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Self-consistent electronic response and collective excitations of a multiwire superlattice of finite barrier height

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Dielectric response and plasma excitations of a multiwire superlattice consisting of quantum wires (along z axis) periodically repeated in both the x and y directions are investigated. The quantum wells are considered to be separated by barriers of finite height, with consequent tunneling through the potential barriers which we treat employing tight-binding-type envelope wave functions. The intraminiband electron density-density correlation function is derived, and its normal modes (plasmons) are examined for various potential barrier heights.

Quasi-one-dimensional systems and semiconductor quantum-wire superlattices are currently the subject of considerable research effort. In particular, the electronic response and collective excitations of these novel structures are under intensive scrutiny both experimentally[1-3] and theoretically.[4-10] Most of these investigations are concerned with one-dimensional (1D) arrays of wires (wires repeated in one direction), whereas two-dimensional arrays of wires (wires repeated in two directions) with equally strong coupling in both directions are less well understood. In the latter case of finite potential barrier heights, electrons on adjacent wires couple not only through their mutual Coulomb repulsions, but also through the overlap of their wave functions. Such a quasi-one-dimensional system has properties intermediate between a one-dimensional electron gas and a three-dimensional electron gas, which can be tuned directly from 1D to 3D, bypassing the 2D stage, by controlling the potential barrier height, the superlattice period, and the electron density. Existing studies[7,9,11] are devoted almost exclusively to the Coulomb-coupled quantum wires, leaving largely unanswered the important question of the effect of wave-function overlap upon the dielectric properties and collective excitations of such quasi-1D systems. In this paper, we report on our theoretical investigation of the electronic response properties of a lateral quantum-wire superlattice with finite potential barrier heights, examining the consequences of the incomplete electron confinement. In this, we will first outline the derivation of the electron density-density correlation function (the inverse dielectric function) which encompasses both the intrawire and the interwire Coulomb interactions, as well as the wave-function overlap among neighboring wires, followed by an analysis of the collective and single-particle spectra of the dielectric response function.

Our model of the quantum-wire superlattice is comprised of cylindrical wires of radius r_0 along the z axis, centered on the 2D square lattice sites $\bar{R}=(n_1\hat{\mathbf{x}}+n_2\hat{\mathbf{y}})d$, where n_1 and n_2 are integers and d is the lattice constant. Electrons, of linear density n_0 per wire, are free to move in the z direction, but are partially confined within the cylindrical quantum wells of potential $U(\bar{r})=0$ for $r<r_0$, and $U(\bar{r})=V_0$ for $r>r_0$. ($\bar{r}$ denotes a 2D position vector in the x-y plane, with magnitude r.) The electron eigenstates are of the form $\psi_{\mathbf{k}}(\mathbf{r})=L^{-1/2}e^{ik_z z}\phi_{\bar{k}}(\bar{r})$, with energy eigenvalues $\varepsilon_{\mathbf{k}}=k_z^2/2m+E_{\bar{k}}$. To describe the motion in the x-y plane we employ the tight-binding scheme which has proven to be quite useful in treating planar superlattices,[12-15] and quantum-wire superlattices with wires strongly coupled in one direction only.[4,5,10] The tight-binding wave function is given by $\phi_{\bar{k}}(\bar{r})=A_{\bar{k}}N^{-1/2}\times\sum_{\bar{R}}e^{i\bar{k}\cdot\bar{R}}u(\bar{r}-\bar{R})$, corresponding to the miniband energy $E_{\bar{k}}$. N is the total number of lattice points (equal to the total number of wires), and $u(\bar{r})$ is the normalized single-well wave function for the lowest bound state in the cylindrical well. Furthermore, $A_{\bar{k}}=(1+2\alpha\cos k_x d+2\alpha\cos k_y d)^{-1/2}$ is a normalization factor, and $\alpha=\int d^2r\,u(\bar{r})^*u(\bar{r}-d\hat{\mathbf{x}})$. Only the lowest miniband is considered, and the wave functions are considered to be strongly localized in the wells such that only nearest-neighbor wave-function overlap is taken into account. Within these approximations the tight-binding miniband energy is given by $E_{\bar{k}}=\Delta(2-\cos k_x d-\cos k_y d)$, with a miniband full width 4Δ. Here, $\Delta=2\int d^2r\,u(\bar{r})^*\times U(\bar{r})u(\bar{r}-d\hat{\mathbf{x}})$ is the overlap integral.

In terms of the second-quantized electron operators $c_{\mathbf{k}}^\dagger$ and $c_{\mathbf{k}}$ (suppressing spin indices) the system Hamiltonian can be written as

$$H=\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}c_{\mathbf{k}}^\dagger c_{\mathbf{k}}+\frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}V(\mathbf{q},\bar{k},\bar{k}')c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}'-\mathbf{q}}^\dagger c_{\mathbf{k}'}c_{\mathbf{k}}\,, \quad (1)$$

where the Coulomb matrix element is given as

$$V(\mathbf{q},\bar{k},\bar{k}')=(2e^2/\kappa)\int d^2r\,d^2r'\,\phi_{\bar{k}+\bar{q}}(\bar{r})^*\phi_{\bar{k}'-\bar{q}}(\bar{r}')^*\times K_0(q_z|\bar{r}-\bar{r}'|)\phi_{\bar{k}'}(\bar{r}')\phi_{\bar{k}}(\bar{r})\,, \quad (2)$$

in which κ is the background dielectric constant (considered to be the same in and out the quantum wells), and $K_0(x)$ is the zero-order modified Bessel function. As is well known, the solvability of the random-phase approximation (RPA) integral equation for the density-density correlation function of an interacting electron system depends critically on the form of the Coulomb matrix element. To facilitate such a solution, we cast the Coulomb matrix element in a matrix form following previous treatments of planar superlattices[12–15] based on wave-function overlap involving nearest-neighbor quantum wires only, thus we obtain

$$V(\mathbf{q},\bar{k},\bar{k}')=A_{\bar{k}+\bar{q}}A_{\bar{k}'-\bar{q}}A_{\bar{k}'}A_{\bar{k}}\hat{T}(\bar{k})\hat{V}(\mathbf{q})\hat{T}(\bar{k}')^T , \quad (3)$$

where $\hat{T}(\bar{k})$ is a column matrix [$\hat{T}(\bar{k})^T$ is its transpose] given by

$$\hat{T}(\bar{k})^T=(1,\cos k_x d,\sin k_x d,\cos k_y d,\sin k_y d) . \quad (4)$$

In Eq. (3), $\hat{V}(\mathbf{q})$ is a 5×5 square matrix whose elements are

$$V_{ij}(\mathbf{q})=(4\pi e^2/\kappa)\sum_{\bar{G}} I_i(\bar{q}+\bar{G})I_j(\bar{q}+\bar{G})^*/[(\bar{q}+\bar{G})^2+q_z^2] , \quad (5)$$

where $\bar{G}$ is the 2D reciprocal-lattice vector conjugate to $\bar{R}$, and the form factor $\hat{I}(\bar{q})$ is again a column matrix with elements

$$I_1(\bar{q})=\int d^2r\exp(i\bar{q}\cdot\bar{r})\,|u(\bar{r})|^2 , \quad (5a)$$

$$I_2(\bar{q})=\int d^2r\exp(i\bar{q}\cdot\bar{r})u(\bar{r})^*[u(\bar{r}-d\hat{\mathbf{x}})+u(\bar{r}+d\hat{\mathbf{x}})] , \quad (5b)$$

$$I_3(\bar{q})=i\int d^2r\exp(i\bar{q}\cdot\bar{r})u(\bar{r})^*[u(\bar{r}-d\hat{\mathbf{x}})-u(\bar{r}+d\hat{\mathbf{x}})] , \quad (5c)$$

$$I_4(\bar{q})=\int d^2r\exp(i\bar{q}\cdot\bar{r})u(\bar{r})^*[u(\bar{r}-d\hat{\mathbf{y}})+u(\bar{r}+d\hat{\mathbf{y}})] , \quad (5d)$$

and

$$I_5(\bar{q})=i\int d^2r\exp(i\bar{q}\cdot\bar{r})u(\bar{r})^*[u(\bar{r}-d\hat{\mathbf{y}})-u(\bar{r}+d\hat{\mathbf{y}})] . \quad (5e)$$

In the same spirit the electron density operator can be written as

$$\rho(\mathbf{q})=\hat{\rho}(\mathbf{q})^T\hat{I}(\bar{q}) , \quad (6)$$

where

$$\hat{\rho}(\mathbf{q})=\sum_{\mathbf{k}}\hat{T}(\bar{k})A_{\bar{k}+\bar{q}}A_{\bar{k}}c^\dagger_{\mathbf{k}+\mathbf{q}}c_{\mathbf{k}} . \quad (7)$$

To formulate the RPA integral equation we consider the equation of motion of the electron density matrix $i\partial\tilde{\rho}/\partial t=[H+H',\tilde{\rho}]$, where H is given by Eq. (1) and $H'=\sum_{\mathbf{q}}\phi(\mathbf{q},t)\rho(\mathbf{q},t)$. Here, $\phi(\mathbf{q},t)=\phi(\mathbf{q},\omega)\exp(i\omega t)$ is an arbitrary external potential. Following standard procedures, we evaluate the commutator to linear order in ϕ and employ the result to generate the RPA integral equation for the density-density correlation function

$$\pi(\mathbf{q},\omega)=-i\int dt\,e^{i\omega t}\Theta(t)\langle[\rho(\mathbf{q},t),(-\mathbf{q},0)]\rangle , \quad (8a)$$

where $\Theta(t)$ is the Heaviside unit step function. This has a matrix counterpart $\hat{\pi}(\mathbf{q},\omega)$ through the relation

$$\pi(\mathbf{q},\omega)=\hat{I}(\bar{q})^T\hat{\pi}(\mathbf{q},\omega)\hat{I}(\bar{q}) , \quad (8b)$$

which obeys an algebraic-matrix RPA equation in Fourier space corresponding to

$$\hat{I}(\bar{q})^T\hat{\pi}(\mathbf{q},\omega)\hat{I}(\bar{q})=\hat{I}(\bar{q})^T\hat{\pi}^{(0)}(\mathbf{q},\omega)\hat{I}(\bar{q}) + \hat{I}(\bar{q})^T\hat{\pi}^{(0)}(\mathbf{q},\omega)\hat{V}(\mathbf{q})\hat{\pi}(\mathbf{q},\omega)\hat{I}(\bar{q}) , \quad (9)$$

where the noninteracting electron density-density correlation function is also cast in matrix form $\pi^{(0)}(\mathbf{q},\omega)=\hat{I}(\bar{q})^T\hat{\pi}^{(0)}(\mathbf{q},\omega)\hat{I}(\bar{q})$ with

$$\hat{\pi}^{(0)}(\mathbf{q},\omega)=\sum_{\mathbf{k}}\hat{T}(\bar{k}+\bar{q})\hat{T}(\bar{k})^TA^2_{\bar{k}+\bar{q}}A^2_{\bar{k}} \times[f_0(\varepsilon_{\mathbf{k}+\mathbf{q}})-f_0(\varepsilon_{\mathbf{k}})]/(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}}+\omega+i\delta) , \quad (10)$$

and $f_0(\varepsilon)$ is the Fermi distribution function. The matrix form of Eq. (9), $\hat{\pi}(\mathbf{q},\omega)=\hat{\pi}^{(0)}(\mathbf{q},\omega)+\hat{\pi}^{(0)}(\mathbf{q},\omega)\hat{V}(\mathbf{q})\times\hat{\pi}(\mathbf{q},\omega)$, is readily solved by a 5×5 matrix inversion as

$$\hat{\pi}(\mathbf{q},\omega)=[1-\hat{V}(\mathbf{q})\hat{\pi}^{(0)}(\mathbf{q},\omega)]^{-1}\hat{\pi}^{(0)}(\mathbf{q},\omega) . \quad (11)$$

The collective modes of the interacting electron system are given by the singularities of the function $\hat{\pi}(\mathbf{q},\omega)$, which are the roots of the secular equation

$$\det|1-\hat{V}(\mathbf{q})\hat{\pi}^{(0)}(\mathbf{q},\omega)|=0 . \quad (12)$$

The dielectric response properties of the multiwire superlattice under consideration are completely embodied in the real and imaginary parts of $\pi(\mathbf{q},\omega)$ given by Eq. (8) jointly with Eqs. (10) and (11). These explicit expressions are of essential importance in studies such as high-frequency transport and static and dynamic screening. Our present purpose is to utilize them in examining the collective excitation (plasmon) spectrum of the system. To proceed we need first the solution of the single-well Schrödinger equation, $u(\bar{r})$. For cylindrical quantum wells this is given in terms of the Bessel functions $J_0(r)$ and $K_0(r)$, subject to the boundary conditions that both $u(\bar{r})$ and $du(\bar{r})/dr$ be continuous at $r=r_0$. However, to simplify subsequent numerical computations we employ a variational ground-state wave function $u(\bar{r})=(C/\pi r_0^2)^{1/2}\times\exp(-Cr^2/2r_0^2)$, with $C=\ln(2mr_0^2V_0)$, in lieu of the exact wave function. A comparison of these two functions shows a small difference (less than 10%) for the values of r_0 and V_0 used in the present work. Use of this variational wave function renders the integrals of Eqs. (5a)–(5e) elementary, and they are readily evaluated as

$$I_1(\bar{q})=A(q) , \quad (5a')$$

$$I_2(\bar{q})=B(q)\cos(q_xd/2) , \quad (5b')$$

$$I_3(\bar{q})=-B(q)\sin(q_xd/2) , \quad (5c')$$

$$I_4(\bar{q})=B(q)\cos(q_yd/2) , \quad (5d')$$

and

$$I_5(\bar{q})=-B(q)\sin(q_yd/2) , \quad (5e')$$

where $A(q)=\exp(-q^2r_0^2/4C)$, and $B(q)=2A(q)\times\exp(-Cd^2/4r_0^2)$.

Before turning our attention to numerical solutions of Eq. (12), we should point out that a closed-form analytic solution is attainable in the long-wavelength (close-pack) limit. Under these limiting conditions $qd\ll 1$ and $q_zd\ll 1$, we arrive at the conclusion (after some lengthy algebra) that

$$\omega^2=\omega_p^2\cos^2\theta+\omega_g^2\sin^2\theta\,, \qquad (13)$$

where $\omega_p^2=4\pi n_0e^2/\kappa d^2$ is the square of the bulk close-pack plasma frequency and $\omega_g^2=4e^2\Delta^2V_{11}(2m/\varepsilon_F)^{1/2}$. Also, $\cos^2\theta=q_z^2/(q^2+q_z^2)$ and $\sin^2\theta=q^2/(q^2+q_z^2)$. The Fermi energy ε_F is assumed to lie above the lowest miniband, and its value is self-consistently determined for a given electron density n_0.

The most striking difference between the present result and that of an infinite-barrier model[11] is the appearance of the second term in Eq. (13). While the latter model features a plasma band bounded at the top by the "optical" branch whose long-wavelength limit is given by ω_p, going down continuously in frequency with increasing θ to the "acoustic" branch having $\omega\rightarrow 0$ as $q_z\rightarrow 0$ $(\theta\rightarrow\pi/2)$, the introduction of finite wave-function overlap elevates the lower branch of the plasma band to a nonvanishing value having $\omega\rightarrow\omega_g$ as $q_z\rightarrow 0$. Moreover, the linear dependence of ω_g on the miniband width 4Δ is consistent with the understanding that the lower limit of plasma frequency is at the top of the single-particle spectrum, which in the infinite-barrier model is given by $\varepsilon_{\mathbf{q}}=q_z^2/2m$, for $q=0$, whereas in the case of a tunneling superlattice it is given by $\varepsilon_{\mathbf{q}}=q_z^2/2m+4\Delta$. Similar considerations apply to planar superlattices, where the effect of finite potential barrier height on the plasmon dispersion relation is well documented.[13–15]

The model system we consider in the ensuing numerical calculation is a GaAs(wells)-$Al_xGa_{1-x}As$(barriers) multiwire superlattice. Material parameters pertaining to such a system are electron effective mass $m=0.07m_0$ (m_0 is the free-electron mass), and background dielectric constant $\kappa=12.9$. The wire radius is taken as $r_0=50$ Å, and the 2D lattice constant $d=150$ Å. The linear density of electrons per wire is assumed to be $n_0=10^7\ \mathrm{m}^{-1}$, and two values of the potential barrier height $V_0=100$ meV and $V_0=200$ meV are considered. With these parameters the intraminiband plasma frequency has the value $\omega_p=8.2$ meV. Our computations are carried out at zero temperature.

The plasmon dispersion relation for $V_0=100$ meV is graphed in Fig. 1. The upper bound of the plasma band is defined by $q_x=q_y=0$, representing the parallel propagation of plasma excitations along the direction of the wires $(\theta=0)$. The curve defining the lower bound of the plasma band corresponds to a spread of propagation angle θ for various q_z values. The largest angle possible $(\theta=\pi/2)$ is at $q_z=0$ and $q\neq 0$, for which the minimum excitation frequency is ω_g, which is 1.1 meV for the given value of $V_0=100$ meV. For a chosen q_z value, the maximum propagation angle (corresponding to minimum excitation frequency for that q_z value) is determined by requiring that both the real and imaginary parts of Eq. (12) vanish

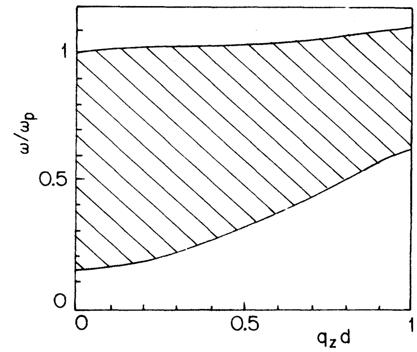

FIG. 1. Plasmon dispersion relation for a multiwire superlattice: $r_0=50$ Å, $d=150$ Å, $V_0=100$ meV, and $n_0=10^7\ \mathrm{m}^{-1}$.

jointly. In contrast to the infinite-barrier model,[11] where the minimum excitation frequencies always obtain for perpendicular propagation $(\theta=\pi/2)$ and vanish in the limit $q_z=0$, wave-function overlap makes such minima finite, even for $q_z=0$. As V_0 is reduced to zero, the plasma band collapses into the upper curve of Fig. 1, which is just the 3D plasma dispersion relation for a bulk electron gas of effective density n_0/d^2. Thus it is possible to examine the continuous transition from insulated 1D wires to a 3D bulk system by varying the barrier height V_0. This is further supported by Fig. 2, where a higher value of the potential barrier is assumed, i.e., $V_0=200$ meV, and all other parameters are unchanged. The upper bound of the plasma band is essentially unaffected by the increased barrier height, while the minimum plasma frequencies are much reduced. In particular, the long-wavelength limit of the lower bound is now at $\omega_g=0.1$ meV, showing the tendency toward infinite-barrier behavior.

Plasma excitations for small propagation angles $(qd\ll 1)$ are essentially undamped in the range of q_z shown in Figs. 1 and 2. These excitations represent the collective oscillations (parallel to the wires) of electron density in the periodic array of wires, which experience strong Coulomb restoring forces, whence they propagate with higher frequencies. Large-angle propagation, on the other hand, projects a large Coulomb force component perpendicular to the wires, which is canceled by the

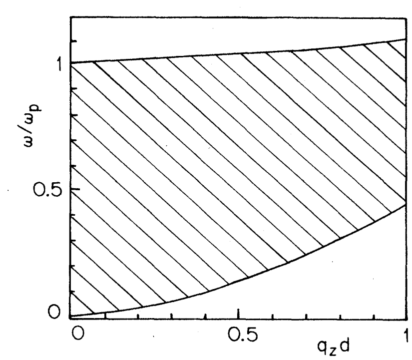

FIG. 2. Plasmon dispersion relation for a multiwire superlattice. $r_0=50$ Å, $d=150$ Å, $V_0=200$ meV, and $n_0=10^7\ \mathrm{m}^{-1}$.

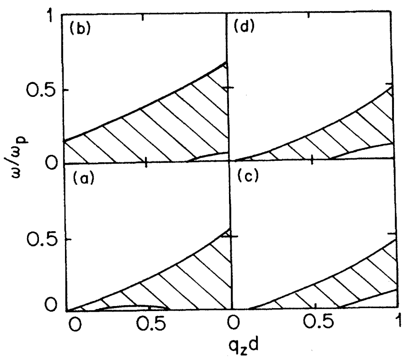

FIG. 3. Single-particle excitations of a multiwire superlattice. $r_0=50$ Å, $d=150$ Å, $n_0=10^7$ m^{-1}. (a) $V_0=100$ meV, $q_x=q_y=0$; (b) $V_0=100$ meV, $q_x=q_y=\pi$; (c) $V_0=200$ meV, $q_x=q_y=0$; (d) $V_0=200$ meV, $q_x=q_y=\pi$.

confining force of the potential walls, thus lessening the restoring force and leading to much reduced frequencies. Since the walls are not rigid, the force cancellation can never be complete, and the frequencies depend upon the "hardness" of the walls as measured in terms of potential barrier height, with lower frequencies for harder walls having higher barriers. These features are clearly exhibited in Figs. 1 and 2, and are also known to exist for multiwire systems with infinite-barrier height,[11] except for the fact that the restoring force in the latter case vanishes identically for perpendicular propagation of long-wavelength excitations, and consequently $\omega\rightarrow 0$. However, unlike the infinite-barrier case, in which the plasma band never merges with the single-particle spectrum, the low-frequency and large-propagation-angle plasma modes for finite V_0 are Landau damped into electron-hole pairs. Such damping is more pronounced for lower barrier height, as the 3D limit is approached. Single-particle spectra of representative values of q are shown in Fig. 3. The "holes" in the single-particle spectra are characteristic of 1D electron systems, associated with the restricted nature of the phase space.[11] Departures from purely 1D characteristics are seen as the "holes" are not extended in q_z from zero to twice the Fermi wave number, and that they move to the right as q is increased. These features are direct consequences of the finite barrier height. Another effect of finite V_0 is that the single-particle spectrum acquires a finite width for $q_z=0$ and nonzero q, a common signature of tunneling superlattices,[15] as is evident in Fig. 3(b).

In summary, we have examined the electronic response and plasma excitations of a multiwire tunneling superlattice having finite potential barrier height. Within a tight-binding scheme we solved the RPA integral equation in closed form, as a 5×5 matrix inversion, obtaining an explicit expression for the density-density correlation function of the interacting electron system. Plasma spectrum influenced by the finite wave-function overlap between neighboring quantum wires is discussed, along with the single-particle excitations, emphasizing the role of the barrier height as the key parameter in controlling the dimensionality of the electron system. Many of the features of the quasi-1D plasma spectrum are of strong current interest, and may be examined experimentally in comparison with this analysis. We must point out, however, that the present treatment considers intraminiband excitations only. Interband effects can be incorporated in the tight-binding scheme in principle, and will be taken up in a future study.

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