Many-Body Properties of a Quasi-One-Dimensional Semiconductor Quantum Wire

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We study the many-body exchange-correlation properties of electrons confined to the lowest subband of a quantum wire, including effects of impurity scattering. Without impurity scattering, virtual excitations of arbitrarily low-energy plasmons destroy the Fermi surface of the electrons, whereas the presence of impurity scattering damps out these plasmons and *restores* the Fermi surface. The electron inelastic scattering rate Γ in the absence of impurity scattering is zero below k_c corresponding to the plasmon emission threshold, above which Γ diverges as $(k-k_c)^{-1/2}$. For typical wire widths and electron densities currently available, the band-gap renormalization is found to be $\sim$10–20 meV.

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There has been a great deal of recent interest [1] in ultranarrow confined semiconductor systems, called quantum wire structures, where electron dynamics is essentially restricted to be one dimensional. Such quantum wires, with active widths (along the plane of confinement) smaller than 300 Å and of negligible (less than 100 Å) thickness, have recently been fabricated [2,3] and continued improvement in growth and fabrication techniques should lead to even more confined and better defined wires in the near future. While there is much excitement about the potential applications of these semiconductor quantum wires as high-speed transistors and efficient photodetectors and lasers, these systems have also generated great fundamental physics interest as examples of *real* one-dimensional Fermi gases, where one-dimensional electron dynamics can be studied in a controlled and quantitative manner (just as semiconductor inversion layers, heterojunctions, and quantum wells have been serving as useful physical models for two-dimensional Fermi systems for the last decade or so). Recent fabrication breakthroughs [2,3] have allowed the attainment of the *truly* one-dimensional electric quantum limit, in the sense that only one quantum subband is populated by the electrons in the quantum wire so that the one-dimensional interacting Fermi-gas model is valid. Theory predicts very unusual properties for interacting one-dimensional Fermi systems, and the semiconductor quantum wires should be ideal for experimentally observing these properties. However, thus far, all experimental results [1–4] of electronic properties of quantum wires seem to be explicable on the basis of a normal one-dimensional Fermi-liquid model.

The purpose of this Letter is twofold. (1) We want to address the issue of why the one-dimensional quantum wire electrons seem to behave as normal Fermi liquids despite convincing well-accepted theoretical claims that both disorder and interaction effects are singularly nonperturbative in one dimension and should lead to ground states which are drastically different from normal Fermi liquids (such as strongly localized systems or Luttinger liquids [5]). (2) We present calculated results for two important experimentally measurable Fermi-liquid properties for the quantum wire electrons, the electronic inelastic mean free path and the band-gap renormalization. Our calculation is, to the best of our knowledge, the first complete realistic theory of many-body exchange-correlation effects in one-dimensional quantum wire systems; similar early calculations [6] in two-dimensional electron-gas systems were useful and important in the development of that subject.

Addressing point (1) of the paper, we begin by mentioning three important ways in which an *ideal* one-dimensional electron gas is *theoretically* expected to be *strikingly different* from their higher-dimensional counterparts. In each case, a perturbation to the system, which in higher dimensions tends to leave the system in a Fermi-liquid state, theoretically *drastically* changes the behavior of the system in one dimension (i.e., the Fermi-liquid behavior is a highly unstable fixed point in one dimension). We then argue that *actual* semiconductor quantum wires may behave differently from the theoretical zero temperature ideal because of the effects of finite temperature, finite size, and scattering, which may serve to stabilize Fermi-liquid behavior in the semiconductor quantum wires.

First, the presence of any electron-phonon coupling (which is invariably present) in a one-dimensional system theoretically should result in a lattice Peierls distortion [7], accompanied by a charge-density-wave ground state at zero temperature. However, in actual semiconductor quantum wires, the electron-phonon interaction via the deformation potential coupling is so weak that even at the low temperatures, at which experiments on these systems are performed, the Peierls distortion does not occur. The second important consideration for quantum wires is disorder-induced Anderson localization [8]—in one dimension (unlike higher dimensions), the presence of *any* disorder localizes all electronic states. The currently fabricated semiconductor quantum wires are obviously not disorder free, and hence, in the electric quantum limit, all the quantum wire electronic states are exponentially Anderson localized, and the concept of an electron gas strictly should not apply here. However, we argue that in the state-of-the-art high-quality semiconductor quantum wires incorporating modulation doping techniques, typical localization lengths are very long (many microns) and therefore in these wires the electrons may be considered to be extended for all experimental purposes.

The third important way in which ideal one-dimensional Fermi gases differ from equivalent higher-dimensional systems is that the presence of particle-particle interactions theoretically makes the Fermi-liquid model inapplicable to one-dimensional systems [5]. Instead, the paradigm for interacting one-dimensional Fermi systems is the strongly correlated Luttinger (also called Tomonaga-Luttinger) liquid. Hence, in the electric quantum limit semiconductor quantum wires should behave as Luttinger liquids. In experiments involving luminescence, inelastic light scattering, far-infrared spectroscopy, capacitance studies, etc., on the other hand, quantum wires have shown no obvious sign of Luttinger-liquid behavior, seemingly behaving instead as *normal* one-dimensional Fermi liquids. For instance, an essential feature of a Luttinger liquid is that it has no Fermi surface (i.e., the momentum distribution function n_k is continuous through the Fermi momentum k_F) and yet luminescence experiments show large Fermi edge singularities [2]. In this paper, we suggest, based on our theoretical results, that in the real quantum wires impurity effects can suppress Luttinger-liquid behavior in semiconductor quantum wires, causing them to behave as normal one-dimensional Fermi liquids. Thus, the effects of the strong correlations of the Luttinger liquid, just as the Peierls instability and Anderson localization, may be negligible in real quantum wires.

In this work, we calculate the zero-temperature leading-order (in the dynamically screened interaction) self-energy $\Sigma(k,\omega)$ of electrons that are confined to the lowest-energy subband of quantum wire of width a and of zero thickness with infinite potential barriers. We ignore contributions from higher-energy subbands on the grounds that they should be irrelevant in the limit where the electron Fermi energy is much smaller than the subband energy separation. (The calculation can of course be extended to include higher subbands.) Knowledge of $\Sigma(k,\omega)$ allows one to calculate many experimentally observable one-electron properties of a system. We calculate $\Sigma(k,\omega)$ using the so-called GW approximation [9], which has been highly successful in describing properties of real two- and three-dimensional electron systems. $\Sigma(k,\omega)$ is determined by the dynamical screening properties of the electron gas in the wire, which is quantified by the dielectric function $\epsilon(q,\omega)$. We assume that $\epsilon(q,\omega)$ is given by the random-phase approximation (RPA) [10,11], which has recently been shown [12] to exactly reproduce the plasmon dispersion of one-dimensional systems. We include the effects of impurity scattering on $\epsilon(q,\omega)$ through the modification given by Mermin [13], in which the scattering is described by a single relaxation rate γ.

A system is a Fermi liquid if it possesses a Fermi surface (i.e., a discontinuity in n_k) whose presence is indicated by a δ function in the spectral function $A(k,\omega)$ at $k=k_F$ and $\omega=0$. The existence of a $\delta(\omega)$ in $A(k_F,\omega)$ depends crucially on the behavior of $\mathrm{Im}[\Sigma(k_F,\omega)]$ as $\omega\rightarrow 0$. If $|\mathrm{Im}[\Sigma(k_F,\omega)]|$ goes to zero faster than $|\omega|$, then $A(k_F,\omega)$ has a $\delta(\omega)$, indicating that the system is a Fermi liquid. The discontinuity in n_k at k_F is proportional to the weight of this δ function and is called the renormalization factor Z_F [14]. In contrast, if $|\mathrm{Im}[\Sigma(k_F,\omega)]|$ goes to zero slower than $|\omega|$, then there is *no* δ function in $A(k_F,\omega)$, implying that the system is *not* a Fermi liquid [5,15]. Two- and three-dimensional systems with and without disorder in general are Fermi liquids [16]. Through a study of $\mathrm{Im}[\Sigma_{\mathrm{ret}}(k_F,\omega)]$, we show that in one dimension the system is (is not) a Fermi liquid in the presence (absence) of impurity scattering.

The imaginary part of $\Sigma(k_F,\omega)$ is a measure of the virtual transition rate to all states of energy less than ω away from the Fermi energy. At low energies in two and three dimensions, single-particle scattering is far more important than plasmon scattering because the single-particle excitation spectrum is gapless and the phase space available for single-particle scattering extends around the entire Fermi surface, whereas the plasmon dispersion either rises quickly or has a gap at $q=0$. Therefore, for small ω, the major contribution to $\mathrm{Im}[\Sigma(k_F,\omega)]$ in two and three dimensions comes from *virtual single-particle excitations.* In contrast, in one dimension, the single-particle excitation spectrum has a gap except at $|q|=0,2k_F$, and the phase space available for single-particle scattering is severely restricted, while the plasmon dispersion is gapless at $q=0$. Hence, in one dimension, $\mathrm{Im}[\Sigma(k_F,\omega)]$ at small ω is dominated not by virtual single-particle excitations but by the *virtual excitation of plasmons.* This unique feature of one-dimensional systems gives rise to interesting consequences, which we describe next.

In the case of a clean quantum wire ($\gamma=0$), we find within the RPA that the dominance of the virtual low-energy plasmon excitations results in $|\mathrm{Im}[\Sigma(k_F,\omega)]| \sim|\omega|\,|\ln(|\omega|)|^{1/2}$, indicating, as noted earlier, that the Fermi surface does not exist (in agreement with Luttinger-liquid theory). In other words, because of the ease with which particles at the Fermi surface can emit virtual low-energy plasmons, the Fermi surface smears out to the extent that a sharp discontinuity in n_k no longer exists. However, the inclusion of impurity scattering causes the electrons to diffuse at long wavelengths which damps out the plasmons at small q. Hence, the plasmon contribution to $\mathrm{Im}[\Sigma(k_F,\omega)]$ at small $|\omega|$ is removed, resulting in $\mathrm{Im}[\Sigma(k_F,\omega)]|\sim\omega^2|\ln(|\omega|)|^3$ as $|\omega| \rightarrow 0$, which implies that the Fermi surface is restored. This result indicates the Fermi surface is resurrected in dirty systems because the low-energy virtual plasmon emission responsible for its destruction in clean systems has been suppressed by impurity scattering.

In Fig. 1, we show our calculated Fermi distribution function $n_k=(2\pi)^{-1}\int d\omega\, A(k,\omega)$ for various values of the impurity scattering rate γ. We emphasize that γ was

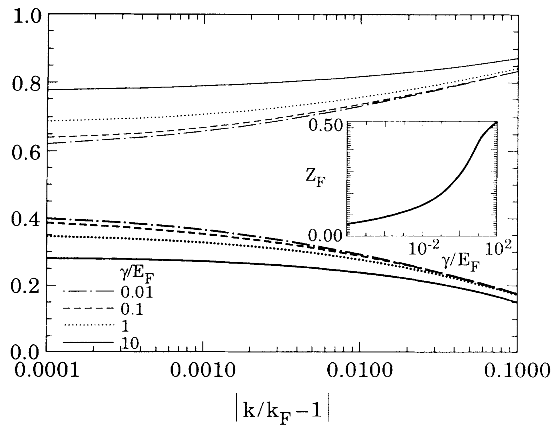

FIG. 1. Momentum distribution function n_k of a quasi-one-dimensional electron gas around $k/k_F=1$, for $k_Fa=0.9$ and $r_s=2m_ee^2/\pi\hbar^2k_F\epsilon_0=0.7$ (corresponding to $a=100$ Å and density of 0.56×10^6 cm^{-1} in GaAs), for various impurity scattering rates γ. The bold lines refer to $k>k_F$, and the thin lines to $k<k_F$. For $\gamma=0$, n_k is continuous at $k=k_F$, implying that the system is non-Fermi-liquid, but for $\gamma\neq0$ a discontinuity occurs at $k=k_F$, signaling the presence of a Fermi surface. Inset: The Fermi surface renormalization factor Z_F, which gives the magnitude of the discontinuity in n_{k_F}, is shown as a function of γ.

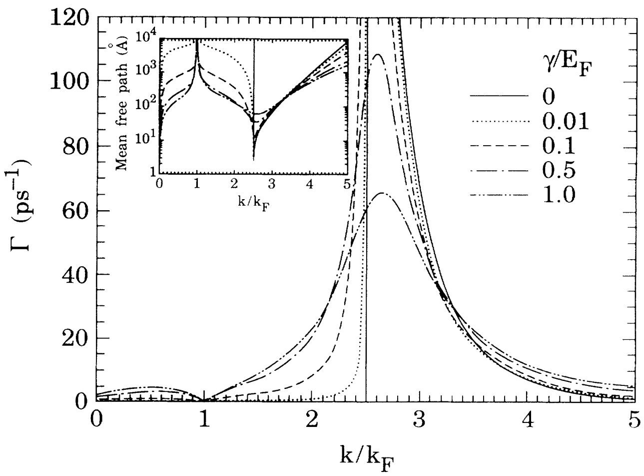

FIG. 2. Inelastic scattering rates $\Gamma(k)$, as a function of k, for various γ's (electron-impurity scattering rates), for $k_Fa=0.9$ and $r_s=0.7$. Within RPA, for $\gamma=0$, the $\Gamma(k)$ is identically zero below $k=k_c$ because energy and momentum conservation prohibits single-particle excitations and plasmon emissions. Above k_c, the scattering rate is caused by plasmon emissions. For $\gamma\neq0$, the plasmon line broadens and momentum conservation is relaxed, resulting in a nonzero Γ for $k<k_c$. Inset: The corresponding mean free path $l(k)=k/m\Gamma(k)$.

included only in the dynamical screening function and *not* in the single-electron Green's function because we wanted to determine if the suppression of the emission of low-energy virtual plasmons produces a discontinuity in n_k. Figure 1 clearly shows a discontinuity in n_k at $k=k_F$ for $\gamma/E_F\neq0$. Note that if we included effects of γ (or finite temperature) in the single-electron Green's function, n_k would have been broadened in the usual way and the result would look very similar to nonsingular higher-dimensional broadened Fermi functions. These details will be published elsewhere. In the inset, we show the calculated Z_F as a function of the impurity scattering rate. For $\gamma=0$, $Z_F=0$ indicating that there is no Fermi surface, but as scattering is increased Z_F also increases until it saturates at very large γ (where our results should not be trusted because our treatment ignores localization). Note that Z_F goes to zero slowly as $\gamma\rightarrow0$, implying that even a small amount of impurity scattering results in a fairly pronounced discontinuity in n_k at k_F.

Figure 2 shows the inelastic scattering rates of quasiparticles in the conduction band $\Gamma(k)=2|\mathrm{Im}[\Sigma(k,\omega=\xi_k)]|$, where ξ_k is the electron energy relative to the chemical potential, for parameters corresponding to $a=100$ Å and a density of $n=0.56\times10^6$ cm^{-1} in GaAs. For $\gamma=0$, below a threshold wave vector k_c, there is *no* electron-electron scattering (within the RPA) because in a strictly one-dimensional system conservation of energy and momentum restricts electron-electron scattering to an exchange of particles, which is not a randomizing process because electrons are indistinguishable [17]. (Our treatment ignores multiparticle excitations, which will give rise to a nonzero scattering rate for $k<k_c$.) For $k>k_c$, a new scattering channel opens in which electrons genuinely emit plasmons (as opposed to the virtual plasmon excitations at the Fermi surface). The inelastic scattering rate diverges as $\sim(k-k_c)^{-1/2}$ as one approaches k_c from above, due to the divergence in the density of states available for scattering right at the plasmon emission threshold. For $\gamma\neq0$, the inelastic scattering rate remains finite because the plasmon line is broadened. Furthermore, the breaking of translational invariance relaxes momentum conservation, permitting inelastic scattering via single-particle excitations for $k<k_c$. The inset in Fig. 2 shows the inelastic mean free path, $l=v(k)/\Gamma(k)$, where v is the electron velocity.

In Fig. 3, we show the results of the calculation of the band-gap renormalization (the sum of $\mathrm{Re}[\Sigma(k=0,\omega=\xi_{k=0})]$ of conduction-band electrons and valence-band holes) due to the presence of the conduction electrons. These results should be useful in explaining photoluminescence experiments in quantum wires, even though we only have electrons in our calculation while the experiments contain both electrons and holes, because we expect the holes to have a negligible effect on the band-gap renormalization due to their large mass (and hence their inability to screen effectively).

Finally, we discuss differences between our model and the Luttinger model, on which the properties of the Luttinger liquid are based. We assume a finite density of electrons in a parabolic energy dispersion, whereas the

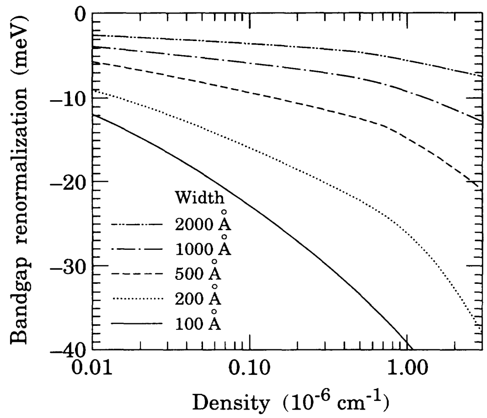

FIG. 3. Total band-gap renormalization $[\mathrm{Re}(\Sigma_e+\Sigma_h)$ at $k=0$, $\omega=\xi_{k=0}]$ as a function of electron density in the quantum wire for various wire widths with parameters corresponding to GaAs.

Luttinger model assumes an *infinite* density of negative energy electrons in a completely linear dispersion. We use the *actual* Coulomb interaction [18] between electrons for a rectangular well (a reasonably realistic model for confinement [19]), whereas the Luttinger model assumes an unrealistic short-range potential. On the other hand, we carry out only the leading-order self-energy calculation in the dynamically screened interaction, whereas the solution of the Luttinger model includes all vertex corrections and is exact.

In conclusion, we have shown that in a one-dimensional system, within the RPA, the Fermi surface disappears in a clean system because particles at the Fermi surface can excite low-energy virtual plasmons. When impurity scattering is included, the Fermi surface *reappears* because the low-energy virtual plasmon excitations which are responsible for the disappearance of the Fermi surface are suppressed by the impurity scattering. In the absence of impurity scattering, there is a divergence in the inelastic scattering rate as k approaches the plasma emission threshold from above. The band-gap renormalization is found to be on the order of 10–20 meV for typical experimental parameters.

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