Theory of one-dimensional solitons, polarons, and multipolarons: An alternative formulation

Kihong Kim*
Department of Molecular Science and Technology, Ajou University, Suwon 442-749, Korea

Dong-Hun Lee
Department of Astronomy and Space Science, Kyung Hee University, Yongin 449-900, Korea
(Received 4 August 1999)

We develop an alternative formulation of the theory of solitons, polarons, and multipolarons in quasi-one-dimensional degenerate and nondegenerate conducting polymers, starting from the continuum Hamiltonian introduced by Brazovskii and Kirova. Based on a convenient real-space representation of the electron Green function in one dimension, we present a simple method of calculating the Green function and the density of states in the presence of a single soliton or polaron defect, through which we derive exact expressions for the soliton, polaron, and multipolaron excitation energies and the self-consistent gap functions for an arbitrary value of the electron-phonon coupling constant. We apply our results to *cis*-polyacetylene.

I. INTRODUCTION

A wide variety of fascinating physical phenomena occur in quasi-one-dimensional materials with a Peierls-Frölich ground state.[1,2] In particular, the proposal[3–7] that nonlinear excitations such as solitons and polarons play a crucial role in the electronic properties of conjugated conducting polymers and other related materials have attracted great interest over the past two decades.[2,8–11] Experimental and theoretical efforts to confirm the existence of these nonlinear excitations and to clarify their properties are being continued to the present day.[12–16]

In a large number of theoretical studies of solitons and polarons, the electron-electron interaction is ignored[17] and the lattice motion is treated classically. A simple lattice model of noninteracting electrons in one dimension coupled to phonons was introduced by Su, Schrieffer, and Heeger[4] and has been applied mainly to numerical studies of *trans*-polyacetylene $[(\mathrm{CH})_x]$, which is a representative conjugated polymer with two degenerate ground states. A continuum version of this model derived by Takayama, Lin-Liu, and Maki[18] admits exact soliton and polaron solutions and has been the starting point in a number of analytical studies.[7,19] In order to treat nondegenerate materials with a unique ground state and a higher-energy metastable state such as *cis*-polyacetylene, Brazovskiĭ and Kirova derived a generalized version of the continuum model, which contains a new parameter, Δ_e, representing the *extrinsic* gap in the electronic spectrum that exists even in the absence of the Peierls distortion.[6] When $\Delta_e=0$, the model of Brazovskiĭ and Kirova reduces to that of Takayama, Lin-Liu, and Maki. If $\Delta_e\neq 0$, it does not admit the soliton solution, but allows the so-called multipolaron solutions in addition to the polaron solution.

In this paper, we reformulate the theory of solitons, polarons, and multipolarons, starting from the continuum Hamiltonian introduced by Brazovskiĭ and Kirova, which can describe both degenerate and nondegenerate conducting polymers depending on the value of Δ_e. We develop an efficient method for calculating the Green functions associated with the nonlinear excitations, based on a convenient real-space representation of the Green function in one dimension. Using the density of states expression obtained from the Green function, we compute the soliton, polaron, and multipolaron excitation energies and the related self-consistent gap functions *exactly* for an *arbitrary* value of the electron-phonon coupling constant. These results are usually presented in the weak electron-phonon coupling limit in the literature and, to the best of our knowledge, have never been written down explicitly before. Our method, which involves only concepts familiar in condensed-matter physics, is simple and transparent and has the advantage of being readily generalizable to more difficult problems such as the influence of disorder on solitons and polarons.

In the next section, we introduce the Hamiltonian and the soliton wave function. The polaron case will be discussed in Appendix A. In Sec. III and Appendixes A and B, we describe our method for calculating the Green function and the density of states. In Sec. IV, we compute the soliton, polaron, and multipolaron excitation energies and the self-consistent gap functions and apply the results to *cis*-polyacetylene. In Sec. V, we conclude the paper with some remarks.

II. HAMILTONIAN AND WAVE FUNCTIONS

We consider the continuum Hamiltonian of quasi-one-dimensional conducting polymers and related materials first introduced by Brazovskiĭ and Kirova,[6,20]

$$H=\sum_s \int dx\, \Psi_s^\dagger(x)\left\{-i\hbar v_F\sigma_3\frac{d}{dx} +[\Delta_i(x)+\Delta_e]\sigma_1\right\}\Psi_s(x)+\frac{1}{\pi\hbar v_F\lambda}\int dx\,\Delta_i^2(x), \tag{1}$$

where v_F is the Fermi velocity and λ is the dimensionless electron-phonon coupling constant. (For a precise definition of λ in terms of the parameters of the lattice model, refer to Ref. 21.) σ_i's $(i=1,2,3)$ are Pauli matrices. The (real-valued) gap function is written as $\Delta(x)=\Delta_i(x)+\Delta_e$, where

$\Delta_i(x)$ is the *intrinsic* gap function, which is sensitive to electron-phonon coupling and varies slowly on the scale of a lattice spacing, and Δ_e is a constant *extrinsic* component. The time derivative of $\Delta_i(x)$ is assumed to be sufficiently small that the lattice kinetic energy can be ignored. $\Psi_s(x)$, with $s=\uparrow,\downarrow$ being the spin index, is the two-component electron wave function for noninteracting electrons moving to the right (ψ_{1s}) and to the left (ψ_{2s}):

$$\Psi_s(x)=\begin{pmatrix}\psi_{1s}(x)\\ \psi_{2s}(x)\end{pmatrix}. \tag{2}$$

From the Hamiltonian, we obtain the Dirac-type equation for the electron wave functions

$$\begin{pmatrix} -i\hbar v_F\dfrac{d}{dx} & \Delta(x)\\ \Delta(x) & i\hbar v_F\dfrac{d}{dx}\end{pmatrix}\begin{pmatrix}\psi_{1s}(x)\\ \psi_{2s}(x)\end{pmatrix}=E\begin{pmatrix}\psi_{1s}(x)\\ \psi_{2s}(x)\end{pmatrix} \tag{3}$$

and the self-consistent gap equation

$$\Delta_i(x)=\Delta(x)-\Delta_e=-\frac{\pi\hbar v_F\lambda}{2}{\sum}'\,[\psi_{1s}(x)\psi_{2s}^*(x)+\psi_{2s}(x)\psi_{1s}^*(x)], \tag{4}$$

where the prime on the summation symbol indicates the sum is over all *occupied* electronic states.

We distinguish between the two cases with $\Delta_e=0$ and $\Delta_e>0$. Let us first consider the case with $\Delta_e=0$. Then the Hamiltonian has two degenerate ground states with $\Delta(x)=\Delta_i(x)=\pm\Delta_0$, where $\Delta_0(>0)$ is the self-consistent uniform Peierls gap parameter. In this paper, we focus on nonuniform solutions for the gap function. The best-known ones are the single soliton and the single polaron. Here we discuss the soliton and put all the algebra for the polaron in Appendix A. The spatial variation is set by the coherence length, a scale defined by the Fermi velocity and the uniform gap:

$$\xi=\frac{\hbar v_F}{\Delta_0}. \tag{5}$$

A second dimensionless parameter κ is important for polarons and is defined and discussed in Appendix A. The spatial variation of the order parameter for a single soliton located at $x=0$ is

$$\frac{\Delta(x)}{\Delta_0}=\tanh\left(\frac{x}{\xi}\right). \tag{6}$$

The resulting (unnormalized) wave functions for unbound states with $|E|\geqslant\Delta_0$ can be written as

$$\begin{aligned}\psi_{1s}(x)&=\phi_1(x)=e^{ikx}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}-ik\xi\right],\\ \psi_{2s}(x)&=\phi_2(x)=-ie^{ikx}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}-ik\xi\right],\end{aligned} \tag{7}$$

where the quantum number k is related to the energy eigenvalue by $E^2=(\hbar v_F k)^2+\Delta_0^2$.[22] For a reason to be explained in the next section, we introduce another equivalent set of wave functions

$$\begin{aligned}\psi_{1s}(x)&=\tilde{\phi}_1(x)=ie^{-ikx}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}+ik\xi\right],\\ \psi_{2s}(x)&=\tilde{\phi}_2(x)=e^{-ikx}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}+ik\xi\right],\end{aligned} \tag{8}$$

which are trivially obtained from Eq. (7) by replacing k with $-k$ and multiplying the wave functions by i. We omitted the spin indices in the notations $\phi_1,\phi_2,\tilde{\phi}_1$, and $\tilde{\phi}_2$ because the wave functions are spin independent. There is also a soliton bound state located at $E=0$ and described by the wave functions

$$\psi_{1s}(x)=\frac{1}{2\sqrt{\xi}}\,\mathrm{sech}\left(\frac{x}{\xi}\right),\quad \psi_{2s}(x)=\frac{-i}{2\sqrt{\xi}}\,\mathrm{sech}\left(\frac{x}{\xi}\right). \tag{9}$$

Though there is no electronic state for $0<|E|<\Delta_0$, we can still use the wave functions (7) and (8) for computing the subgap Green functions.

When the extrinsic component of the gap function, Δ_e, is nonzero, the double degeneracy of the ground state is broken and a higher-energy metastable state with a uniform gap appears. For $\Delta_e>0$, the constant intrinsic gap Δ_i can be taken to be positive in the Peierls ground state and negative in the metastable state.[21] In both states, the uniform Peierls gap parameter is given by $\Delta_0=|\Delta_i+\Delta_e|$. We caution the readers that we will use the same notation Δ_0 and the definition (5), regardless of the value of Δ_e. It turns out that the soliton solution is not allowed in nondegenerate cases because Eqs. (6) and (7) do not satisfy the gap equation (4) for nonzero Δ_e.

III. GREEN FUNCTION AND THE DENSITY OF STATES

In this section, we compute the retarded and advanced 2×2 matrix Green functions G^+ and G^- associated with Eq. (3). For that purpose, we introduce two linearly independent wave functions ψ and $\tilde{\psi}$ that satisfy Eq. (3) in the interval $-L\leqslant x\leqslant L$ and the boundary conditions in which $\psi(-L)$ and $\tilde{\psi}(L)$ do not diverge as L becomes large, whereas $\psi(L)$ and $\tilde{\psi}(-L)$ diverge.[15] We write the Green function in the form

$$G(x,y|E)=\begin{pmatrix}G_{11}(x,y|E) & G_{12}(x,y|E)\\ G_{21}(x,y|E) & G_{22}(x,y|E)\end{pmatrix}=\begin{cases}\dfrac{i}{\hbar v_F(\psi_1\tilde{\psi}_2-\psi_2\tilde{\psi}_1)}\begin{pmatrix}\tilde{\psi}_1(x)\psi_2(y) & \tilde{\psi}_1(x)\psi_1(y)\\ \tilde{\psi}_2(x)\psi_2(y) & \tilde{\psi}_2(x)\psi_1(y)\end{pmatrix} & \text{if } x>y\\ \dfrac{i}{\hbar v_F(\psi_1\tilde{\psi}_2-\psi_2\tilde{\psi}_1)}\begin{pmatrix}\psi_1(x)\tilde{\psi}_2(y) & \psi_1(x)\tilde{\psi}_1(y)\\ \psi_2(x)\tilde{\psi}_2(y) & \psi_2(x)\tilde{\psi}_1(y)\end{pmatrix} & \text{if } x<y,\end{cases} \tag{10}$$

where $(\psi_1\tilde{\psi}_2-\psi_2\tilde{\psi}_1)$ is a constant independent of x.[15,23,24] We obtain $G^+(G^-)$ by solving for wave functions with Im E a small positive (negative) number.

The wave functions for the single-soliton case, (ϕ_1,ϕ_2) and $(\tilde{\phi}_1,\tilde{\phi}_2)$, defined by Eqs. (7) and (8), do not satisfy the necessary boundary conditions, and therefore cannot be used in the representation (10). However, it is possible to construct two new solutions (ψ_1,ψ_2) and $(\tilde{\psi}_1,\tilde{\psi}_2)$, which satisfy the boundary conditions, by a linear superposition of (ϕ_1,ϕ_2) and $(\tilde{\phi}_1,\tilde{\phi}_2)$:

$$\begin{aligned}
\psi_1&=e^{ikL}\phi_1+e^{-ikL}\tilde{\phi}_1\\
&=e^{ik(x+L)}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}-ik\xi\right]\\
&\quad+ie^{-ik(x+L)}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}+ik\xi\right],\\
\psi_2&=e^{ikL}\phi_2+e^{-ikL}\tilde{\phi}_2\\
&=-ie^{ik(x+L)}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}-ik\xi\right]\\
&\quad+e^{-ik(x+L)}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}+ik\xi\right],\\
\tilde{\psi}_1&=e^{-ikL}\phi_1+e^{ikL}\tilde{\phi}_1\\
&=e^{ik(x-L)}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}-ik\xi\right]\\
&\quad+ie^{-ik(x-L)}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}+ik\xi\right],\\
\tilde{\psi}_2&=e^{-ikL}\phi_2+e^{ikL}\tilde{\phi}_2\\
&=-ie^{ik(x-L)}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}-ik\xi\right]\\
&\quad+e^{-ik(x-L)}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}+ik\xi\right].
\end{aligned}\tag{11}$$

First, we calculate the Green function for $E\geqslant\Delta_0$. We introduce a small imaginary part $\tilde{E}$ to the energy and replace E by $E+i\tilde{E}$. Then the quantum number k acquires an imaginary part and is replaced by $k+i\tilde{k}$ such that $E\tilde{E}=(\hbar v_F)^2k\tilde{k}$. If we choose $\hbar v_Fk=-\sqrt{E^2-\Delta_0^2}\leqslant 0$,[25] $\tilde{E}$ and $\tilde{k}$ have opposite signs. In order to obtain the retarded Green functions, we assume $\tilde{E}>0$ and take the $L\to\infty$ limit first to simplify Eq. (11) using the fact that $\tilde{k}$ is negative and $e^{\tilde{k}L}$ vanishes in this case. Finally, we take the $\tilde{E}\to 0$ limit to obtain the simplified wave functions for use in calculating the retarded Green functions:

$$\begin{aligned}
\psi_1&=e^{ik(x+L)}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}-ik\xi\right],\\
\psi_2&=-ie^{ik(x+L)}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}-ik\xi\right],\\
\tilde{\psi}_1&=ie^{-ik(x-L)}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}+ik\xi\right],\\
\tilde{\psi}_2&=e^{-ik(x-L)}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}+ik\xi\right].
\end{aligned}\tag{12}$$

Similarly, for the advanced Green functions, we assume $\tilde{E}<0$ and obtain

$$\begin{aligned}
\psi_1&=ie^{-ik(x+L)}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}+ik\xi\right],\\
\psi_2&=e^{-ik(x+L)}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}+ik\xi\right],\\
\tilde{\psi}_1&=e^{ik(x-L)}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}-ik\xi\right],\\
\tilde{\psi}_2&=-ie^{ik(x-L)}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}-ik\xi\right].
\end{aligned}\tag{13}$$

These wave functions satisfy the required boundary conditions that $\psi_{1,2}(L)$ and $\tilde{\psi}_{1,2}(-L)$ diverge as L goes to infinity, whereas $\psi_{1,2}(-L)$ and $\tilde{\psi}_{1,2}(L)$ do not diverge. Substituting Eqs. (12) and (13) into Eq. (10), we find

$$\begin{aligned}
G^{\pm}(x,x')&=\frac{\mp i}{\hbar v_F}\frac{\exp[\pm i\sqrt{(E/\Delta_0)^2-1}\ \ |x-x'|/\xi]}{4\sqrt{(E/\Delta_0)^2-1}}\\
&\quad\times\left\{2\left[\frac{E}{\Delta_0}\mathbf{1}+\sigma_1\pm\sqrt{(E/\Delta_0)^2-1}\ \ \mathrm{sgn}(x-x')\sigma_3\right]\right.\\
&\quad+\frac{\Delta_0}{E}[1-t_0t_0'\mp i\sqrt{(E/\Delta_0)^2-1}\ \ |t_0-t_0'|]\\
&\quad\left.\times(\sigma_2-\mathbf{1})+(t_0+t_0'-2)\sigma_1+i(t_0-t_0')\sigma_3\right\},
\end{aligned}\tag{14}$$

where $\mathbf{1}$ is the unit matrix and t_0 and t_0' are defined by

$$t_0=\tanh\left(\frac{x}{\xi}\right),\qquad t_0'=\tanh\left(\frac{x'}{\xi}\right).\tag{15}$$

When $E\leqslant-\Delta_0$, we choose $\hbar v_Fk=\sqrt{E^2-\Delta_0^2}$.[25] Then $\tilde{E}$ and $\tilde{k}$ have opposite signs. A calculation similar to that for $E\geqslant\Delta_0$ leads to the symmetry relationship

$$\begin{aligned}
G_{11}^{\pm}(x,x'|E)&=-G_{22}^{\mp}(x,x'|-E),\\
G_{12}^{\pm}(x,x'|E)&=G_{21}^{\mp}(x,x'|-E).
\end{aligned}\tag{16}$$

The subgap Green function for $0<|E|<\Delta_0$ will be derived in Appendix B.

With the exact Green function in hand, it is a straightforward matter to compute the local electronic density of states (per spin) $\rho_s(x,E)$:

$$\rho_s(x,E) = -\frac{1}{\pi}\mathrm{Im}\ \mathrm{Tr}\ G^+(x,x|E) = \begin{cases} \dfrac{1}{\pi\hbar v_F}\dfrac{1}{\sqrt{E^2-\Delta_0^2}}\left[|E| - \dfrac{\Delta_0^2}{2|E|\cosh^2(x/\xi)}\right] & \text{if} \quad |E| \geq \Delta_0 \\ 0 & \text{if} \quad 0<|E|<\Delta_0 . \end{cases} \tag{17}$$

The spatially averaged density of states $\rho_s(E)$ is given by

$$\rho_s(E) = \frac{1}{2L}\int_{-L}^{L} dx\, \rho_s(x,E) = \begin{cases} \rho_0(E) + \delta\rho_s(E) & \text{if} \quad |E| \geq \Delta_0 \\ 0 & \text{if} \quad 0<|E|<\Delta_0 , \end{cases} \tag{18}$$

where the density of states in the Peierls ground state, $\rho_0(E)$, and the correction to the density of states in the presence of a single soliton, $\delta\rho_s(E)$, are

$$\rho_0(E) = \frac{1}{\pi\hbar v_F}\frac{|E|}{\sqrt{E^2-\Delta_0^2}},$$
$$\delta\rho_s(E) = -\frac{1}{2\pi\hbar v_F}\frac{\Delta_0^2}{|E|\sqrt{E^2-\Delta_0^2}}\frac{\xi}{L}\tanh\left(\frac{L}{\xi}\right). \tag{19}$$

In the polaron case, we derive the local electronic density of states $\rho_p(x,E)$ for $|E| \geq \Delta_0$ from the Green functions derived in Appendix A:

$$\rho_p(x,E) = \frac{1}{\pi\hbar v_F}\frac{|E|}{\sqrt{E^2-\Delta_0^2}} \times \left\{1 - \frac{\kappa^2\Delta_0^2}{2(E^2-E_0^2)}\left[\frac{1}{\cosh^2[\kappa(x+x_0)/\xi)} + \frac{1}{\cosh^2[\kappa(x-x_0)/\xi]}\right]\right\}, \tag{20}$$

where $E_0 = \Delta_0\sqrt{1-\kappa^2}$ and x_0 is defined by Eq. (A1). The density of states when $0 \leq |E| < \Delta_0$ and $E \neq \pm E_0$ is zero. The spatially averaged density of states, $\rho_p(E)$, for $|E| \geq \Delta_0$ is given by

$$\rho_p(E) = \rho_0(E) + \delta\rho_p(E),$$
$$\delta\rho_p(E) = -\frac{1}{\pi\hbar v_F}\frac{|E|}{\sqrt{E^2-\Delta_0^2}}\frac{\kappa\Delta_0^2}{(E^2-E_0^2)}\frac{\xi}{2L} \times \left[\tanh\left(\frac{\kappa(L+x_0)}{\xi}\right) + \tanh\left(\frac{\kappa(L-x_0)}{\xi}\right)\right]. \tag{21}$$

IV. SOLITON, POLARON, AND MULTIPOLARON ENERGIES

A. Self-consistency in the uniform case

In this subsection, we reformulate the self-consistency equation (4) in the uniform case with a constant gap function in terms of the Green functions. First, we write the total energy (E_T) per unit length in terms of the electronic density of states per spin $\rho(E,\Delta_0)$:

$$\frac{E_T}{2L} = \frac{\Delta_i^2}{\pi\hbar v_F\lambda} + \sum_s \int_{-E_c}^{-\Delta_0} dE\ \ E\rho(E,\Delta_0)$$
$$= \frac{\Delta_i^2}{\pi\hbar v_F\lambda} - 2\int_{\Delta_0}^{E_c} dE\, E\rho(E,\Delta_0), \tag{22}$$

where the cutoff energy E_c, introduced to overcome the well-known difficulty of the continuum model that its energy spectrum is unbounded, is a function of the gap parameter $\Delta_0 = |\Delta_i + \Delta_e|$ and satisfies the requirement that the integrated density of states,

$$N(E_c(\Delta_0),\Delta_0) = \int_{\Delta_0}^{E_c} dE\, \rho(E,\Delta_0), \tag{23}$$

is a constant independent of Δ_0. As mentioned earlier, in nondegenerate cases with $\Delta_e > 0$, the intrinsic gap Δ_i can be taken to be positive in the ground state and negative in the metastable state. Equivalently, the absolute value $|\Delta_i|$ satisfies $|\Delta_i| = \Delta_0 - \Delta_e$ in the ground state and $|\Delta_i| = \Delta_0 + \Delta_e$ in the metastable state. Applying the self-consistency condition

$$\frac{\partial}{\partial\Delta_0}\left[\frac{E_T(\Delta_0)}{2L}\right] = 0 \tag{24}$$

to Eq. (22) and using the relationships[26]

$$\frac{\partial N(E,\Delta_0)}{\partial E} = \rho(E,\Delta_0),$$
$$\frac{d}{d\Delta_0}N(E_c(\Delta_0),\Delta_0) = 0, \tag{25}$$
$$\frac{\partial N(E,\Delta_0)}{\partial\Delta_0} = \frac{1}{\pi}\,\mathrm{Im}[G_{12}^+(x,x|E) + G_{21}^+(x,x|E)],$$

we derive a new form of the self-consistency equation,

$$|\Delta_i| = -\pi\hbar v_F \lambda \int_{\Delta_0}^{E_c} dE \frac{\partial N(E,\Delta_0)}{\partial \Delta_0}$$
$$= -\hbar v_F \lambda \int_{\Delta_0}^{E_c} dE \, \mathrm{Im}[G_{12}^{+}(x,x|E) + G_{21}^{+}(x,x|E)], \tag{26}$$

in a straightforward manner. Since in the uniform case

$$G_{12}^{+}(x,x|E) = G_{21}^{+}(x,x|E) = \frac{-i}{2\hbar v_F} \frac{\Delta_0}{\sqrt{E^2-\Delta_0^2}}, \tag{27}$$

we obtain

$$|\Delta_i| = \lambda \int_{\Delta_0}^{E_c} dE \frac{\Delta_0}{\sqrt{E^2-\Delta_0^2}}$$
$$= \lambda \Delta_0 \cosh^{-1}\left(\frac{E_c}{\Delta_0}\right) = \lambda \Delta_0 \ln\left(\frac{E_c + \sqrt{E_c^2-\Delta_0^2}}{\Delta_0}\right), \tag{28}$$

which reduces to

$$E_c = \Delta_0 \cosh\left(\frac{1}{\lambda}\right) \tag{29}$$

in the degenerate case where $\Delta_0 = |\Delta_i|$. One can easily see that, in the weak-coupling limit, Eq. (28) is approximated by

$$\Delta_0 = 2E_c \exp\left[-\frac{1}{\lambda}\left(1 \mp \frac{\Delta_e}{\Delta_0}\right)\right], \tag{30}$$

where the upper (lower) sign corresponds to the ground (metastable) state. The total energy per unit length, obtained from Eq. (22), is given by

$$\frac{E_T}{2L} = \frac{\Delta_i^2}{\pi\hbar v_F \lambda} - \frac{\Delta_0^2}{\pi\hbar v_F}\left\{\cosh^{-1}\left(\frac{E_c}{\Delta_0}\right) + \frac{1}{2}\sinh\left[2\cosh^{-1}\left(\frac{E_c}{\Delta_0}\right)\right]\right\}, \tag{31}$$

which, using the gap equation (28), can be rewritten as

$$\frac{E_T}{2L} = \frac{\Delta_i^2}{\pi\hbar v_F \lambda} - \frac{\Delta_0^2}{\pi\hbar v_F}\left[\frac{|\Delta_i|}{\lambda\Delta_0} + \frac{1}{2}\sinh\left(\frac{2|\Delta_i|}{\lambda\Delta_0}\right)\right]. \tag{32}$$

B. Soliton energy

We compute the soliton excitation energy E_s in the degenerate case using the density of states expression obtained in Sec. III. Regardless of the number of electrons occupying the midgap state with $E=0$, E_s is given by

$$E_s = \frac{1}{\pi\hbar v_F \lambda}\int_{-L}^{L} dx \, \Delta_0^2[\tanh^2(x/\xi) - 1]$$
$$-4L\left[\int_{\Delta_0}^{E_c^s} dE \, E\rho_s(E) - \int_{\Delta_0}^{E_c^0} dE \, E\rho_0(E)\right], \tag{33}$$

where E_c^s is the energy cutoff in the presence of a soliton defect, while $E_c^0[=\Delta_0 \cosh(1/\lambda)]$ is the cutoff in the Peierls ground state. E_c^s and E_c^0 are related by the condition that the total number of electronic states in both cases has to be the same:

$$\frac{1}{2} + 2L\int_{\Delta_0}^{E_c^s} dE \, \rho_s(E) = 2L\int_{\Delta_0}^{E_c^0} dE \, \rho_0(E), \tag{34}$$

where the number 1/2 on the left-hand side accounts for the midgap state (per spin). Substituting Eqs. (18) and (19) into Eq. (34) and using the fact that E_c^s differs from E_c^0 by a term of order $1/L$, we derive

$$\frac{E_c^s}{\Delta_0} = \frac{E_c^0}{\Delta_0} - \frac{\xi}{2L}\tanh\left(\frac{1}{\lambda}\right)\cot^{-1}\left[\sinh\left(\frac{1}{\lambda}\right)\right] + O\left(\frac{1}{L^2}\right). \tag{35}$$

Using this in Eq. (33), we find, in the $L\to\infty$ limit,

$$E_s = \frac{2}{\pi}\Delta_0 \cosh\left(\frac{1}{\lambda}\right)\cot^{-1}\left[\sinh\left(\frac{1}{\lambda}\right)\right], \tag{36}$$

which reduces to the well-known value of the soliton excitation energy in the weak-coupling limit, $2\Delta_0/\pi$, as λ goes to zero and increases monotonically to Δ_0 as λ grows to infinity. In Fig. 1, we plot the energy of a single soliton-antisoliton pair, $2E_s$, together with the polaron energy in the degenerate case to be obtained in the next subsection [Eq. (42)], as a function of λ.

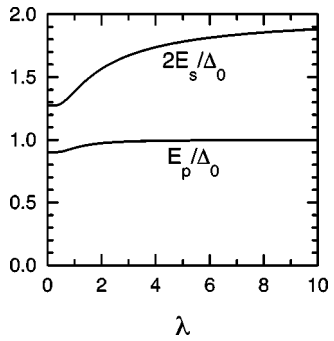

FIG. 1. The energy of a soliton-antisoliton pair, $2E_s$, and the polaron energy in the degenerate case, E_p, versus the electron-phonon coupling constant, λ.

C. Polaron and multipolaron energies

The polaron excitation energy E_p is obtained in a manner similar to that in the previous subsection. Defining the electron occupation numbers of the subgap states at $E=E_0$ and $-E_0$ as n_+ and $n_-(n_+, n_- = 0,1,2)$, we have

$$E_p = \frac{1}{\pi\hbar v_F \lambda}\int_{-L}^{L} dx \, \Delta_i^2\left\{\left[1 - \frac{\Delta_0}{\Delta_i}\kappa(t_+ - t_-)\right]^2 - 1\right\}$$
$$+(n_+ - n_-)E_0 - 4L\left[\int_{\Delta_0}^{E_c^p} dE \, E\rho_p(E) - \int_{\Delta_0}^{E_c^0} dE \, E\rho_0(E)\right], \tag{37}$$

where the constant $\Delta_i(=\Delta_0 - \Delta_e > 0)$ satisfying Eq. (28) is the intrinsic gap in the ground state and E_c^p is the energy

TABLE I. Polaron and multipolaron states in *cis*-polyacetylene when $\lambda=0.4$ and $\Gamma=0.15$. $N=n_+-n_-+2$ is the effective occupation number, $Q=2-n_+-n_-$ is the effective charge, θ is the angle (in radians) defined by Eq. (41) and E_p is the excitation energy.

n_+	n_-	N	Q	θ	E_p/Δ_0	Interpretation
1	2	1	−1	0.66	0.93	Electron (e) polaron
0	1	1	+1	0.66	0.93	Hole (h) polaron
2	2	2	−2	1.19	1.51	*e-e* bipolaron
1	1	2	0	1.19	1.51	*e-h* bipolaron (or exciton)
0	0	2	+2	1.19	1.51	*h-h* bipolaron
2	1	3	−1	1.41	1.75	*e-e-h* tripolaron
1	0	3	+1	1.41	1.75	*e-h-h* tripolaron
2	0	4	0	1.48	1.87	*e-e-h-h* quadripolaron

cutoff in the presence of a polaron defect. We emphasize that the coherence length ξ appearing in the definitions of t_+ and t_- [Eq. (A3)] is defined by $\hbar v_F/\Delta_0$, not by $\hbar v_F/\Delta_i$. Equation (34) is replaced by

$$1+2L\int_{\Delta_0}^{E_c^p} dE\,\rho_p(E)=2L\int_{\Delta_0}^{E_c^0} dE\,\rho_0(E). \tag{38}$$

Substituting Eq. (21) into the above equation, we find

$$\frac{E_c^p}{\Delta_0}=\frac{E_c^0}{\Delta_0}-\frac{\xi}{L}\tanh\left(\frac{\Delta_i}{\lambda\Delta_0}\right)\cot^{-1}\left[\frac{1}{\kappa}\sinh\left(\frac{\Delta_i}{\lambda\Delta_0}\right)\right]+O\left(\frac{1}{L^2}\right). \tag{39}$$

The polaron energy E_p to order 1 follows from this and Eq. (37) and is equal to

$$\begin{aligned}E_p=&(n_+-n_-+2)E_0\\&+\frac{4}{\pi}\Delta_0\cosh\left(\frac{\Delta_i}{\lambda\Delta_0}\right)\cot^{-1}\left[\frac{1}{\kappa}\sinh\left(\frac{\Delta_i}{\lambda\Delta_0}\right)\right]\\&-\frac{4}{\pi}E_0\tan^{-1}\left[\frac{\kappa\Delta_0}{E_0}\coth\left(\frac{\Delta_i}{\lambda\Delta_0}\right)\right]\\&+\frac{4}{\pi}\Delta_0\Gamma(\tanh^{-1}\kappa-\kappa),\end{aligned} \tag{40}$$

where $\Gamma\equiv\Delta_e/\lambda\Delta_0$. The self-consistency condition is equivalent to the condition that E_p has to be minimized with respect to κ for given values of n_+ and n_-. Applying a weaker condition for which E_p takes an extremal value, that is, $\partial E_p/\partial\kappa=0$, to Eq. (40), we obtain

$$\tan^{-1}\left[\tan\theta\coth\left(\frac{1}{\lambda}-\Gamma\right)\right]+\Gamma\tan\theta=\frac{\pi}{4}(n_+-n_-+2), \tag{41}$$

$$0\leqslant\theta\leqslant\frac{\pi}{2}$$

where θ is defined by $\kappa=\sin\theta$ and $E_0=\Delta_0\cos\theta$. It turns out that, in the degenerate case with $\Gamma=0$, stable solutions that satisfy Eq. (41) and minimize Eq. (40) exist only for the electron polaron state ($n_+=1$, $n_-=2$), with the effective charge $Q\equiv2-n_+-n_-=-1$ and the spin $S=1/2$, and the hole polaron state ($n_+=0$, $n_-=1$), with $Q=+1$ and $S=1/2$. In both cases, $\theta=\tan^{-1}[\tanh(1/\lambda)]$ and

$$\kappa=\frac{\tanh(1/\lambda)}{\sqrt{\tanh^2(1/\lambda)+1}},\quad E_0=\frac{\Delta_0}{\sqrt{\tanh^2(1/\lambda)+1}},$$
$$E_p=\frac{4}{\pi}\Delta_0\cosh(1/\lambda)\cot^{-1}[\sqrt{\cosh^2(1/\lambda)+\sinh^2(1/\lambda)}], \tag{42}$$

which reduce to $\kappa=1/\sqrt{2}$, $E_0=\Delta_0/\sqrt{2}$ and $E_p=2\sqrt{2}\Delta_0/\pi$ in the weak-coupling limit. The behavior of E_p as a function of λ in the degenerate case is shown in Fig. 1.

In the nondegenerate case with $\Gamma>0$, stable polaron and multipolaron (bipolaron, tripolaron, quadripolaron) solutions exist for all possible combinations of n_+ and n_- except for $n_+=0$ and $n_-=2$. There are three bipolaron solutions with effective occupation number $N\equiv n_+-n_-+2=2$. Both the electron-electron bipolaron ($n_+=n_-=2$, $Q=-2$) and the hole-hole bipolaron ($n_+=n_-=0$, $Q=+2$) have zero, spin while the electron-hole bipolaron ($n_+=n_-=1$, $Q=0$), which can also be called an exciton, exists in either spin singlet ($S=0$) or triplet ($S=1$) forms. More details about the interpretation of multipolaron solutions can be found in Refs. 2 and 9. Explicit values of κ,E_0, and E_p for given values of λ and Γ can be obtained only numerically. As a specific example of applying Eqs. (40) and (41), we consider the case of *cis*-polyacetylene. There is a considerable uncertainty in the precise values of λ and $\Gamma(=\Delta_e/\lambda\Delta_0)$. In order to make a rough estimate of the excitation energy, we use a set of the approximate values close to those assumed in, Ref. 21 which are $\lambda=0.4$, $\Delta_e=0.06$ eV, $\Delta_0=1$ eV, and therefore, $\Gamma=0.15$. The results are listed in Table I.

V. CONCLUSION

In the present paper, we have reformulated the theory of solitons, polarons, and multipolarons in both degenerate and nondegenerate conducting polymers. Especially, we have developed a simple method for calculating the Green function and the density of states in the presence of a soliton or polaron defect and computed the soliton, polaron, and multipolaron excitation energies and the self-consistent gap functions exactly for an arbitrary value of the electron-phonon coupling constant [see Eqs. (36) and (40)–(42)]. Our method can be generalized in a straightforward way to more complicated situations. In a previous work, Kim and Wilkins have devised an efficient numerical method for calculating the *exact* disorder-averaged Green function in the presence of a soliton or polaron defect and disorder.[15] It appears that, by combining this method with the results of the present work, one can study the disordered soliton or polaron problem in an exact and self-consistent manner. Work in this direction will be presented in a separate publication.

ACKNOWLEDGMENTS

We are grateful to John Wilkins for reading the manuscript and making valuable comments. This work has been supported by the Korea Research Foundation through Grant No. KRF-1999-015-DI0034 and the U.S. DOE, Basic Energy Sciences, Division of Materials Sciences.

APPENDIX A: POLARON GREEN FUNCTION

The spatial variation of the order parameter for a single polaron located at $x=0$ is given by

$$\frac{\Delta(x)}{\Delta_0}=1-\kappa\left\{\tanh\left[\frac{\kappa(x+x_0)}{\xi}\right]-\tanh\left[\frac{\kappa(x-x_0)}{\xi}\right]\right\}, \tag{A1}$$

$$\frac{x_0}{\xi}=\frac{1}{4\kappa}\ln\left(\frac{1+\kappa}{1-\kappa}\right), \quad 0<\kappa<1.$$

The dimensionless parameter κ appearing in this equation determines the shape of the polaron, which changes from an extremely shallow well centered at $x=0$ for $0<\kappa\ll 1$ to a well-separated pair of a soliton and an antisoliton located at x_0 and $-x_0$, respectively, as $\kappa\to 1$. This parameter cannot take an arbitrary value, since the self-consistent gap equation is not satisfied for every value of κ. When $\Delta_e=0$ and in the weak electron-phonon coupling limit (that is, the $\lambda\to 0$ limit), it turns out that κ has the unique value of $1/\sqrt{2}$, as will be shown in Sec. IV C.

In case of the single-polaron configuration, the exact unnormalized wave functions for unbound states with $|E|\geqslant\Delta_0$ can be written as[22]

$$\psi_{1s}(x)=\phi_1(x)=e^{ikx}\left[k\xi+\frac{E}{\Delta_0}-1+\gamma(1+i)t_+ -\delta(1-i)t_-\right], \tag{A2}$$

$$\psi_{2s}(x)=\phi_2(x)=e^{ikx}\left[k\xi-\frac{E}{\Delta_0}+1-\gamma(1-i)t_+ +\delta(1+i)t_-\right],$$

where t_+, t_-, γ, and δ are defined by

$$t_+=\tanh\left[\frac{\kappa(x+x_0)}{\xi}\right], \qquad t_-=\tanh\left[\frac{\kappa(x-x_0)}{\xi}\right], \tag{A3}$$

$$\gamma=\frac{\kappa}{2}\left(1+\frac{i\hbar k_F k}{E+\Delta_0}\right), \qquad \delta=\frac{\kappa}{2}\left(1-\frac{i\hbar k_F k}{E+\Delta_0}\right).$$

Similarly to the soliton case, we introduce an equivalent set of wave functions

$$\psi_{1s}(x)=\tilde{\phi}_1(x)=e^{-ikx}\left[k\xi-\frac{E}{\Delta_0}+1-\delta(1+i)t_+ +\gamma(1-i)t_-\right], \tag{A4}$$

$$\psi_{2s}(x)=\tilde{\phi}_2(x)=e^{-ikx}\left[k\xi+\frac{E}{\Delta_0}-1+\delta(1-i)t_+ -\gamma(1+i)t_-\right],$$

which are obtained from Eq. (A2) by replacing k with $-k$ and multiplying the wave functions by -1. In addition, there are two subgap polaron bound states located at $E=\pm E_0\equiv\pm\Delta_0\sqrt{1-\kappa^2}$, the wave functions for which we do not write down here explicitly. As in the soliton case, we can also use the wave functions (A2) and (A4) for computing the subgap Green functions when $0\leqslant|E|<\Delta_0$ and $E\neq\pm E_0$.

We superpose two independent solutions in the polaron case, Eqs. (A2) and (A4), to make two new wave functions (ψ_1,ψ_2) and $(\tilde{\psi}_1,\tilde{\psi}_2)$ satisfying the necessary boundary conditions. When $E\geqslant\Delta_0$, following the same procedure as in Sec. III, we obtain the simplified wave functions

$$\psi_1=e^{ik(x+L)}\left[k\xi+\frac{E}{\Delta_0}-1+\gamma(1+i)t_+ -\delta(1-i)t_-\right],$$

$$\psi_2=e^{ik(x+L)}\left[k\xi-\frac{E}{\Delta_0}+1-\gamma(1-i)t_+ +\delta(1+i)t_-\right], \tag{A5}$$

$$\tilde{\psi}_1=e^{-ik(x-L)}\left[k\xi-\frac{E}{\Delta_0}+1-\delta(1+i)t_+ +\gamma(1-i)t_-\right],$$

$$\tilde{\psi}_2=e^{-ik(x-L)}\left[k\xi+\frac{E}{\Delta_0}-1+\delta(1-i)t_+ -\gamma(1+i)t_-\right],$$

with $\hbar v_F k=-\sqrt{E^2-\Delta_0^2}$ [25] for computing the retarded Green functions and

$$\psi_1=e^{-ik(x+L)}\left[k\xi-\frac{E}{\Delta_0}+1-\delta(1+i)t_+ +\gamma(1-i)t_-\right],$$

$$\psi_2=e^{-ik(x+L)}\left[k\xi+\frac{E}{\Delta_0}-1+\delta(1-i)t_+ -\gamma(1+i)t_-\right], \tag{A6}$$

$$\tilde{\psi}_1=e^{ik(x-L)}\left[k\xi+\frac{E}{\Delta_0}-1+\gamma(1+i)t_+ -\delta(1-i)t_-\right],$$

$$\tilde{\psi}_2=e^{ik(x-L)}\left[k\xi-\frac{E}{\Delta_0}+1-\gamma(1-i)t_+ +\delta(1+i)t_-\right],$$

for the advanced Green functions. The Green functions obtained by substituting Eqs. (A5) and (A6) into Eq. (10) are

$$G^{\pm}(x,x')=\frac{\mp i}{\hbar v_F}\frac{\exp[\pm i\sqrt{(E/\Delta_0)^2-1}|x-x'|/\xi]}{4\sqrt{(E/\Delta_0)^2-1}}\left\{2\left(\frac{E}{\Delta_0}\mathbf{1}+\sigma_1\pm\sqrt{(E/\Delta_0)^2-1}\ \ \mathrm{sgn}(x-x')\sigma_3\right)\right.$$
$$+\frac{\kappa^2\Delta_0^2}{E_0^2-E^2}\left[\frac{E}{\Delta_0}\{([1-t_-t'_-\mp i\sqrt{(E/\Delta_0)^2-1}|t_--t'_-|/\kappa](\mathbf{1}-\sigma_2)\right.$$
$$+[1-t_+t'_+\mp i\sqrt{(E/\Delta_0)^2-1}|t_+-t'_+|/\kappa](\mathbf{1}+\sigma_2))\}+\{[1-(E/\Delta_0)^2]$$
$$\times(t_-+t'_--t_+-t'_+)/\kappa+2-t_-t'_+-t_+t'_-\mp i\sqrt{(E/\Delta_0)^2-1}[t_+t'_--t_-t'_+$$
$$+(t_--t'_-+t_+-t'_+)/\kappa]\mathrm{sgn}(x-x')\}\sigma_1+i\{\mp i\sqrt{(E/\Delta_0)^2-1}[2-t_-t'_+-t_+t'_-$$
$$\left.\left.+(t_-+t'_--t_+-t'_+)/\kappa]\mathrm{sgn}(x-x')+[1-(E/\Delta_0)^2](t_--t'_-+t_+-t'_+)/\kappa+t_+t'_--t_-t'_+\}\sigma_3\right]\right\}, \tag{A7}$$

The Green functions for $E\leqslant-\Delta_0$ are obtained using the symmetry relationship Eq. (16), which is valid in the polaron case, too.

When $0\leqslant|E|<\Delta_0$ and $E\neq\pm E_0$, we obtain

$$\psi_1=e^{q(x+L)}\left[-iq\xi+\frac{E}{\Delta_0}-1+\gamma(1+i)t_+-\delta(1-i)t_-\right],$$
$$\psi_2=e^{q(x+L)}\left[-iq\xi-\frac{E}{\Delta_0}+1-\gamma(1-i)t_+-\delta(1+i)t_-\right],$$
$$\tilde{\psi}_1=e^{-q(x-L)}\left[-iq\xi-\frac{E}{\Delta_0}+1-\delta(1+i)t_++\gamma(1-i)t_-\right], \tag{A8}$$
$$\tilde{\psi}_2=e^{-q(x-L)}\left[-iq\xi+\frac{E}{\Delta_0}-1+\delta(1-i)t_+-\gamma(1+i)t_-\right],$$

where $q=ik=\sqrt{1-(E/\Delta_0)^2}/\xi$ (see Appendix B) and γ and δ are given by Eq. (A3) with ik replaced by q. Substituting Eq. (A8) into Eq. (10), we obtain

$$G^{\pm}(x,x')=-\frac{1}{\hbar v_F}\frac{\exp[-\sqrt{1-(E/\Delta_0)^2}|x-x'|/\xi]}{4\sqrt{1-(E/\Delta_0)^2}}\left\{2\left(\frac{E}{\Delta_0}\mathbf{1}+\sigma_1+i\sqrt{1-(E/\Delta_0)^2}\mathrm{sgn}(x-x')\sigma_3\right)\right.$$
$$+\frac{\kappa^2\Delta_0^2}{E_0^2-E^2}\left[\frac{E}{\Delta_0}\{[1-t_-t'_-+\sqrt{1-(E/\Delta_0)^2}|t_--t'_-|/\kappa](\mathbf{1}-\sigma_2)+[1-t_+t'_++\sqrt{1-(E/\Delta_0)^2}|t_+-t'_+|/\kappa](\mathbf{1}+\sigma_2)\}\right.$$
$$+\{[1-(E/\Delta_0)^2](t_-+t'_--t_+-t'_+)/\kappa+2-t_-t'_+-t_+t'_-+\sqrt{1-(E/\Delta_0)^2}$$
$$\times[t_+t'_--t_-t'_++(t_--t'_-+t_+-t'_+)/\kappa]\mathrm{sgn}(x-x')\}\sigma_1+i\{\sqrt{1-(E/\Delta_0)^2}$$
$$\times[2-t_-t'_+-t_+t'_-+(t_-+t'_--t_+-t'_+)/\kappa]\mathrm{sgn}(x-x')$$
$$\left.\left.+[1-(E/\Delta_0)^2](t_--t'_-+t_+-t'_+)/\kappa+t_+t'_--t_-t'_+\}^{\sigma_3}\right]\right\}, \tag{A9}$$

where t'_+ and t'_- are defined similarly to t_+ and t_- except that x is replaced by x'.

APPENDIX B: SUBGAP GREEN FUNCTION IN THE SOLITON CASE

Here we calculate the Green function for $0<|E|<\Delta_0$. In this case, we have $k\xi=\pm i\sqrt{1-(E/\Delta_0)^2}\equiv\pm iq\xi$. We choose $k=-iq$[25] and take the $L\to\infty$ limit to simplify Eq. (11) using the fact that q is positive and e^{-qL} vanishes:

$$\psi_1=e^{q(x+L)}\left[\tanh\left(\frac{x}{\xi}\right)-i\frac{E}{\Delta_0}-q\xi\right],\quad \psi_2=-ie^{q(x+L)}\left[\tanh\left(\frac{x}{\xi}\right)+i\frac{E}{\Delta_0}-q\xi\right], \tag{B1}$$

$$\tilde{\psi}_1 = ie^{-q(x-L)}\left[\tanh\left(\frac{x}{\xi}\right) - i\frac{E}{\Delta_0} + q\xi\right], \quad \tilde{\psi}_2 = e^{-q(x-L)}\left[\tanh\left(\frac{x}{\xi}\right) + i\frac{E}{\Delta_0} + q\xi\right].$$

The Green functions are obtained in a straightforward manner by substituting Eq. (B1) directly into Eq. (10). We find that the retarded and advanced Green functions are the same in the present case and given by

$$G^{\pm}(x,x') = -\frac{1}{\hbar v_F}\frac{\exp[-\sqrt{1-(E/\Delta_0)^2}|x-x'|/\xi]}{4\sqrt{1-(E/\Delta_0)^2}}\left\{2\left[\frac{E}{\Delta_0}\mathbf{1} + \sigma_1 + i\sqrt{1-(E/\Delta_0)^2}\,\mathrm{sgn}(x-x')\sigma_3\right]\right.$$
$$\left. + \frac{\Delta_0}{E}[1 - t_0t_0' + \sqrt{1-(E/\Delta_0)^2}|t_0 - t_0'|](\sigma_2 - \mathbf{1}) + (t_0 + t_0' - 2)\sigma_1 + i(t_0 - t_0')\sigma_3\right\}. \quad \text{(B2)}$$

*E-mail: khkim@madang.ajou.ac.kr

[1] G. Grüner, *Density Waves in Solids* (Addison-Wesley, Redwood City, 1994).

[2] S. Roth, *One-Dimensional Metals* (VCH, Weinheim, 1995).

[3] S.A. Brazovskiĭ, Pis'ma Zh. Éksp. Teor. Fiz. **28**, 656 (1978) [JETP Lett. **28**, 606 (1978)]; **78**, 677 (1980); Sov. Phys. JETP **51**, 342 (1980)].

[4] W.-P. Su, J.R. Schrieffer, and A.J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979); Phys. Rev. B **22**, 2099 (1980).

[5] M.J. Rice, Phys. Lett. **71A**, 152 (1979).

[6] S.A. Brazovskiĭ and N.N. Kirova, Pis'ma Zh. Éksp. Teor. Fiz. **33**, 6 (1981) [JETP Lett. **33**, 4 (1981)].

[7] D.K. Campbell and A.R. Bishop, Phys. Rev. B **24**, 4859 (1981).

[8] S.A. Brazovskiĭ and N.N. Kirova, Sov. Sci. Rev., Sect. A **5**, 99 (1984).

[9] D. K. Campbell, in *Molecular Electronic Devices II*, edited by F. L. Carter (Dekker, New York, 1987).

[10] A.J. Heeger, S. Kivelson, J.R. Schrieffer, and W.-P. Su, Rev. Mod. Phys. **60**, 781 (1988).

[11] *Conjugated Conducting Polymers*, edited by H. Kiess (Springer, Berlin, 1992).

[12] K.A. Coplin, S. Jasty, S.M. Long, S.K. Manohar, Y. Sun, A.G. MacDiarmid, and A.J. Epstein, Phys. Rev. Lett. **72**, 3206 (1994).

[13] S.M. Long, Y. Sun, A.G. MacDiarmid, and A.J. Epstein, Phys. Rev. Lett. **72**, 3210 (1994).

[14] H. Okamoto, Y. Oka, T. Mitani, and M. Yamashita, Phys. Rev. B **55**, 6330 (1997).

[15] K. Kim and J.W. Wilkins, Synth. Met. **83**, 13 (1996).

[16] M.V. Mostovoy, M.T. Figge, and J. Knoester, Phys. Rev. B **57**, 2861 (1998).

[17] It is well known that the electron-electron interaction is relevant in polyacetylene in several respects. For detailed discussions, see, e.g., Refs. 10 and 11.

[18] H. Takayama, Y.R. Lin-Liu, and K. Maki, Phys. Rev. B **21**, 2388 (1980).

[19] K. Fesser, A.R. Bishop, and D.K. Campbell, Phys. Rev. B **27**, 4804 (1983).

[20] We caution that the continuum model is strictly valid only when the coherence length is much larger than the lattice constant. Since this condition is not met when $\lambda \gg 1$, we do not expect our results to be quantitatively applicable to real conducting polymers in that case.

[21] D. Boyanovsky, C.A.A. de Carvalho, and E.S. Fraga, Phys. Rev. B **50**, 2889 (1994).

[22] D.K. Campbell and A.R. Bishop, Nucl. Phys. B **200**, 297 (1980).

[23] A.A. Ovchinnikov and N.S. Érikhman, Zh. Éksp. Teor. Fiz. **78**, 1448 (1980) [Sov. Phys. JETP **51**, 728 (1980)].

[24] K. Kim, R.H. McKenzie, and J.W. Wilkins, Phys. Rev. Lett. **71**, 4015 (1993).

[25] The same expression for the Green function is obtained for a different sign choice for k.

[26] Equation (25) follows from the definition of $N(E,\Delta_0)$, which is equal to $\sqrt{E^2-\Delta_0^2}/\pi\hbar v_F$ for $E>\Delta_0$, and Eq. (27).