RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 47, NUMBER 3 15 JANUARY 1993-I

# Finite-temperature generalization of the "line and pole" decomposition for self-energies: Application to one-dimensional quantum wires

Ben Yu-Kuang Hu
*Department of Physics, University of Maryland, College Park, Maryland 20742-4111*
(Received 20 July 1992)

We present a method for obtaining expressions for the analytic continuation of finite-temperature self-energies which are suitable for use in numerical computations. In the case of the *GW* approximation for the self-energy, this method gives the finite-temperature generalization of the zero-temperature "line and pole" decomposition. This formalism is used to calculate the finite-temperature self-energy and band-gap renormalization of electrons in the extreme quantum limit of a quantum wire.

Powerful field-theoretic techniques, including Feynman diagram perturbation methods, were developed several decades ago as a tool for calculating physical properties of interacting quantum systems. First to be introduced was the zero-temperature formalism, which allowed the ground-state properties of an interacting system to be calculated. Subsequently, Matsubara[1] introduced a similar formalism for finite-temperature systems, which was formally identical to the zero-temperature formalism. Generally, the zero-temperature formalism has been used for many-body quasiparticle calculations for metals[2] because the energy scales intrinsic to the problem (Fermi energy, plasmon energy, etc.) are usually much larger than the temperature $T$. However, in semiconductors, especially in artificial structures of reduced dimensionality, because of the low electron densities and large dielectric constants involved, the experimental temperature can be comparable to the intrinsic energy scales of the electron gas. In these cases, the zero-temperature formalism may not provide an adequate description of the system, and therefore the finite-temperature formalism is needed.[3]

While the finite-temperature formalism is easier to handle than the zero-temperature formalism in some ways, using it involves an extra hurdle. With the finite-temperature formalism, one obtains an expression for the electron self-energy $\sigma(i\nu_n)$ that is only valid at discrete points on the complex frequency plane, $i\nu_n \equiv i(2n+1)\pi T$, there $n$ is an integer. (In this paper, we set $\hbar = k_B = 1$.) The $\sigma(i\nu_n)$ must be *analytically continued* to the complex plane to obtain the self-energy $\Sigma(z)$ that is valid for all complex frequencies,[4] from which the retarded self-energy, the quantity relevant to experiments, can be obtained by setting $z = \omega + i0^+$. (In this paper, we use the convention that functions denoted by upper case characters are analytic in the frequency variable, while those denoted by lower case characters may be nonanalytic.)

In principle, from $\sigma(i\nu_n)$, one can obtain a formal expression for $\Sigma(z)$ in terms of integrals over spectral representations,[5] but the expressions for $\Sigma(z)$ obtained in this manner involve integration over one or more frequency variables, which makes them inefficient for use in numerical computations. On previous occasions various approximations such as the plasmon-pole approximation were used to obtain the finite-temperature self-energy.[3] In this paper, we present a more direct method of analytically continuing the $\sigma(i\nu_n)$ to $\Sigma(z)$ which yields an exact expression which is much more amenable to numerical calculation. We then apply this method to calculate various many-body properties of electrons in a quantum wire.

In a nutshell, the method uses the properties which the analytic continuation of $\sigma(i\nu_n)$ must satisfy to lead us to its analytic continuation, $\Sigma(z)$. These properties are as follows: (i) $\Sigma(z)$ is analytic on the entire complex frequency plane, with the exception of branch cuts on the real axis[4] (henceforth, when we say a function is "analytic" it is with the implicit understanding that it could have branch cuts on the real axis); (ii) $\Sigma(z = i\nu_n) = \sigma(i\nu_n)$ for all $i\nu_n$; and (iii) $\Sigma(z)$ goes to a constant as $|z| \to \infty$. These properties ensure a unique analytic continuation.[6] By systematically fulfilling each of the above conditions, we are led directly to the desired analytic continuation.

We elucidate this method by examining a simple example, that of the self-energy within the *GW* approximation [see Fig. 1(a)] of a translationally invariant system. The self-energy can be written as a sum of a frequency independent exchange and a frequency-dependent correlation part,[5] $\sigma(\mathbf{k}, i\nu_n) = \sigma_{ex}(\mathbf{k}) + \sigma_{cor}(\mathbf{k}, i\nu_n)$. The exchange part, which is frequency independent (and hence already analytic), is given by $\sigma_{ex}(\mathbf{k}) = -(2\pi)^{-d} \int d\mathbf{q}\, V_c(\mathbf{q}) n_F(\xi_{\mathbf{k}+\mathbf{q}})$, where $V_c(\mathbf{q})$ is the bare Coulomb interaction, $n_F(x) = [\exp(x/T)+1]^{-1}$ is the Fermi function, $\xi_{\mathbf{k}+\mathbf{q}}$ is the kinetic relative to the chemical potential, and $d$ is the dimension of the system. The $\sigma_{cor}(\mathbf{k}, i\nu_n)$ is given by

$$\sigma_{cor}(\mathbf{k}, i\nu_n) = -\int \frac{d\mathbf{q}}{(2\pi)^d} h_{\mathbf{k},\mathbf{q}}(i\nu_n) , \tag{1}$$

where

$$h_{\mathbf{k},\mathbf{q}}(i\nu_n) = T\sum_{i\omega_n} \frac{w(\mathbf{q}, i\omega_n)}{i\nu_n + i\omega_n - \xi_{\mathbf{k}+\mathbf{q}}} . \tag{2}$$

Here, the frequency summation is over the boson frequencies $i\omega_n = i2\pi nT$ ($n$ are integers), and $w(\mathbf{q}, i\omega_n) = V_c(\mathbf{q})[\epsilon^{-1}(\mathbf{q}, i\omega_n) - 1]$ is the difference between the screened and bare Coulomb interactions. The problem is to analytically continue $\sigma_{cor}(\mathbf{k}, i\nu_n)$ to $\Sigma_{cor}(\mathbf{k}, z)$.

Finding an analytic continuation $\Sigma_{cor}(\mathbf{k}, z)$ of $\sigma_{cor}(\mathbf{k}, i\nu_n)$ is equivalent, by Eq. (1), to finding the analyt-

 

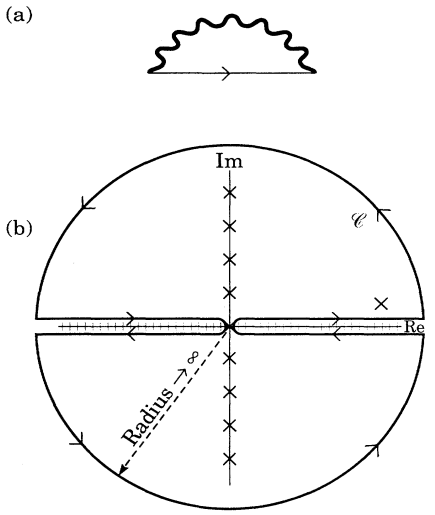


FIG. 1. (a) The diagram for the *GW* approximation of the self-energy. The thick wavy line indicates the screened Coulomb interaction, while the straight line is the bare electron Green function. (b) The contour of integration $\mathcal{C}$ for Eq. (4). The hatched real axis indicates a branch cut due to $w(\mathbf{q},\omega)$ in the integrand of Eq. (4). The crosses mark the poles due to the integrand; the ones on the imaginary axis are due to $n_B(\omega)$, and the isolated pole is due to the denominator. The residues of the poles on the imaginary axis give $h_{\mathbf{k},\mathbf{q}}(z)$, while the residue of the isolated pole gives $\tilde{h}_{\mathbf{k},\mathbf{q}}(z)$.

ic continuation $H_{\mathbf{k},\mathbf{q}}(z)$ of $h_{\mathbf{k},\mathbf{q}}(i\nu_n)$. Thus, if we construct a function $H_{\mathbf{k},\mathbf{q}}(z)$ such that (1) it is analytic (in the sense mentioned above), and (2) $H_{\mathbf{k},\mathbf{q}}(z=i\nu_n)=h_{\mathbf{k},\mathbf{q}}(i\nu_n)$, then

$$\Sigma_{\rm cor}(\mathbf{k},z)=-\int\frac{d\mathbf{q}}{(2\pi)^d}H_{\mathbf{k},\mathbf{q}}(z) \tag{3}$$

automatically satisfies the conditions (i) and (ii) above.[7] Note that the simple replacement $i\nu_n\rightarrow z$ in Eq. (2) gives a function $h_{\mathbf{k},\mathbf{q}}(z)$ that has poles at $z=\xi_{\mathbf{k}+\mathbf{q}}-i\omega_n$ for all $n$ and thus, because it violates condition (1), it is not the desired analytic continuation $H_{\mathbf{k},\mathbf{q}}(z)$.

The outline of the procedure for obtaining the function $H_{\mathbf{k},\mathbf{q}}(z)$ which satisfies conditions (1) and (2) is as follows. First, we write down a function $H^A_{\mathbf{k},\mathbf{q}}(z)=h_{\mathbf{k},\mathbf{q}}(z)+\tilde{h}_{\mathbf{k},\mathbf{q}}(z)$, where $\tilde{h}_{\mathbf{k},\mathbf{q}}(z)$ is chosen so that it *cancels* all the singularities in $h_{\mathbf{k},\mathbf{q}}(z)$ on the complex plane. Thus, $H^A_{\mathbf{k},\mathbf{q}}(z)$ is *analytic,* fulfilling condition (1). However, $\tilde{h}_{\mathbf{k},\mathbf{q}}(z)$ is, in general, nonzero at $z=i\nu_n$, and hence $H^A_{\mathbf{k},\mathbf{q}}(i\nu_n)\neq h_{\mathbf{k},\mathbf{q}}(i\nu_n)$, violating condition (2). The second step is therefore to add an additional analytic term $H'_{\mathbf{k},\mathbf{q}}(z)$ which *cancels* $\tilde{h}_{\mathbf{k},\mathbf{q}}(z)$ at all $z=i\nu_n$. Since the function $H^A_{\mathbf{k},\mathbf{q}}(z)+H'_{\mathbf{k},\mathbf{q}}(z)$ is analytic and equals $h_{\mathbf{k},\mathbf{q}}(z)$ for all $z=i\nu_n$, fulfilling both conditions (1) and (2), it is desired analytic continuation $H_{\mathbf{k},\mathbf{q}}(z)$. With this $H_{\mathbf{k},\mathbf{q}}(z)$, $\Sigma_{\rm cor}(\mathbf{k},z)$ given by Eq. (3) satisfies conditions (i) and (ii) above. Condition (iii) can be checked in the end; in the case of *GW* approximation (and in other cases we have studied) it is satisfied.

In the case of *GW* self-energy, $H^A_{\mathbf{k},\mathbf{q}}(z)$ is given by

$$H^A_{\mathbf{k},\mathbf{q}}(z)=\int_{\mathcal{C}}\frac{d\omega}{2\pi i}\frac{w(\mathbf{q},\omega)n_B(\omega)}{z+\omega-\xi_{\mathbf{k}+\mathbf{q}}}\ , \tag{4}$$

where $n_B(\omega)=[\exp(\omega/T)-1]^{-1}$ is the Bose distribution function, and the contour of integration $\mathcal{C}$ is shown in Fig. 1(b). $H^A_{\mathbf{k},\mathbf{q}}(z)$ is clearly analytic (off the real axis) in the variable $z$. By the residue theorem, $H^A_{\mathbf{k},\mathbf{q}}(z)$ is given by the sum of the residues of the poles from $n_B(\omega)$ and the denominator in the integrand of Eq. (4) [note that $w(\mathbf{q},\omega)$ is analytic everywhere except for a branch cut of the real axis], yielding

$$H^A_{\mathbf{k},\mathbf{q}}(z)=h_{\mathbf{k},\mathbf{q}}(z)+\tilde{h}_{\mathbf{k},\mathbf{q}}(z)\ , \tag{5}$$

where

$$\begin{aligned}h_{\mathbf{k},\mathbf{q}}(z)&=T\sum_{i\omega_n}\frac{w(\mathbf{q},i\omega_n)}{z+i\omega_n-\xi_{\mathbf{k}+\mathbf{q}}}\ ,\\ \tilde{h}_{\mathbf{k},\mathbf{q}}(z)&=w(\mathbf{q},\xi_{\mathbf{k}+\mathbf{q}}-z)n_B(\xi_{\mathbf{k}+\mathbf{q}}-z)\ .\end{aligned} \tag{6}$$

Despite being the sum of two nonanalytic functions, $H^A_{\mathbf{k},\mathbf{q}}(z)$ is analytic because the poles that occur at $z=\xi_{\mathbf{k}+\mathbf{q}}-i\omega_n$ for $h_{\mathbf{k},\mathbf{q}}(z)$ are exactly canceled by the poles in $\tilde{h}_{\mathbf{k},\mathbf{q}}(z)$.[8] However, because $\tilde{h}_{\mathbf{k},\mathbf{q}}(i\nu_n)\neq 0$, $H^A_{\mathbf{k},\mathbf{q}}(z)$ does not fulfill condition (2). In order to fulfill condition (2), we need to add an analytic function which cancels $\tilde{h}_{\mathbf{k},\mathbf{q}}(z)$ at $z=i\nu_n$.

Since $i\nu_n=i(2n+1)\pi T$, for all integers $n$, $n_B(\xi_{\mathbf{k}+\mathbf{q}}-i\nu_n)\equiv -n_F(\xi_{\mathbf{k}+\mathbf{q}})$, and thus $\tilde{h}_{\mathbf{k},\mathbf{q}}(i\nu_n)=-w(\mathbf{q},\xi_{\mathbf{k}+\mathbf{q}}-i\nu_n)n_F(\xi_{\mathbf{k}+\mathbf{q}})$. Therefore the analytic term needed to cancel $\tilde{h}_{\mathbf{k},\mathbf{q}}(i\nu_n)$ is

$$H'_{\mathbf{k},\mathbf{q}}(z)=w(\mathbf{q},\xi_{\mathbf{k}+\mathbf{q}}-z)n_F(\xi_{\mathbf{k}+\mathbf{q}})\ . \tag{7}$$

Hence, $H_{\mathbf{k},\mathbf{q}}(z)=H^A_{\mathbf{k},\mathbf{q}}(z)+H'_{\mathbf{k},\mathbf{q}}(z)$ is given by Eqs. (5), (6), and (7), and the correlation self-energy in the *GW* approximation is, from Eq. (3),

$$\begin{aligned}\Sigma_{\rm cor}(\mathbf{k},z)&=-\int\frac{d\mathbf{q}}{(2\pi)^d}[H^A_{\mathbf{k},\mathbf{q}}(z)+H'_{\mathbf{k},\mathbf{q}}(z)]\\ &=-\int\frac{d\mathbf{q}}{(2\pi)^d}T\sum_{i\omega_n}\frac{w(\mathbf{q},i\omega_n)}{z+i\omega_n-\xi_{\mathbf{k}+\mathbf{q}}}\\ &\quad-\int\frac{d\mathbf{q}}{(2\pi)^d}w(\mathbf{q},\xi_{\mathbf{k}+\mathbf{q}}-z)\\ &\quad\times[n_B(\xi_{\mathbf{k}+\mathbf{q}}-z)+n_F(\xi_{\mathbf{k}+\mathbf{q}})]\ .\end{aligned} \tag{8}$$

The retarded self-energy, $\Sigma_{\rm ret}(\mathbf{k},\omega)$ is obtained by setting $z\rightarrow\omega+i0^+$. The first and second terms on the right-hand side of Eq. (8) are, respectively, the finite-temperature generalization of the so-called "line" and "pole" components of the *GW* approximation of the $T=0$ correlation self-energy.[9] As in the zero-temperature case, the line contribution is completely real because $w(\mathbf{q},-i\omega_n)$ and $w(\mathbf{q},i\omega_n)$ are complex conjugates, and hence the total contriubtion to the imaginary part of $\Sigma_{\rm ret}(\mathbf{k},\omega)$ comes from the pole part.

As in the $T=0$ case, in the *GW* approximation the "on-shell" imaginary part of the self-energy,

$|\mathrm{Im}[\Sigma_{\mathrm{ret}}(\mathbf{k},\omega=\xi_{\mathbf{k}})]|$, is half the sum of the Born-approximation electron and hole scattering rates. Using the identity

$$n_B(\xi_{\mathbf{k}+\mathbf{q}}-\omega)+n_F(\xi_{\mathbf{k}+\mathbf{q}})=n_B(\xi_{\mathbf{k}+\mathbf{q}}-\omega)[1-n_F(\xi_{\mathbf{k}+\mathbf{q}})] -n_B(\omega-\xi_{\mathbf{k}+\mathbf{q}})n_F(\xi_{\mathbf{k}+\mathbf{q}}) , \tag{9}$$

we can write $2|\mathrm{Im}[\Sigma_{\mathrm{ret}}(\mathbf{k},\xi_{\mathbf{k}})]|=\gamma_e(\mathbf{k})+\gamma_h(\mathbf{k})$ where

$$\gamma_e(\mathbf{k})=-\int\frac{d\mathbf{q}}{(2\pi)^d}2V_c(\mathbf{q})\mathrm{Im}[\epsilon^{-1}(\mathbf{q},\xi_{\mathbf{k}+\mathbf{q}}-\xi_{\mathbf{k}})] \times n_B(\xi_{\mathbf{k}+\mathbf{q}}-\xi_{\mathbf{k}})[1-n_F(\xi_{\mathbf{k}+\mathbf{q}})] ,$$
$$\gamma_h(\mathbf{k})=\int\frac{d\mathbf{q}}{(2\pi)^d}2V_c(\mathbf{q})\mathrm{Im}[\epsilon^{-1}(\mathbf{q},\xi_{\mathbf{k}+\mathbf{q}}-\xi_{\mathbf{k}})] \times n_B(\xi_{\mathbf{k}}-\xi_{\mathbf{k}+\mathbf{q}})n_F(\xi_{\mathbf{k}+\mathbf{q}}) , \tag{10}$$

are the Born-approximation electron and hole scattering rates, respectively.

The method outlines above can also be used for higher-order diagrams. The procedure is analogous to the one carried out above; i.e., first, one obtains an analytic function $H^A_{\mathbf{k},\mathbf{q}}(z)=h_{\mathbf{k},\mathbf{q}}(z)+\tilde{h}_{\mathbf{k},\mathbf{q}}(z)$ by writing $H^A_{\mathbf{k},\mathbf{q}}(z)$ in terms of integrals of the form Eq. (4). Then, one finds the analytic $H'_{\mathbf{k},\mathbf{q}}(z)$ necessary to cancel out the $\tilde{h}_{\mathbf{k},\mathbf{q}}(z)$ at $z=i\nu_n$. The number of terms needed to obtain $H_{\mathbf{k},\mathbf{q}}(z)$ increases somewhat from the example given above [for the second-order term for the self energy with two screened Coulomb interactions, six terms in addition to $h_{\mathbf{k},\mathbf{q}}(z)$ are needed], but writing $\Sigma_{\mathrm{ret}}(\mathbf{k},z)$ in the manner prescribed above generally reduces integrals over spectral representations to sums over complex frequencies, which aids numerical computation. Further details will be given elsewhere.[10]

*Self-energy of a one-dimensional quantum wire.* Recently, there has been considerable effort focused both experimentally[11] and theoretically[12] on semiconductor quantum wires. Because the energy scales of the electron gas in these structures are small (e.g., Fermi energies of 5 meV $\sim$ 50 K), even small temperatures may affect their many-body properties significantly. We therefore apply

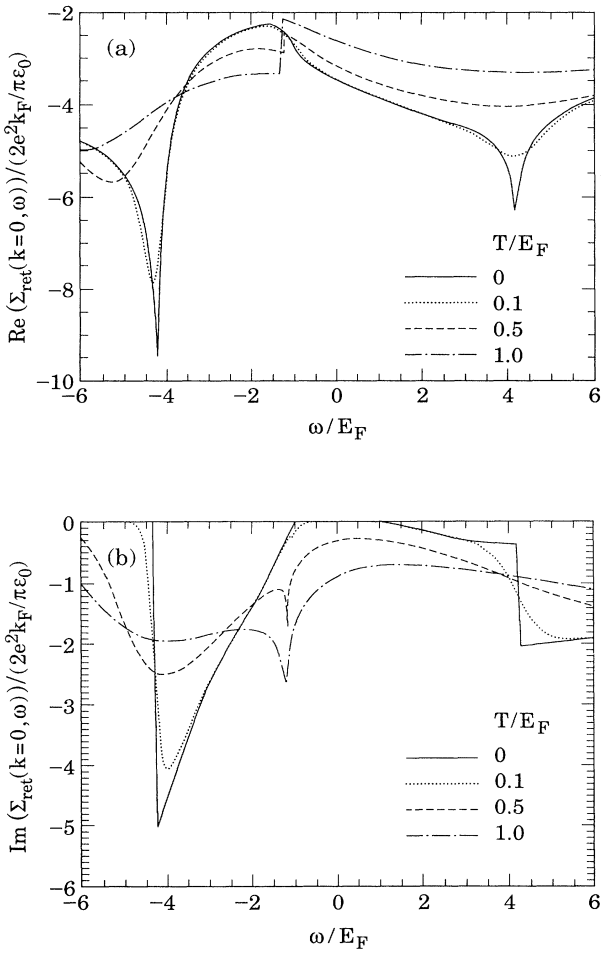


FIG. 2. Real and imaginary parts of the $k=0$ self-energy (in the $GW$ approximation, where $W$ is the screened interaction given by the random-phase approximation) as a function of frequency for a quasi-one-dimensional electron gas, for various temperatures. Parameters used are $k_Fa=0.9$ and $r_s=2m_ee^2/\pi\hbar^2k_F\epsilon_0=0.7$ ($a$ is the wire width, $k_F$ is the Fermi wave vector, $m_e$ is the electron mass, and $\epsilon_0$ is the static lattice dielectric constant), corresponding to $a=100$ Å and density of $0.56\times10^6$ cm$^{-1}$ in GaAs, which gives a Fermi energy $E_F=4.4$ meV = 50 K and $2e^2k_F/\pi\epsilon_0=6.2$ meV. A logarithmic divergence develops at $\omega=\xi_k$ (the on-shell frequency) in $\mathrm{Im}\Sigma_{\mathrm{ret}}(k,\omega)$ for $T\neq0$ because the Born-approximation electron-electron scattering rate at $T\neq0$ in a one-dimensional electron gas is infinite.

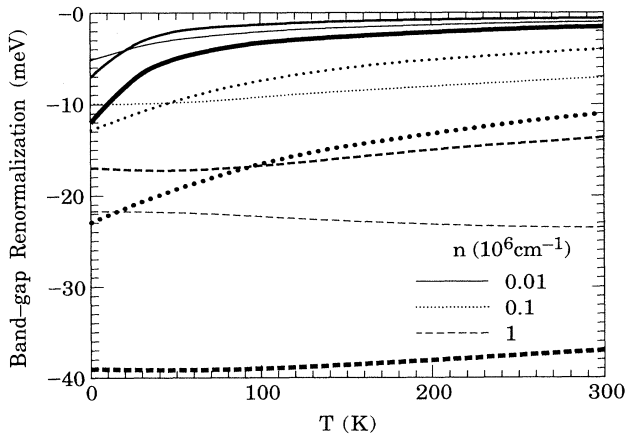


FIG. 3. Band-gap renormalization due to conduction electrons as a function of temperature, for a wire width of 100 Å in GaAs, for electron densities of $10^4$ cm$^{-1}$ (solid lines), $10^5$ cm$^{-1}$ (dotted lines), and $10^6$ cm$^{-1}$ (dashed lines). The thin lines are for the electrons ($\mathrm{Re}[\Sigma_{\mathrm{electron}}(k=0,\xi_{k=0})]$), the light bold lines are for the holes ($\mathrm{Re}[\Sigma_{\mathrm{hole}}(k=0,\xi_{k=0})]$), and the heavy bold lines are for the sum of the two. The densities $n=10^4$, $10^5$, and $10^6$ cm$^{-1}$ correspond to Fermi temperatures of $E_F=1.6\times10^{-2}$, 1.6, and 160 K, respectively.

Eq. (8) to the calculation of the self-energy and band-gap renormalization of electrons in a one-dimensional quantum wire in the extreme quantum limit (i.e., assuming that the electrons only occupy the lowest energy subband). We use the random-phase approximation form for the dielectric function $\epsilon(q,z)$, which we numerically evaluate using the finite-temperature expression given by Maldague.[13]

In Fig. 2, we show the real and imaginary parts of the retarded self-energy of a quantum wire (with a parabolic band in the unconfined direction), as a function of frequency, for $k=0$. The discontinuities in $\mathrm{Im}[\Sigma_{\mathrm{ret}}(\omega)]$ at $T=0$, which arise from virtual plasmon emission thresholds, broaden with increasing temperature because the plasmon peaks are broadened by Landau damping. The logarithmic divergence in the imaginary part of the self-energy that develops at $\omega=\xi_k$ when $T$ is increased from zero is unique to one-dimensional systems—in $d=1$ at $\omega=\xi_k$, there is a nonintegrable $q^{-1}$ singularity in the integrand in Eq. (8) corresponding to a divergence in the Born-approximation electron-electron scattering at small momentum transfer. (In higher dimensions, this singularity is removed by the phase-space factor of $q^{d-1}$.) Concomitant with the divergence in $\mathrm{Im}[\Sigma_{\mathrm{ret}}(k,\xi_k)]$ is a discontinuity in $\mathrm{Re}[\Sigma_{\mathrm{ret}}(k,\xi_k)]$, since the real and imaginary parts are related by the Kramers-Kronig relations.

In Fig. 3 we show the electron and hole band-gap renormalization due to the presence of conduction electrons. These results are relevant to photoluminescence experiments in GaAs, even though the calculation ignores the screening effects of holes, because the holes are ineffective at screening due to their heavy mass. Due to the discontinuity in $\mathrm{Re}[\Sigma_{\mathrm{ret}}(k,\xi_k)]$, we take $\frac{1}{2}\mathrm{Re}[\Sigma_{\mathrm{ret}}(k,\xi_k+0^+)+\Sigma_{\mathrm{ret}}(k,\xi_k-0^+)]$ at $k=0$ to be the band-gap renormalization. We find that for very low densities, where the Fermi temperature is low, the band-gap renormalization can change by approximately an order of magnitude when the temperature increases from $T=0$ to 300 K.

To conclude, we have shown that we can obtain, in a relatively direct manner, expressions for the analytic continuation of the thermal Matsubara self-energies which are suitable for use in numerical computations. Applying this method to the $GW$ approximation for the self-energy, gives Eq. (8), which generalizes the $T=0$ "line and pole" decomposition to finite temperatures. Using Eq. (8) to calculate the finite-temperature many-body properties of a quantum wire, we find that the band-gap renormalization can change significantly between $T=0$ and 300 K for wires with very low electron densities.

Enlightening discussions with S. Das Sarma and useful comments and suggestions by H. A. Fertig, C. A. Stafford, J. W. Wilkins, and X. C. Xie are gratefully acknowledged. This work was supported by the U.S. ARO.

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