^{1/2}}\frac{\omega_0^2}{k^2 v_F^2 + \kappa_0^2 v_F^2} = \frac{1}{\pi}\frac{\omega_0}{v_F}\tan^{-1}\frac{\omega_0}{\kappa_0 v_F} = \frac{1}{\pi}\frac{\omega_0}{v_F}\left[\frac{\pi}{2} - \tan^{-1}\left[\frac{\kappa_0 v_F}{\omega_0} \right] \right] , \tag{A5}$$

we see that the final term in (A3) becomes

$$- \frac{2g^2}{\omega_Q^2}(t_+ - t_0)\left[\frac{1}{\pi}\int_0^K \frac{dk}{(k^2 v_F^2 + \Delta_0^2)^{1/2}}\left[\kappa_0 v_F + \frac{\kappa_0 v_F \omega_0^2}{k^2 v_F^2 + \kappa_0^2 v_F^2} \right] - \frac{\omega_0}{2v_F} \right]$$

$$= - \frac{2g^2}{\omega_Q^2}(t_+ - t_-)\left[\kappa_0 v_F \frac{\omega_Q^2}{g^2} - \frac{1}{\pi}\frac{\omega_0}{v_F}\tan^{-1}\left[\frac{\kappa_0 v_F}{\omega_0} \right] \right] , \tag{A6}$$

which, upon expanding the $\tan^{-1}$, can be seen to be higher order in $\kappa_0 v_F$ than the remaining term—which is just the contribution of the positive-energy localized state—on the right-hand side of (A3). Thus ignoring the higher-order terms is precisely the frozen-valence-band approximation and is clearly valid to leading order. To leading order, then,

$$-\kappa_0 v_F(t_+ - t_-) \simeq -\frac{g^2}{\omega_Q^2}\frac{\omega_0}{2v_F}(t_+ - t_-) , \tag{A7}$$

or, since $\omega_0 = \Delta_0 + O(\kappa_0^2 v_F^2)$, this self-consistency constraint requires

$$\kappa_0 v_F = \frac{g^2 \Delta_0}{2\omega_Q^2 v_F} , \tag{A8}$$

which is precisely the result [(4.13)] found in the text.

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[28]We stress this point because the SSH Hamiltonian can also be studied in cases other than that of a half-filled band. In particular, the $\frac{1}{3}$-filled case predicts exotic nonintegrally charged excitations and may be applicable to, e.g., tetrahiafulvalene-tetracyanoquinodimethane at 19 kbar. See Ref. 15.

[29]The SSH model does not, however, include Coulomb interactions among the electrons. This is potentially its greatest defect, and further work attempting to incorporate both electron-electron and electron-phonon interactions is needed.

[30]This value of α is deduced from an assured dimerization gap of $E_g \equiv 2\Delta_0 = 1.4$ eV.

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[33]For consistency and clarity, in (2.2) we have shown the lattice kinetic energy in the Heisenberg representation, rather than the Schrödinger representation as in Refs. 26, 27, and 31. This should cause no confusion in particular because we shall be treating the lattice degrees of freedom classically (the adiabatic approximation) and shall in any case be interested primarily in static excitations.

[34]As we discuss later, this limit is not achieved in *trans*-$(CH)_x$, and thus there remain quantitative differences between the two polarons. Nonetheless, it is important to realize that these models are in fact describing the same object.

[35]The observation that systems of quite different discrete structures often lead to equivalent polarons in the continuum limit was stressed in Ref. 31, p. 338.

[36]For consistency with previous work, we use units with $\hbar = 1$. With $\hbar \neq 1$, Eq. (2.5b) reads $\hbar v_F = 2t_0 a$.

[37]To obtain the explicit form of (3.2) we have effectively added $2Ja_n^{(0)}$ to both sides of the equation. This simply amounts to a shift of the electronic energy eigenvalue $\epsilon = \epsilon' + 2J$.

[38]For comparative purposes we follow the conventions of Refs. 26, 27, 31, and 32 in which n is a dimensionless site index. Hence no factors of the lattice spacing occur in (3.3).

[39]For an early but extensive review, see A. C. Scott, F. Y. F. Chu, and D. W. McLaughlin, Proc. IEEE 61, 1443 (1973).

[40]We define the polaron binding energy to be the positive amount by which the localized polaron energy is lower than the lowest delocalized electron state.

[41]If, by analogy to (3.5), we take $1/\kappa_0$ as a measure of the

polaron extent, we obtain a width of $\simeq 10a$.

[42]In two of our previous papers (Ref. 20) we have stressed the analogy between the continumm electron-phonon model of *trans*-$(CH)_x$ and a model relativistic field theory. Here the analogy is again useful, for the limit in Eq. (4.1) corresponds precisely to the nonrelativistic limit—all momenta $(\kappa_0 v_F)$ small compared to masses (Δ_0)—of the "Dirac" equation (3.11) Thus the reduction carried out in (4.1)—(4.5) is precisely the familiar nonrelativistic reduction of the Dirac equation to the Schrödinger equation and one could indeed apply the well-known Foldy-Wouthuysen transformation and techniques to make our simple arguments rigorous and to calculate higher terms in $1/\Delta_0$ systematically. For simplicity, we carry out the reduction directly.

[43]Note that this particular reduction holds only for states with $\epsilon_n \simeq \Delta_0 + O(k^2)$. For states in the valence band, $\epsilon_n \simeq -\Delta_0 + O(k^2)$, $\psi^{(2)}$ is the large component and $\psi^{(1)}$

is determined in terms of it. Furthermore, as the derivative in (4.4) suggests, in each case for large k, i.e., states far from the bottom of the band, one cannot make this reduction.

[44]For simplicity, we focus here on the electron polaron. The argument can also be made for a hole polaron.

[45]For the analogous problem in the field-theory context, the weakly bound limit can be achieved by letting N, the internal symmetry index, become large. For the quasi-one-dimensional condensed-matter system, one always has $N = 2$, since N corresponds to the two spin states of the electron.

[46]M. Nakahara and K. Maki, Phys. Rev. B 25, 7789 (1982); E. Fradkin and J. Hirsch, Phys. Rev. Lett. 49, 402 (1982); Phys. Rev. B (in press).

[47]By the electron-hole symmetry referred to earlier, the other allowed localized transition for the electron polaron, valance band $\rightarrow +\omega_0$, equals α_3.