Properties of polyacetylene obtained from Green's functions in the coordinate representation

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An electronic Green's function for polyacetylene with a soliton is obtained with the use of the continuum model but in a coordinate representation. This representation eliminates the necessity of imposing any specific boundary conditions for eigenstates of the Hamiltonian. The Green's function is easily used to obtain both the electronic density of states and the spatial charge density for the midgap state as well as the conduction and valence bands. It is further used to find an optical-absorption coefficient that satisfies the optical sum rule for the polymer chain with a single soliton.

I. INTRODUCTION

The proposal that domain walls between two energetically degenerate but topologically different configurations of *trans*-polyacetylene, $(CH)_x$, play an important role in determining its electronic properties has contributed a large share of the theoretical[1-4] and experimental[5] interest in this material. Moreover, the suggestion that these domain walls—charged solitons—are created at low dopant concentrations has received considerable experimental support, especially from optical-absorption measurements.[6-9]

In the soliton model an electronic state forms in the middle of the dimerization gap which should then give rise to optical absorption at energies deep within the gap. Based on a continuum model of $(CH)_x$ several calculations of the optical absorption[7,10-13] have been made. Although they all give the same midgap absorption, not all of them give the same reduction in the interband transition, nor do they all satisfy the optical-sum rule. The source of these inconsistencies apparently lies in the way each calculation treats the boundary conditions for the broken symmetry of the polymer chain with a soliton.[13]

In the present work we propose to avoid some pitfalls associated with the boundary conditions by working in a coordinate representation to obtain electronic Green's functions for $(CH)_x$ with a soliton. From these Green's functions the electronic density of states and the spatial charge density follow almost immediately. The Green's functions are then used to calculate an optical-absorption coefficient which satisfies the optical-sum rule.

In an Appendix, detailed comparison between the present approach and that of Kivelson *et al.*[13] is made and the formal equivalence between the two is discussed. The real part of the dielectric function is also given there.

II. GREEN'S FUNCTION IN THE COORDINATE REPRESENTATION

In the continuum model the electronic part of the Hamiltonian for trans-$(CH)_x$ with a soliton localized at $x = 0$ is given by[3]

$$H_e = \sum_s \int dx\, \Psi_{i,s}^\dagger(x) \left[-iv_f(\sigma_3)_{ij}\frac{\partial}{\partial x} + \Delta(x)(\sigma_1)_{ij} \right] \Psi_{j,s}(x) ,$$

$$(2.1a)$$

where

$$\Delta(x) = \Delta \tanh\Delta x/v_f , \qquad (2.1b)$$

Δ is the dimerization gap, Ψ is the electron spinor, and σ's are the Pauli spin matrices. The Green's functions in the Matsubara representation are defined as

$$G_{ij,ss'}(x,x',\tau) = -\langle T\Psi_{i,s}(x,\tau)\Psi_{j,s'}^\dagger(x',0)\rangle . \qquad (2.2)$$

Recognizing that the anticommutator

$$\{\Psi_{i,s}^\dagger(x),\ \Psi_{j,s'}(x)\} = \delta_{ij}\delta_{ss'}\delta(x-x') \qquad (2.3)$$

yields the equations of motion

$$-\frac{\partial}{\partial\tau}G_{ij}(x,x',\tau) + \left[iv_f(\sigma_3)_{im}\frac{\partial}{\partial x} - \Delta(x)(\sigma_1)_{im} \right]G_{mj}(x,x',\tau)$$

$$= \delta_{ij}\delta(x-x')\delta(\tau) , \qquad (2.4)$$

where, for convenience, the spin indices have been suppressed and the chemical potential is set equal to zero. [This is correct for $(CH)_x$ with a neutral soliton and introduces no loss in generality.] Expanding in Matsubara frequencies, $\omega_n = (2n+1)\pi/\beta$, these equations become

$$i\omega_n G_{ij}(x,x',\omega_n) + \left[iv_f(\sigma_3)_{im}\frac{\partial}{\partial x} - \Delta(x)(\sigma_1)_{im} \right]G_{mj}(x,x',\omega_n)$$

$$= \delta_{ij}\delta(x-x') . \qquad (2.5)$$

These four first-order differential equations couple G_{11} and G_{21} as well as G_{22} and G_{12}. To decouple the equations for G_{11} and G_{21}, define

$$G_{+1} = G_{11} + iG_{21} , \quad G_{+2} = G_{22} + iG_{12} , \qquad (2.6a)$$

and

$$G_{-1} = G_{11} - iG_{21} , \quad G_{-2} = G_{22} - iG_{12} . \tag{2.6b}$$

However, since the correct free-particle Green's function in one dimension satisfies

$$\left[-v_f^2 \frac{\partial^2}{\partial x^2} + \Delta^2 + \omega_n^2 \right] G_0(x,x',\omega_n) = \delta(x - x') , \tag{2.7}$$

with

$$G_0(x,x',\omega_n) = \frac{\exp(-k \, | \, x - x' \, | \,)}{2v_f^2 k} , \tag{2.8a}$$

and

$$v_f^2 k^2 = \Delta^2 + \omega_n^2 , \tag{2.8b}$$

it follows that this Green's function can be used to solve any particular solution of the free-particle operator. Thus

$$G_{21}(x,x',\omega_n) = [-iv_f k \, \text{sgn}(x - x') - i\Delta(x) + i\omega_n][-iv_f k \, \text{sgn}(x - x') + i\Delta(x') - i\omega_n] \frac{G_0(x,x',\omega_n)}{2\omega_n} \tag{2.9a}$$

and

$$G_{11}(x,x',\omega_n) = [iv_f k \, \text{sgn}(x - x') + i\Delta(x) + i\omega_n][-iv_f k \, \text{sgn}(x - x') + i\Delta(x') - i\omega_n] \frac{G_0(x,x',\omega_n)}{2i\omega_n} . \tag{2.9b}$$

The two coupled equations for G_{22} and G_{12} can be obtained from those for G_{11} and G_{21} with the substitution of $-v_f$ for v_f. Consequently, substituting $-v_f$ for v_f in G_{11} and G_{21} yields G_{22} and G_{12}, respectively.

Certain properties of the system can be immediately obtained from these functions. Analytically continuing $i\omega_n$ to obtain the retarded Green's function gives the electronic density of states $\rho(\epsilon)$,

$$\rho(\epsilon) = \pi^{-1} \text{Im} \int dx \sum_{i,s} G_{ii,ss}(x,x,\epsilon + i\delta) . \tag{2.10}$$

This trace is easily evaluated as

$$\rho(\epsilon) = \begin{cases} \dfrac{2L}{\pi v_f} \dfrac{\epsilon}{(\epsilon^2 - \Delta^2)^{1/2}} - \dfrac{2\Delta}{\pi\epsilon(\epsilon^2 - \Delta^2)^{1/2}}, & \epsilon > \Delta \tag{2.11a} \\[2mm] 2\delta(\epsilon), \quad | \, \epsilon \, | < \Delta & \tag{2.11b} \\[2mm] \dfrac{-2L}{\pi v_f} \dfrac{\epsilon}{(\epsilon^2 - \Delta^2)^{1/2}} + \dfrac{2\Delta}{\pi\epsilon(\epsilon^2 - \Delta^2)^{1/2}}, & \epsilon < -\Delta, \end{cases}$$

$$\tag{2.11c}$$

where the correct signs are obtained by evaluating the square root just above the branch cut. The terms proportional to L give the correct density of states for *trans*-polyacetylene without a soliton, $\rho_0(\epsilon)$, while the delta function lying at midgap is the well-known electronic state associated with the domain wall separating the two-degenerate ground states. (The factors of 2 come from spin.) The change in the continuum density of states produced by the soliton, $\delta\rho(\epsilon)$, is easily integrated to give

$$\int_{-\infty}^{-\Delta} \delta\rho(\epsilon)d\epsilon + \int_{\Delta}^{\infty} \delta\rho(\epsilon)d\epsilon = -2 , \tag{2.12}$$

which explicitly shows that one-spin degenerate quantum state (half an electronic state) from each of the two bands contributes to the midgap state. In neutral (undoped) polyacetylene this results in one electron from the previously filled valence band being forced into the midgap state.

The spatial charge density at $T=0$ for the singly occupied midgap state is given by

$$\rho_s(x) = \pi^{-1} \text{Im} \int_{-\Delta}^{\Delta} d\epsilon \sum_i G_{ii,ss}(x,x,\epsilon + i\delta) , \tag{2.13}$$

with no spin sum because of the single occupancy. This trace is also easily evaluated and is

$$\rho_s(x) = \frac{\Delta}{2v_f} \frac{1}{\cosh^2(\Delta x / v_f)} . \tag{2.14}$$

Similarly the change in the spatial charge density for the valence band is expressed as

$$\delta\rho_v(x) = \pi^{-1} \text{Im} \int_{-\infty}^{-\Delta} d\epsilon \sum_{i,s} G_{ii,ss}(x,x,\epsilon + i\delta) \; -\rho_{0v}(x) , \tag{2.15}$$

which gives

$$\delta\rho_v(x) = \frac{-\Delta}{2v_f} \frac{1}{\cosh^2(\Delta x / v_f)} . \tag{2.16}$$

This emphasizes that the charge in the valence band is spatially redistributed to exactly cancel the space charge due to the electron in the midgap state. Therefore, it is easily concluded from these Green's functions in the coordinate representation that *trans*-polyacetylene with a soliton and a singly occupied midgap state is "locally" as well as globally charge neutral." The unusual charge-spin relations of a soliton in $(CH)_x$, $q=0$, $s=\frac{1}{2}$ or $q=\pm e$, $s=0$, directly follow.

III. FREQUENCY-DEPENDENT CONDUCTIVITY

In the continuum model the current-density operator for polyacetylene is given by

$$J = ev_f \sum_s \int dx \, \Psi_{i,s}^{\dagger}(x)\sigma_{3ij}\Psi_{j,s}(x) . \tag{3.1}$$

In the Matsubara formalism the current-current correlation is

$$\Pi(\tau) = -\langle TJ(\tau)J(0)\rangle . \tag{3.2}$$

The retarded current-current correlation is obtained by Fourier expanding in Matsubara frequencies and then analytically continuing $i\omega_n$ to $\omega + i\delta$. The frequency-dependent conductivity is derived from this as

$$\sigma(\omega) = \mathrm{Re}\frac{i\Pi(\omega + i\delta)}{\omega} \; . \tag{3.3}$$

Considering only the time-dependent part of the current-current correlation,

$$\Pi(\tau) = 2e^2 v_f^2 \int dx \int dx'(\sigma_3)_{ij}(\sigma_3)_{nm}$$

$$\times G_{jn}(x,x,',\tau)G_{mi}(x',x,-\tau) \; , \tag{3.4}$$

hence

$$\Pi(\omega_n) = 2e^2 v_f^2 \int dx \int dx' \frac{1}{\beta}\sum_{\omega_n'} \frac{G_0(x,x',\omega_n')G_0(x',x,\omega_n'-\omega_n)}{\omega_n'(\omega_n'-\omega_n)}$$

$$\times \{\omega_n'^2(\omega_n'-\omega_n)^2 + v_f^4 k^2(\omega_n')k^2(\omega_n'-\omega_n) - 2\omega_n'(\omega_n'-\omega_n)v_f^2 k(\omega_n')k(\omega_n'-\omega_n)$$

$$- v_f^2[k^2(\omega_n') + k^2(\omega_n'-\omega_n)]\Delta(x)\Delta(x') + 2\omega_n'(\omega_n'-\omega_n)\Delta(x)\Delta(x') + \Delta^2(x)\Delta^2(x')\} \; . \tag{3.5}$$

The frequency-dependent conductivity or optical absorption is reduced to evaluating the imaginary part Eq. (3.5), the calculations are straightforward but tedious, and the technique for evaluating the integrals over x and x' therefore will be given in Appendix A, but the results merely stated are

$$H(a) = \int dx \int dx' \exp(-a\,|x-x'|) = \frac{2L'}{a} - \frac{2}{a^2} + \frac{2\exp(-aL')}{a^2} \; , \tag{3.6a}$$

$$I(a) = \int dx\tanh x \int dx'\tanh x' \exp(-a\,|x-x'|)$$

$$= \frac{2L}{a} + \frac{2}{a^2} - 8\sum_{n=0}\frac{1}{(2n+a)^2} - \frac{2\exp(-aL')}{a^2} + \frac{4\pi}{a}\frac{\exp(-aL'/2)}{\sin(\pi a/2)} \; , \tag{3.6b}$$

$$J(z) = \int dx\,\tanh^2 x \int dx'\tanh^2 x' \exp(-a\,|x-x'|)$$

$$= \frac{2L'}{a} - \frac{2}{a^2} - \frac{8}{a} - 4 - 4a + 8a^2\sum_{n=0}\frac{1}{(2n+a)^2} + \frac{2\exp(-aL')}{a^2} + \frac{4\pi\exp(-aL'/2)}{\sin(\pi a/2)} \; , \tag{3.6c}$$

where $L' = \Delta L/v_f$ and $a = [k(\omega_n') + k(\omega_n'-\omega_n)]v_f/\Delta$, and Eqs. (2.8a) and (2.1b) have been explicitly used.

Combining all the terms proportional L, the chain length, results in the current-current correlation for *trans*-polyacetylene without a soliton:

$$\Pi_0(\omega_n) = \frac{2e^2 v_f^2 L}{\beta}\sum_{\omega_n'}\frac{-\omega_n'(\omega_n'-\omega_n) + v_f^2 k(\omega_n')k(\omega_n'-\omega_n) - \Delta^2}{v_f^2 k(\omega_n')k(\omega_n'-\omega_n)v_f[k(\omega_n') + k(\omega_n'-\omega_n)]} \; . \tag{3.7}$$

This Matsubara sum is performed with the appropriate contour integral. Upon analytic continuation of $i\omega_n$ this contour is deformed analogous to the contour used in calculating optical absorption in a superconductor.[14] The resulting conductivity for a chain without a soliton at $T=0$ is

$$\sigma_0(\omega) = 4e^2 v_f L\frac{\Delta^2}{\omega^2(\omega^2 - 4\Delta^2)^{1/2}}\quad \omega > 2\Delta \; . \tag{3.8}$$

This expression is easily integrated over frequency to obtain the sum rule

$$\int \sigma_0(\omega)d\omega = e^2 v_f L \; . \tag{3.9}$$

The midgap absorption essentially comes from the pole structure of $\Pi(\omega_n)$. Upon analytically continuing $i\omega_n \to \omega + i\delta$ and changing to a real variable of integration the relevant pole is of the form

$$1/(x-\omega-i\delta) = 1/(x-\omega) + \pi i\delta(x-\omega) \; ,$$

and the imaginary parts of the integrals are then evaluated

trivially. With the use of the identity[15]

$$\sum_{n=0}^{\infty}\frac{(2n+1)^2 - (\omega^2/\Delta^2 - 1)}{[(2n+1)^2 + \omega^2/\Delta^2 - 1]^2} = \frac{\pi^2/8}{\cosh^2[\pi/2(\omega^2/\Delta^2 - 1)^{1/2}]} \; , \tag{3.10}$$

the expression obtained for the midgap absorption is the same as that obtained by others[10–13] and is

$$\sigma_s(\omega) = \frac{\pi^2}{2}\frac{e^2 v_f^2}{\Delta(\omega^2 - \Delta^2)^{1/2}}\frac{1}{\cosh^2[\pi/2(\omega^2/\Delta^2 - 1)^{1/2}]} \; ,$$

$$\omega > \Delta \; . \tag{3.11}$$

The reduction of the interband transition is obtained almost as easily. The only term that can be evaluated explicitly comes from the third term $(-8/a)$ in Eq. (3.6c). The rest of the bleaching in the interband transition comes from an imaginary principal part integration arising from the $1/(2n+a)^2$ terms in (3.6b) and (3.6c). The final result is given by

$$\sigma_i(\omega) = [1 - (4\Delta v_f)/(L\omega^2)]\sigma_0(\omega) - F(\omega) \; , \tag{3.12}$$

where $F(\omega)$ is determined numerically from the principal value integration. Figure 1 gives the results for the changes in the optical absorption owing to the presence of a soliton in the chain. Note, however, the sign for the reduction in the interband transition has been changed so that $\Delta\sigma_i(\omega)$ is positive in Fig. 1. The optical-sum rule has been verified numerically to four significant figures, which, although lacking the elegance of an analytical result, is in satisfactory agreement. On initial inspection the results arrived at here are in agreement only with Horowitz[12] who creates a somewhat artificial dilute lattice of solitons. However, the results of Kivelson et al.[13] may be rearranged to be (apart from a missing numerical factor) identical to those found here as well. Examination of their Eqs. (B13) and (B15) show that each contains a cancelling factor of $(2v_f/\Delta L)\sigma_0(\omega)$ which then gives an optical absorption in agreement with that found here. The agreement with Kivelson (which is further discussed in Appendix B) is satisfying because it demonstrates the equivalence of the alternatives of a coordinate space calculation or an eigenfunction expansion, both of which deal directly with the unusual boundary conditions confronted in trans-polyacetylene with a soliton. This equivalence should provide flexibility in carrying out further Green's-function-based studies on this and related polymers.

IV. CONCLUSIONS

The symmetry of trans-polyacetylene with a soliton is substantially different from the translationally invariant dimerized chain. Although vestiges of translational invariance remain because of the domain-wall topology, care must be taken in determining the way this topology is translated into boundary conditions and ultimately into the eigenstates of the system, and there appears to be some inconsistency in the literature on this point.

The presence of a soliton is sufficiently analogous to the introduction of any localized effect that we have considered the problem of optical absorption from a coordi-
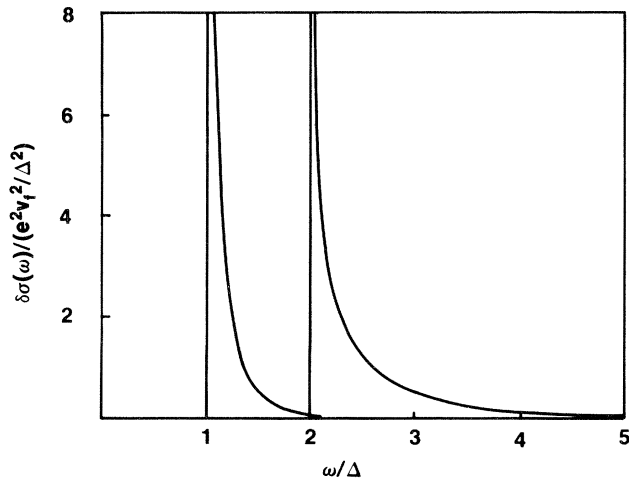

FIG. 1. Change in the optical absorption owing to the presence of a soliton in the chain; the sign for the reduction in the interband transition is changed so that it appears positive in this figure.

nate representation point of view. The continuum approximation to the Su-Schrieffer-Heeger model is used without reference to boundary conditions for a chain of finite length. In this way details of the system's eigenstates become unimportant.

The coordinate representation Green's function for the chain with a soliton, which is required for the optical-absorption calculation, permits a surprisingly simple calculation of the density of states. The subsequent optical-absorption calculation is conceptually straightforward but mathematically more tedious. However, the contour integrals that arise are very similar to several already familiar from superconductivity theory and those techniques have been applied here. The results confirm the eigenfunction expansions of Kivelson et al. and suggest a flexible Green's-function approach to this class of one-dimensional systems.

ACKNOWLEDGMENTS

APPENDIX A: INTEGRATIONS OVER x and x'

To evaluate $\Pi(\omega_n)$ requires the integration of three separate integrals, $H(a)$, $I(a)$, and $J(a)$ in Eq. (3.6). The correct expression for $H(a)$ can be obtained using the techniques shown below or by direct integration and will not be discussed in this appendix. However, the evaluation of $I(a)$ and $J(a)$ is not quite as straightforward and the procedures used will be outlined here. First consider the integral

$$I(a)= \int dx\,\tanh x \int dx'\tanh x'\exp(-a\,|x-x'|)\,. \quad \text{(A1)}$$

It is convenient to use the following integral representation for $\exp(-a\,|x-x'|)$,

$$\exp(-a\,|x-x'|)=\frac{a}{\pi}\int\frac{dq}{q^2+a^2}\exp[iq(x-x')]\,. \quad \text{(A2)}$$

Following this substitution

$$I(a)=\frac{a}{\pi}\int\frac{dq}{q^2+a^2}f^2(q)\,, \quad \text{(A3)}$$

where

$$f(q)=\int_{-L'/2}^{L'/2}dx\,\sin(qx)\tanh x\,. \quad \text{(A4)}$$

Integration by parts and assuming $L'=\Delta L/v_f\gg1$ yields

$$f(q)=\frac{\pi}{\sinh(\pi q/2)}-\frac{2\cos(L'/2)}{q}\,. \quad \text{(A5)}$$

At this point it is convenient to use the following identity for $1/\sinh^2(\pi q/2)$,[16]

$$\frac{1}{\sinh^2(\pi q/2)}=\frac{4}{\pi^2}\left[\frac{1}{q^2}-\int_0^\infty\frac{x\cos(qx)\exp(-x)dx}{\sinh x}\right]\,. \quad \text{(A6)}$$

Substituting the expression (A5) and (A6) into (A3) and combining terms so that second-order poles cancel enables the q integrations to be done using simple pole residue techniques. The only remaining integral to be done comes from the identity expressed in (A6). This integral is of the form of a Laplace transform and can be found in most tables. The result is in the form of an infinite sum or

$$\int_0^\infty \frac{xe^{-(a+1)x}}{\sinh x}dx = \frac{-2}{a^2} + 2\sum_{n=0}^\infty \frac{1}{(2n+a)^2} \ . \qquad (A7)$$

With the use of this expression the final result is

$$I(a) = \frac{2L'}{a} + \frac{2}{a^2} - 8\sum_{n=0}^\infty \frac{1}{(2n+a)^2} - \frac{2\exp(-aL')}{a^2}$$
$$+ \frac{4\pi}{a}\frac{\exp(-aL'/2)}{\sin(\pi a/2)} \ . \qquad (A8)$$

Now consider

$$J(a) = \int dx\, \tanh^2 x \int dx'\tanh^2 x'\exp(-a\,|x-x'|) \ . \qquad (A9)$$

Substituting the expression $1-\mathrm{sech}^2 x$ for $\tanh^2 x$ results in three integrals, two of which can be performed without difficulty. The remaining integral is

$$J_3(a) = \int dx\, \mathrm{sech}^2 x \int dx'\mathrm{sech}^2 x'e^{-a\,|x-x'|} \ . \qquad (A10)$$

Again, use of the integral representation in Eq. (A2) yields

$$J_3(a) = \frac{a}{\pi}\int \frac{dq}{q^2+a^2}g^2(q) \ , \qquad (A11a)$$

where

$$g(q) = \int_{-L'/2}^{L'/2} dx\frac{\cos(qx)}{\cosh^2 x} \ . \qquad (A11b)$$

The identity given in (A6) once again enables the q integration to be done. However, in this case some care must be taken with respect to the convergence of the q integration, since one of the integrals is of the form

$$\int_{-\infty}^\infty \frac{q^2 e^{iqx}}{q^2+a^2}dx = 2\pi\delta(x) - a^2\int_{-\infty}^\infty \frac{e^{iqx}}{q^2+a^2}dq \ . \qquad (A12)$$

The last integral from the identity (A6) is again performed using (A7). Now combining the two terms that were done directly yields

$$J(a) = \frac{2L'}{a} - \frac{2}{a^2} - \frac{8}{a} - 4 - 4a + 8a^2\sum_{n=0}^\infty \frac{1}{(2n+a)^2}$$
$$+ \frac{2\exp(-aL')}{a^2} + \frac{4\pi\exp(-aL'/2)}{\sin(\pi a/2)} \ . \qquad (A13)$$

APPENDIX B: COMPARISON OF THE OPTICAL-ABSORPTION RESULTS WITH KIVELSON et al.

Given the Hamiltonian in Eq. (2.1) a set of eigenstates defined by

$$H_e\psi_k = \epsilon_k\psi_k \qquad (B1)$$

is generated where the ψ_k's are the spinors discussed in the work by Kivelson et al.[13(b)] The quantum number k can either label the set of states in the conduction band ck, the set of states in the valence band vk, or the midgap state s. The energies associated with these states are

$$\epsilon_{ck} = -\epsilon_{vk} = \epsilon_k = (v_f^2 k^2+\Delta^2)^{1/2} \qquad (B2)$$

and $\epsilon_s = 0$. It is important to note that these states form an orthonormal set, i.e.,

$$\int \psi_k^\dagger(x)\psi_{k'}(x)dx = \delta_{kk'} \ , \qquad (B3)$$

only with the proper normalization and proper boundary conditions,

$$kL = 2n\pi+\phi_k \quad \text{(conduction band)} \ , \qquad (B4a)$$

$$kL = (2n+1)\pi+\phi_k \quad \text{(valence band)} \ , \qquad (B4b)$$

$$|A_k|^2 = (L-v_f\Delta/\epsilon_k^2)^{-1} \ , \qquad (B4c)$$

where $\varphi_k = \tan^{-1}(v_f k/\Delta)$ and $-\pi/2 < \varphi_k \le \pi/2$. Recognizing that with these boundary conditions any sum over k is changed to an integral in the following way:

$$\sum_k \to \frac{1}{2\pi}\int dk(L-v_f\Delta/\epsilon_k^2) \ . \qquad (B5)$$

Then it is easy to show directly that

$$\sum_k \psi_{ik}^*(x)\psi_{jk}(x') = \delta_{ij}\delta(x-x') \ , \qquad (B6)$$

where the sum over k includes all the states in both continuum bands as well as the midgap state. Now a field operator can be expanded as

$$\Psi_i(x,\tau) = \sum_k \psi_{ik}(x)a_k(\tau) \ , \qquad (B7)$$

where a_k $(a_k^\dagger)$ annihilates (creates) an eigenstate of the Hamiltonian in the Matsubara representation. Note that the eigenstate is a spinor while the operator, a_k $(a_k^\dagger)$, itself is not a spinor. With this expansion it is straightforward to show that the anticommutator

$$\{\Psi_{i,s}^\dagger(x),\ \Psi_{j,s'}(x)\} = \delta_{ij}\delta_{ss'}\delta(x-x') \ , \qquad (B8)$$

which was the assumption in Eq. (3).

Now the eigenfunction expansion of the Green's function is

$$G_{ij}(x,x',\omega_n) = \sum_k \frac{\psi_{ik}(x)\psi_{jk}^*(x')}{i\omega_n-\epsilon_k} \ , \qquad (B9a)$$

$$G_{kk'}(\omega_n) = \delta_{kk'}/(i\omega_n-\epsilon_k) \ . \qquad (B9b)$$

The Green's functions in Eq. (B9a) can be shown to be identical to those in Eq. (9) by simply performing the sum over k in the prescribed way and the Green's function in (B9b) is exactly what would be expected from an eigenfunction expansion of a Green's function.

Now the Green's function from (B9a) can be used in Eq. (20) with the integrals over x and x' performed prior to the sum over k and k'.

The integrals of interest are

$$\int_{-L/2}^{L/2} \Psi_{1ck}(x)\Psi_{1vq}^*(x)dx = -A_k A_q^* \left[\frac{1}{\epsilon_k} + \frac{1}{\epsilon_q} \right] \frac{\pi v_f}{[\sinh(\pi v_f(k-q)/2\Delta]} \tag{B10}$$

and

$$\int_{-L/2}^{L/2} \Psi_{1ck}(x)\Psi_{1s}^*(x)dx = \int_{-L/2}^{L/2} \Psi_{1vk}(x)\Psi_{1s}^*(x)dx = A_k \frac{\pi}{4}\left[\frac{v_f}{\Delta} \right]^{1/2} \frac{1}{\cosh(\pi v_f k/2\Delta)} . \tag{B11}$$

Performing the Matsubara sum with the appropriate contour integral yields (in the low-temperature limit)

$$\pi(\omega_n) = \pi_s(\omega_n) + \pi_b(\omega_n) , \tag{B12}$$

where

$$\Pi_s(\omega_n) = e^2 v_f^2 \frac{\pi^2 v_f}{2\Delta} \sum |A_k|^2 \frac{1}{\cosh^2(\pi v_f k/2\Delta)} \left[\frac{1}{i\omega_n - \epsilon_k} - \frac{1}{i\omega_k + \epsilon_k} \right] , \tag{B13}$$

and

$$\Pi_b(\omega_n) = 2e^2 v_f^2 \Delta^2 \sum_{k,q} |A_k|^2 |A_q|^2 \left[\frac{1}{\epsilon_k} + \frac{1}{\epsilon_q} \right]^2 f(k-q) \left[\frac{1}{i\omega_n - (\epsilon_k + \epsilon_q)} - \frac{1}{i\omega_n + \epsilon_k + \epsilon_q} \right] , \tag{B14}$$

with $f(k-q) = \pi v_f \{ 2\Delta \sinh[\pi v_f(k-q)/2\Delta] \}^{-2}$ and A_k being the correct normalization given in Ref. 13(b).
Upon analytical continuation of $i\omega_n$

$$\sigma_s(\omega) = \mathrm{Re}\frac{i\Pi_s(\omega+i\delta)}{\omega} = e^2 v_f^2 \frac{\pi^2}{4} \frac{v_f}{\Delta\omega} \int dk \frac{\delta(\omega - \epsilon_k)}{\cosh^2(\pi/2v_f k/\Delta)} , \tag{B15}$$

with

$$\mathrm{Re}\Pi_s(\omega) = e^2 v_f^3 \frac{\pi}{2} \int dk \frac{1}{\cosh^2(\Pi/2v_f k/\Delta)} \frac{\epsilon_k}{\omega^2 - \epsilon_k^2} , \tag{B16}$$

and

$$\sigma_b(\omega) = \mathrm{Re}\frac{i\Pi_b(\omega+i\delta)}{\omega} = \frac{2\pi e^2 v_f^2 \Delta^2}{\omega} \sum |A_k|^2 |A_g|^2 \left[\frac{1}{\epsilon_k} + \frac{1}{\epsilon_q} \right]^2 f(k-q)\delta(\omega - \epsilon_k - \epsilon_q) , \tag{B17}$$

with

$$\mathrm{Re}\Pi_b(\omega) = 4e^2 v_f^2 \Delta^2 \sum |A_k|^2 |A_q|^2 \left[\frac{1}{\epsilon_k} + \frac{1}{\epsilon_q} \right]^2 f(k-q) \frac{\epsilon_k + \epsilon_q}{\omega^2 - (\epsilon_k + \epsilon_q)^2} . \tag{B18}$$

Within a constant factor the conductivities are identical to those in Ref. 13(b) and the real part of the dielectric response has been obtained as well.

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