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Screening and elementary excitations in narrow-channel semiconductor microstructures

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The dielectric response of a one-dimensional electron gas occurring in the narrow inversion layers in metal-oxide-semiconductor field-effect transistor (or quantum-well) structures is investigated theoretically. A nonsingular screening function appropriate for dc transport calculations is derived. The plasma frequency in such a system is obtained as an explicit function of wave number. Plasmon dispersion for a lateral two-dimensional superlattice made from such one-dimensional quantum wires is also calculated.

Low-dimensional electronic systems occurring at semiconductor surfaces or interfaces have attracted considerable theoretical and experimental attention over the last fifteen years. Two-dimensional (2D) electron systems occurring in metal-oxide-semiconductor (MOS) structures [e.g., the inversion or accumulation layers in Si-SiO_2 MOS field-effect transistors (MOSFET's)] or in semiconductor heterostructures (e.g., GaAs-$Al_xGa_{1-x}As$ heterojunction) have been studied extensively.[1] Very recently, a one-dimensional (1D) electron system has been produced[2] in silicon MOSFET's by a number of experimental groups[3–6] using a variety of techniques. Preliminary transport measurements in these 1D systems have been reported in several recent publications[2–6] and extensive activity in this potentially technologically important field is expected in the near future. In addition, following a suggestion by Sakaki,[7] Petroff, Gossard, Logan, and Wiegman[8] have recently produced and studied a 1D electron gas in a GaAs heterostructure. These 1D quantum wires in GaAs heterostructures have been claimed[7–9] as an exciting new technological possibility, since the impurity content and distribution around these wires can be selectively controlled, producing enhanced mobility which may even exceed the very high mobility values achieved in modulation-doped 2D GaAs-$Al_xGa_{1-x}As$ heterojunction electron transistors. A number of theoretical papers[10–13] have also appeared in the literature dealing with various aspects of electronic transport in these 1D systems.

In this Rapid Communication we consider theoretically several aspects of these 1D quantum wires. Our calculated results should be significant in the understanding of various electronic properties of these systems as experimental information becomes available. In particular, we calculate the screening properties and the elementary collective-excitation spectrum (plasmons) in 1D electron systems. Our emphasis is on pointing out how the quasi-1D nature of real systems suppresses various divergences inherent (and well known) in the *purely* 1D theory. Ours is necessarily a model calculation, since information about the electronic (as well as geometric) structure of these systems is unavailable at this time. For example, no self-consistent electronic-structure calculation for these 1D systems along the lines of the corresponding 2D calculations for Si inversion layers,[14] or for GaAs heterostructures[15] has been reported yet. In the absence of any such realistic calculation, we make the best possible model approximation for the one-electron wave functions (ψ) in these systems by writing

$$\psi(x,y,z)=\frac{e^{ikx}}{\sqrt{L}}\phi_n(y)\xi_i(z)\ , \tag{1}$$

where $\phi_n(y)$ and $\xi_i(z)$ are bound wave functions indicating quantization in the y and z directions whereas k is the good 1D wave vector along the length of the quantum wire which is taken to be the x direction with L as the macroscopic length of the wire. For ϕ and ξ we choose, respectively, the particle-in-a-box–type confinement[5] and the Stern-Howard variational wave function.[1] The ground-state 1D wave function is thus given by

$$\psi_{00k}(x,y,z)=L^{-1/2}e^{ikx}[(2/a)^{1/2}\sin(\pi y/a)]\times[(b^3/2)^{1/2}ze^{-bz/2}]\ ,$$

where the width of the 1D wire along the y axis is a and its average width along the z axis is $3/b=z_0$ with b as a variational parameter.[1] Typical values of a and z_0 are 50–1000 Å and 20–200 Å, respectively.

Using the wave function of Eq. (1), one can obtain the matrix element of the Coulomb interaction in the system, as

$$V_{(n_1n_2n_3n_4)(ijlm)}(q)=\frac{2e^2}{\kappa}\int_0^a dy\int_0^a dy'\phi_{n_1}(y)\phi_{n_2}(y)\phi_{n_3}(y')\phi_{n_4}(y')\int_0^\infty dz\int_0^\infty dz'\xi_i(z)\xi_j(z)\xi_l(z')\xi_m(z')K_0(qR)\ , \tag{2}$$

where

$$R=\sqrt{(y-y')+(z-z')^2}\ , \tag{3}$$

and $K_0(x)$ is the modified Bessel function of the second kind. For the sake of simplicity we have chosen a constant-average-background lattice dielectric constant κ for the system. In Fig. 1(a) we show the calculated Coulomb matrix element $V(q)$ for the ground state ($n_1=n_2=n_3=n_4=0$ and $i=j=l=m=0$) of the system as a function of qa and for a fixed 2D electron density of $N_s=10^{12}$ cm^{-2} (which for $a=100$ Å gives an average 1D electron density of $n_w=10^6$ cm^{-1}). We have also shown by the dashed curve the corresponding logarithmically divergent result for the purely 1D approximation which gives

$$V(q)\simeq\frac{2e^2}{\kappa}K_0(qa)\approx 2e^2|\ln(qx_0)|/\kappa$$

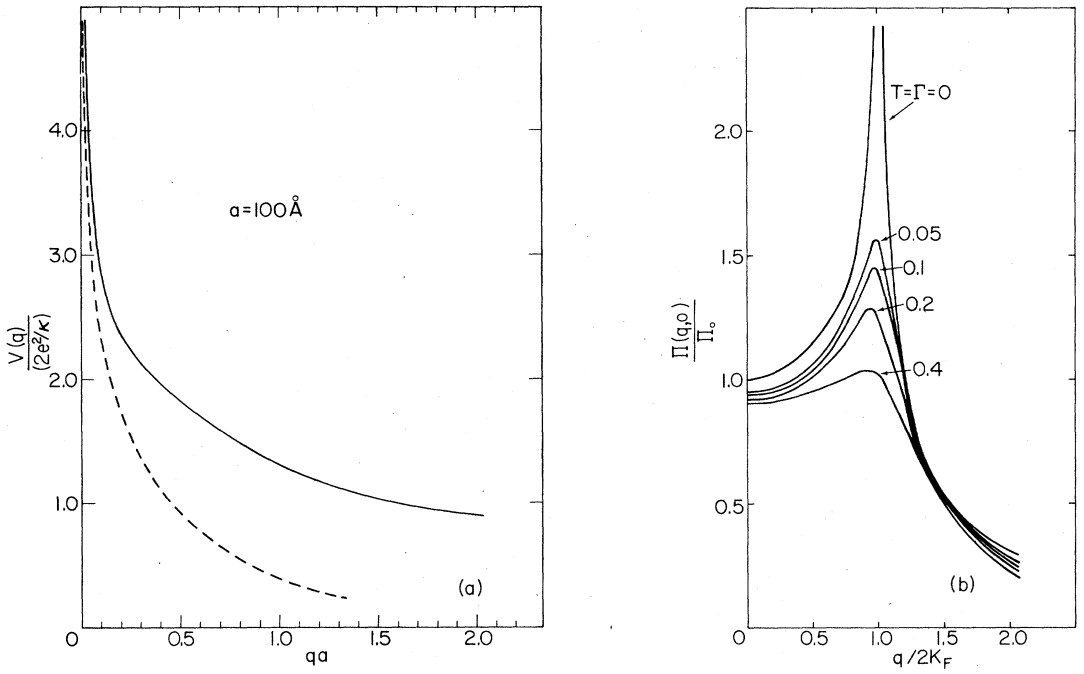

FIG. 1. (a) The calculated Coulomb-interaction matrix element in a quantum wire for the subband-quantized situation [Eq. (2)] (solid curve) and for the 1D model, modified-Bessel-function approximation (dashed curve). (b) The static polarizability of 1D electron gas in the presence of finite temperature and collisional broadening. The top curve is the (singular) result for the pure ($\Gamma=0$) system at zero temperature. The values of the broadening for the other four curves are (from top to bottom) $\Gamma/E_F=0.05$, 0.1, 0.2, and 0.4. The temperature is $T=0.1E_F/k_B$ for these four curves. Π_0 is the magnitude of Π $(q=0,0)$ with $T=\Gamma=0$.

for small qa, where x_0 is a characteristic cutoff length in the problem. In the long-wavelength limit of small q ($qa \ll 1$) it is easy to show that Eq. (2) gives a similar asymptotic behavior

$$V(q \to 0) \simeq 2e^2|\ln(qr_0)|/\kappa \ ,$$

where r_0 is the average value of R which can be taken out as a constant in this limit. We want to emphasize that in a purely 1D theory, $V(q)$ is logarithmically singular for all q, whereas our calculated $V(q)$ as shown in Fig. 1(a) is well behaved for all q except for the usual long-range divergence of the Coulomb interaction for $q \to 0$.

Screening is determined by the static dielectric function $\epsilon(q,0)$ of the system, which, within the random-phase approximation (RPA), is given by

$$\epsilon(q,0)=1-V(q)\Pi(q,0) \ ,$$

where $\Pi(q,0)$ is the static polarizability function of the 1D electron gas. It is well known[16] that the polarizability function of a noninteracting 1D electron gas is logarithmically divergent at $q=2k_F$, where k_F is the 1D Fermi wave vector. This is a simple consequence of the perfect nesting of the Fermi surface in 1D, and is related to the well known Peierls instability. In a real system this $2k_F$ singularity will be softened by thermal and other broadening mechanisms. Since we are primarily interested in low-temperature transport properties, temperature effects[17] on the polarizability are not very important for our purpose. We have calculated the 1D polarizability function by including both the thermal and collisional broadening effects. Collisional broadening arising from impurity scattering is expected to have a significant effect on the polarizability function, particularly around the $q=2k_F$ singular point. We have included impurity scattering effects in the finite-temperature polarizability function by considering the ladder-bubble diagrams. Keeping only the leading-order diagram in the series, we get

$$\Pi(q,0)=-\left[\frac{2g_v m}{\pi q}\right]\int_{-\infty}^{+\infty} dp\left[1-\left[\frac{2}{\pi}\right]\mathrm{Im}\Psi\left[\frac{1}{2}+\frac{\beta\Gamma}{2\pi}+i\frac{\beta E_p}{2\pi}\right]\Big/(2p+q)\right] , \tag{4}$$

where $\beta=(k_BT)^{-1}$, $\Gamma=1/2\tau$ is the collisional broadening associated with a lifetime τ, and $E_p=p^2/2m-\mu$, with μ as the self-consistent chemical potential to be obtained from the total number of particles $n_w=\int dE\, D(E)f(E)$, where D and f are the 1D electronic density of states and the Fermi distribution function, respectively. In Eq. (4), Ψ is the digamma function and g_v is the valley-degeneracy factor[1] [$g_v=2$ for the Si(100) system and $g_v=1$ for GaAs systems].

In Fig. 1(b) we show the calculated $\Pi(q,0)$ as a function of q for several values of Γ and T. It is clear that the inclusion of impurity scattering in the calculation of screening is of fundamental importance at low temperatures in a 1D system (unlike in a 2D system[18] where impurity-scattering effects on the polarizability give rise to higher-order effects). One can easily calculate the low-temperature transport properties of 1D quantum wires using the $V(q)$ and the $\Pi(q)$ ob-

tained in this paper, provided the location and the strength of the charged impurities around the wire are known. We defer the transport calculation to a future publication, since sufficient experimental information on nonlocalized (or "metallic") transport properties is not yet available.

In the second part of this Communication we obtain the collective-excitation spectrum of 1D quantum wires within the RPA. Plasma modes are given by

$$\epsilon(q,\omega)=1-V(q)\Pi_0(q,\omega)=0\ ,$$

where Π_0 is the noninteracting[19] dynamical polarizability. In the long-wavelength ($q\rightarrow 0$) limit we can easily show that the plasmon frequency is given by

$$\omega_p \simeq \omega_0(qa)|\ln(qa)|^{1/2}+O(q^2)\ , \tag{5}$$

where

$$\omega_0=(2n_w e^2/\kappa m a^2)^{1/2}\ .$$

At higher q values, one has a somewhat better approximation given by $\omega_p\simeq\omega_0(qa)\sqrt{K_0(qa)}$. We have, however, solved the exact plasma relation $\epsilon(q,\omega)=0$ by using the numerical values for $V(q)$ as given by Eq. (2) and $\Pi_0(q,\omega)$, and the results are shown in Fig. 2(a), where ω_p/ω_0 is plotted against qa for the exact numerical treatment as well as for the two long-wavelength approximations. It is clear that the long-wavelength approximation is reasonable only for $qa\leq 0.1$. Note that the softening in the plasma frequency for high qa is a spurious effect of the long-wavelength approximation. One very important feature of the 1D plasma dispersion is its strong dependence on the wire dimension a. This is very different from[20] 2D plasmons where information about the subband quantization shows up only in the higher-order dispersion corrections. *This indicates that plasmon spectroscopy (even in the $q\rightarrow 0$ limit) can be used as a characterization tool to obtain quantitative information about the 1D quantization in these wires.*

Since the plasma frequency vanishes in the long-wavelength limit, it is important to include broadening effects in the plasmon dispersion. We expect the plasmon mode to become overdamped at some critical wave number q_c, below which the mode ceases to exist. To include broadening effects, we calculate the polarizability in the diffusion approximation, which can be written as

$$\Pi_D(q,\omega)=\left(1+\frac{i}{\omega\tau}\right)\Pi_0\left(q,\omega+\frac{i}{\tau}\right)\times\left[1+\left(\frac{i}{\omega\tau}\right)\Pi_0\left(q,\omega+\frac{i}{\tau}\right)\Big/\Pi_0(q,0)\right]^{-1}\ , \tag{6}$$

where $\tau=(2\Gamma)^{-1}$ is the relaxation time. In Fig. 2(b) we show the plasmon dispersion calculated on the basis of this diffusion propagator. As is expected, the plasmon vanishes at $q_c a=0.021$ for $\Gamma/\omega_0=0.04$. For small values of qa, the plasmon dispersion is substantially different from the results with $\Gamma=0$. The broadening effect on the plasma dispersion is quantitatively much more important in 1D systems than it is for the corresponding[21] 2D results.

Finally, we have considered the plasmon dispersion in a 1D superlattice formed from a large number of quantum wires placed parallel to each other in a 2D plane. It is easy to show that the plasmon dispersion in such a superlattice is given by the relation

$$1-\Pi_0\sum_{l'}V_{l-l'}(q)e^{ik_y(l-l')d}=0\ ,$$

which in the long-wavelength limit gives

$$\omega=(\omega_0 qa)\left[K_0(qa)+2\sum_{l=1}^{\infty}K_0(lqd)\cos(k_y ld)\right]^{1/2}\ , \tag{7}$$

where d is the superlattice period (i.e., d is the separation

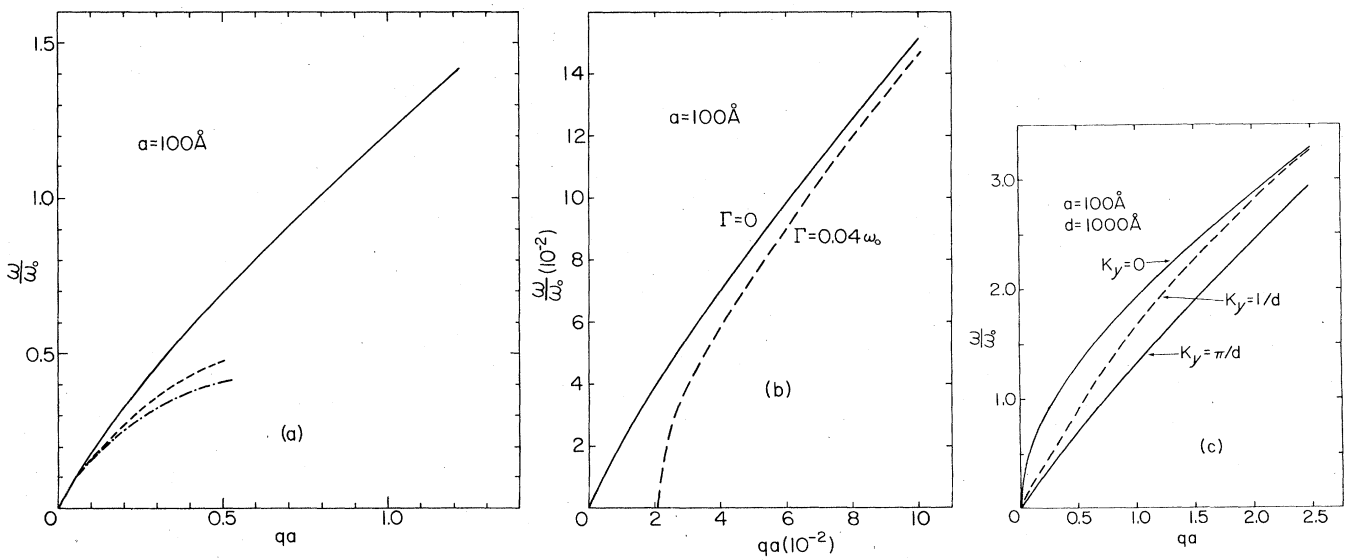

FIG. 2. (a) Calculated plasmon dispersion in a quantum wire as a function of qa where a is the wire width. The solid curve is the actual numerical result, whereas the dashed and the dashed-dotted curves are the long-wavelength Bessel-function approximation and the logarithmic approximations, respectively. (b) The effect of finite broadening on the plasmon dispersion with the solid and the dashed curves giving results without and with broadening, respectively. (c) The plasmon dispersion in a quantum-wire superlattice for three values of $k_y d$, where d is the superlattice period. Results at the plasmon band edges ($k_y=0$ and π/d) correspond, respectively, to purely 2D and 1D plasmons.

between the wires and a is the width of each wire) along the y direction, while k_y is the wave vector associated with the superlattice. We make the usual approximation $d > a$ even though it is not critical for our model.

We have solved the plasma dispersion relation for a superlattice both in the long-wavelength limit, and for arbitrary qa using numerical techniques. Our results are shown in Fig. 2(c). Similar to the situation[22] in 2D superlattices, the plasmons form a superlattice band with k_y as the band wave vector, which varies in the regime $0 \leq k_y \leq |\pi/d|$. For $k_y = 0$, one is looking at long wavelengths in the y direction, and hence the superlattice plasmon looks like a 2D plasmon with $q^{1/2}$ dispersion near $q = 0$. For $k_y = \pi/d$, we are at the zone edge, and the plasmon is 1D in nature. These features are easily seen in Fig. 2(c), where the plasmon for some arbitrary k_y, namely, $K_y d = 1$, is also shown. The plasma band is contained in the region between the two extreme curves at $k_y = 0$ and $k_y = \pi/d$.

In summary, we have considered the screening properties and the elementary excitation spectrum of 1D quantum semiconductor microstructures. We have shown that divergences inherent in strictly 1D theories are suppressed by physical effects like wave-function or impurity-scattering effects. Our results clearly demonstrate that a simple-minded 1D approximation has little quantitative validity in real structures. We have neglected a number of important effects, the most important ones being localization[23] and electron-electron interaction[24] effects (beyond RPA). Both of these effects are of fundamental importance in 1D systems, and their neglect may not be justifiable. Since ours is the first realistic model calculation for these quantum structures, we believe that any effort to incorporate localization or interaction effects should include the basic features considered in this paper. Also, deviations from strict one-dimensionality in the real structures may render invalid some of the general theorems about 1D localization and interaction. On the other hand, if the one-electron wave functions are truly localized in these systems, our work on the screening properties becomes applicable only if the typical localization length (or Thouless length at finite temperature) is larger than the sample width. However, we believe that our calculated plasmon spectrum still remains valid,[25] since localization affects only the very-low-frequency behavior of the dielectric response. Thus our work on plasmons (in both the 1D quantum wire and the superlattice) should be of approximate general validity, whereas our work on screening is applicable only if the one-electron states in the system can be taken to be noninteracting and "delocalized."

Before concluding, we should point out that a rather extensive literature exists[16] on the properties of a one-dimensional electron gas with most of the work carried out in the context of linear-chain organic conductors like tetrathiafulvalene-tetracyanoquinodinethane. New features of our work as presented in this paper are the use of realistic wave functions [Eqs. (1)–(3) and Fig. 1(a)] appropriate for 1D confinement in actual semiconductor structures. Our plasmon dispersion [Fig. 2(a)] relation is thus the first calculated plasmon spectrum for 1D semiconductor quantum wires. For earlier work on 1D plasmons one should consult Refs. 19 and 26. To the best of our knowledge, our calculated plasmon spectrum in the presence of level-broadening effects [Fig.2(b)] and the plasmon spectrum in the 1D superlattice [Fig. 2(c)] are completely new. Finally, our calculated nonsingular screening function [Eq. (4) and Fig. (1)] is, as far as we know, the first such explicit result, even though a one-dimensional dielectric response has earlier been treated[19,27] in the literature including the work of Patton and Sham,[28] who implicitly considered the inclusion of scattering effects in the one-dimensional polarizability.

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[1]T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[2]A. Hartstein, R. A. Webb, A. B. Fowler, and J. J. Wainer, Surf. Sci. **142**, 1 (1984).
[3]A. B. Fowler, A. Hartstein, and R. A. Webb, Phys. Rev. Lett. **48**, 196 (1982).
[4]R. G. Wheeler, K. K. Choi, A. Goel, R. Wisnieff, and D. E. Prober, Phys. Rev. Lett. **49**, 1674 (1982).
[5]W. J. Skocpol, L. D. Jackel, E. L. Hu, R. E. Howard, and L. A. Fetter, Phys. Rev. Lett. **49**, 951 (1982).
[6]R. F. Kwasnick, M. A. Kastner, J. Melngailis, and P. A. Lee, Phys. Rev. Lett. **52**, 224 (1984).
[7]H. Sakaki, Jpn. J. Appl. Phys. **19**, L735 (1980).
[8]P. M. Petroff, A. C. Gossard, R. A. Logan, and W. Wiegman, Appl. Phys. Lett. **41**, 635 (1982).
[9]H. Sakaki, J. Vac. Sci. Technol. **19**, 148 (1981).
[10]V. K. Arora, Phys. Rev. B **23**, 5611 (1981).
[11]J. Lee and H. N. Spector, J. Appl. Phys. **54**, 3921 (1983).
[12]G. W. Bryant, Phys. Rev. B **29**, 6632 (1984).
[13]P. A. Lee, Phys. Rev. Lett. **53**, 2042 (1984).
[14]S. Das Sarma and B. Vinter, Phys. Rev. B **26**, 960 (1982).
[15]F. Stern and S. Das Sarma, Phys. Rev. B **30**, 840 (1984).
[16]For a general review on the 1D electron gas, see *One Dimensional Conductor,* edited by J. T. Devreese, R. P. Evrard, and V. E. van Doren (Plenum, New York, 1979).
[17]A. J. Heeger, in Ref. 16, p. 69.
[18]S. Das Sarma, Phys. Rev. Lett. **50**, 211 (1983).
[19]P. F. Williams and A. N. Bloch, Phys. Rev. B **10**, 1097 (1974).
[20]S. Das Sarma, Phys. Rev. B **29**, 2334 (1984).
[21]G. F. Giuliani and J. J. Quinn, Phys. Rev. B **29**, 2321 (1984).
[22]S. Das Sarma and J. J. Quinn, Phys. Rev. B **25**, 7603 (1982).
[23]D. J. Thouless, Phys. Rev. Lett. **39**, 1167 (1977).
[24]B. L. Altshuler, A. G. Aronov, A. I. Larkin, and P. A. Lee, Phys. Rev. B **22**, 5142 (1980).
[25]We are indebted to R. E. Prange for pointing this out to us.
[26]M. Apostol, Z. Phys. B **22**, 279 (1975); J. J. Ritsko *et al.*, Phys. Rev. Lett. **34**, 1330 (1975).
[27]W. I. Friesen and B. Bergersen, J. Phys. C **13**, 6627 (1980), and references therein.
[28]B. R. Patton and L. J. Sham, Phys. Rev. Lett. **33**, 638 (1974).