Collective excitations, pressure, and compressibility in multilayer systems

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We present a simple method to calculate the spectrum of elementary collective excitations in semiconductor superlattices. It is based on a variational many-body calculation with the hypernetted-chain approximation and the transformation of the structure functions and other quantities depending on the lattice layer indices into Bloch sums. In this method, we can calculate the excitation spectrum for electron and electron-hole superlattices and other more complicated structures. We also calculate the pressure and compressibility in a system of arbitrarily many electron (or hole) gas layers.

The collective excitations in semiconductor superlattices and multilayer systems have been studied theoretically by many authors over recent years.[1–3] A simple model that describes infinite lattices consists of an infinite number of planes stacked upon each other. In general, these planes need not be identical but can consist of electrons or holes that can have different masses on different layers. The layers need not, in general, be at the same distance from each other. For example, they can exist in groups consisting of b planes, these groups in turn being periodically stacked upon each other at a distance c. With our present method one can calculate excitations in both type I (electron layers) and type II (alternate layers of electrons and holes) and also in more complicated structures. We also discuss briefly the pressure and compressibility for finite layer systems. A two-layer system is of particular interest because such a system is used in a recent experiment[4] for measuring compressibility in a two-dimensional electron gas. Another interesting system is a double layer consisting of electrons and holes. Recently, transport measurements on such systems have been reported.[5] We should also point out that the occurrence of the even-denominator fractional quantum Hall effect was predicted[6] and subsequently observed[7] in double-layer electron systems. In all of these studies, the layers are considered to be close enough such that the Coulomb interaction is operative but no tunneling is allowed between the planes.

Our approach is based on the method developed earlier for multicomponent systems[8]. As a starting point we use the Jastrow variational wave function for a system of M species each consisting of n_α, $\alpha = 1, ..., M$ particles. For infinite type-I superlattices we use a model where all planes are stacked at equal distance c from each other. Each plane is assumed to be identical with every other plane. Thus the pair-distribution functions, structure functions, and all other quantities which were dependent on two-layer indices now depend only on the difference of the layer labels, i.e., $f_{\alpha\beta} = f_{\alpha-\beta,0} \equiv f_{\alpha-\beta}$ for any function depending on two layer indices. Using the hypernetted-chain (HNC) approximation for the pair-distribution function, $g_{\alpha\beta} = e^{u_{\alpha\beta}+N_{\alpha\beta}}$, we can now write the energy per particle as

$$\frac{E}{N} = -\frac{\hbar^2}{2m}\bar{\rho}\sum_\alpha \int \sqrt{g_\alpha}\,\nabla^2\sqrt{g_\alpha}\,dr + \frac{\hbar^2}{8m}\bar{\rho}\sum_\alpha \int g_\alpha \nabla^2 N_\alpha\,dr + \tfrac{1}{2}\bar{\rho}\sum_\alpha \int V_\alpha g_\alpha\,dr, \quad (1)$$

where $\bar{\rho}$ is the common areal density of the layers, m is the electron mass, and V_α is the interparticle potential. In order to find the pair-distribution function which minimizes this energy, expression (1) must be varied with respect to $\sqrt{g_\alpha}$. In that case, the nodal sum N_α has to be solved from the Ornstein-Zernike relation.[9] It turns out that by a suitable transformation the Ornstein-Zernike equation can be cast into a linear equation for N.

Let f_α be any quantity depending on layer label α. We define a transform F_κ by

$$F_\kappa = \sum_{\alpha=0}^{M-1} e^{2\pi i\kappa\alpha} f_\alpha. \quad (2)$$

The index κ can have M different values $0, \frac{1}{M}, \ldots, \frac{M-1}{M}$ when periodic boundary conditions $f_{\alpha+M} = f_\alpha$ are im-

posed. The transform thus obeys periodicity $F_{\kappa+1} = F_\kappa$. The crystal momenta k_z and κ are related by $k_z = (2\pi/c)\kappa$. The transforms of the quantities

$$\begin{aligned} S_\alpha(q) &= \bar{\rho} \int e^{i\mathbf{q}\cdot\mathbf{r}}[g_\alpha(r) - 1]d^2r + \delta_{\alpha,0}, \\ N_\alpha(q) &= \bar{\rho} \int e^{i\mathbf{q}\cdot\mathbf{r}} N_\alpha(r) d^2r, \end{aligned} \tag{3}$$

where $S_\alpha(q)$ is the structure factor, can be written as

$$\begin{aligned} S_\kappa(q) &= \sum_\alpha e^{2\pi i\kappa\alpha} S_\alpha \\ N_\kappa(q) &= \sum_\alpha e^{2\pi i\kappa\alpha} N_\alpha. \end{aligned} \tag{4}$$

Using these transformed quantities, the Ornstein-Zernike equation can be solved for N, $N_\kappa = (S_\kappa - 1)^2/S_\kappa$. We can now vary the energy expression with respect to $\sqrt{g_\alpha}$ and get the Euler-Lagrange equations

$$\frac{-\hbar^2}{m}\nabla^2\sqrt{g_\alpha} - \frac{\hbar^2}{4m} W_\alpha(r)\sqrt{g_\alpha} + V_\alpha(r)\sqrt{g_\alpha} = 0, \tag{5}$$

where the induced potential W_α results from the variation of the second term in Eq. (1) and is given by

$$W_\kappa(q) = q^2\left[2S_\kappa(q) - 3 + \frac{1}{S_\kappa(q)^2}\right]. \tag{6}$$

The potential $V_\alpha(r) = e^2/\sqrt{r^2 + \alpha^2c^2}$ is the Coulomb interaction and has a Fourier transform $V_\alpha(q) = (2\pi\bar{\rho}e^2/q)e^{-|\alpha|qc}$. The Bloch transform is easily evaluated to be

$$V_\kappa(q) = \frac{2\pi\bar{\rho}e^2}{q}\frac{\sinh qc}{\cosh qc - \cos 2\pi\kappa}. \tag{7}$$

When the correlations are very weak g_α differ only slightly from unity. In this case, called the uniform limit, we can solve Eq. (5) and get

$$S_\kappa^2(q) = \frac{\hbar^2}{4m}\frac{q^2}{\frac{\hbar}{4m}q^2 + \frac{2\pi\bar{\rho}e^2}{q}\frac{\sinh qc}{\cosh qc - \cos 2\pi\kappa}}. \tag{8}$$

The excitation energy is then evaluated from $\mathcal{E} = (\hbar^2q^2)/2mS_\kappa(q)$, which is a straightforward extension of the Feynman excitation formula.[9] Considering the limit $q \to 0$ while $k_z \neq 0$ we get

$$\mathcal{E} = \sqrt{\frac{\hbar^2\pi e^2\bar{\rho}c}{m}}\frac{q}{|\sin k_zc/2|}, \tag{9}$$

which is a dispersion relation for a sound mode. We are thus dealing with acoustic plasmons, which is consistent with previous calculations on type-I superlattices.[3] This linear dispersion has also been experimentally confirmed.[10]

Figure 1 presents the excitation energies for a type-I superlattice. Clearly, the fully iterated solutions of Eq. (5) give slightly smaller energies than the ones obtained within the uniform limit approximation. This is expected because of the variational nature of the Euler-Lagrange equations. The two curves coincide at larger values of q, where the structure functions $S_\kappa(q)$ go to unity.

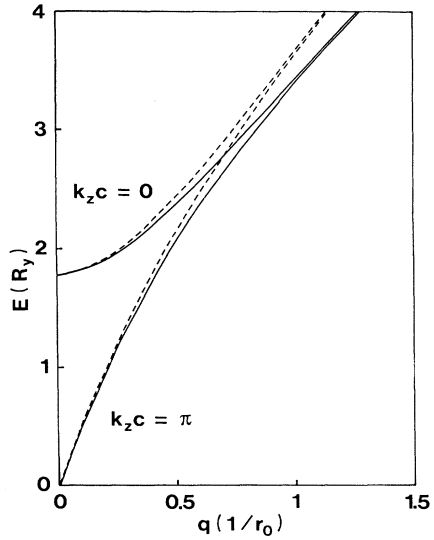

FIG. 1. Excitation curves for a type-I superlattice at values $k_z = 0$ and $k_z = \pi$. The dashed lines represent the uniform limit solution and the solid lines are the fully iterated solutions of the Euler-Lagrange equations. The energy is in units of 1 Ry $= e^2/2\epsilon a_0$, $r_s = 1$ and the layer separation is 0.5 in units $r_s a_0 = 1$, here $a_0 = \epsilon\hbar^2/m_0e^2$.

For a system which consists of different kinds of layers, the above treatment also applies with a few modifications. Consider a system of M groups each consisting of b different layers. The distance between the first layers of adjacent groups is c and the distance from the first layer of a group to the νth layer of the same group is denoted by d_ν. We use the index n for labeling the groups. The Coulomb potential, structure functions, etc. must now be presented in a matrix form. These matrices $A^{\nu_1\nu_2}_{n_1-n_2}$, where $\nu_i = 0, 1, \ldots, b-1$ and $n_i = 0, \ldots, M-1$ have the property $A_{n_1b+\nu_1,n_2b+\nu_2} = A_{(n_1-n_2)b+\nu_1,\nu_2} = A_{\nu_1,(n_2-n_1)b+\nu_2}$. Periodic boundary conditions $A^{\nu_1\nu_2}_n = A^{\nu_1\nu_2}_{n+M}$ are also applied. The Bloch transform is then defined by

$$A^{\nu_1\nu_2}(\kappa) = \sum_{n=0}^{M-1} e^{2\pi i\kappa n} A^{\nu_1\nu_2}_n. \tag{10}$$

The transformed Coulomb potential can now be written as

$$V^{\nu_1\nu_2}(\kappa) = \frac{e_{\nu_1}}{e}\frac{e_{\nu_2}}{e}\sqrt{x_{\nu_1}x_{\nu_2}}\frac{2\pi e^2\rho}{q}\frac{\sinh(qc - q|d_{\nu_1} - d_{\nu_2}|) + e^{-2\pi i\kappa\,\mathrm{sgn}(\nu_1-\nu_2)}\sinh q|d_{\nu_1} - d_{\nu_2}|}{\cosh qc - \cos 2\pi\kappa}, \tag{11}$$

where $e_{\nu_1}(e_{\nu_2})$ is the charge and $x_{\nu_1}(x_{\nu_2})$ is the concentration of the component ν_1 (ν_2). The Euler-Lagrange equations for the transformed quantities can now be solved analytically in the uniform limit. In the two-component case which corresponds to the type-II superlattice, if the components are ordinary electrons and holes the excitation energies are found to be the square roots of the eigenvalues of the matrix

$$\hbar^2 q^2 \begin{pmatrix} \frac{1}{m_1} V^{11}(\kappa) & \frac{1}{\sqrt{m_1 m_2}} V^{12}(\kappa) \\ \frac{1}{\sqrt{m_1 m_2}} V^{21}(\kappa) & \frac{1}{m_2} V^{22}(\kappa) \end{pmatrix} + \hbar^2 q^2 \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix}, \tag{12}$$

where $\sigma_\nu = \frac{\hbar^2 q^2}{4m_\nu^2} \frac{1}{S_{F_\nu}^2}$ and S_{F_ν} is the structure function for the two-dimensional free Fermi gas. The dispersion relation for the sound mode (i.e., acoustic plasmon) is found to be

$$\mathcal{E} = \frac{4}{r_s} Q r_0 \sin\theta \frac{|Z_1 Z_2| \sqrt{x_1 x_2}}{\sqrt{Z_1^2 x_1 \mu_1 + Z_2^2 x_2 \mu_2}} \times \sqrt{\frac{\pi^2}{32} \left(\frac{1}{Z_1^2 \mu_1} + \frac{1}{Z_2^2 \mu_2} \right) + \frac{c-d}{r_0} r_s} \mathrm{Ry}, \tag{13}$$

where $\mathbf{Q} = (\mathbf{q}, k_z)$, $r_0 = r_s a_0$, where a_0 is the Bohr radius, $\epsilon \hbar^2 / m_0 e^2$, where ϵ is the dielectric constant of the background medium, $d = |d_1 - d_2|$, $Z_\nu = e_\nu / e$, and $\mu_\nu = m_\nu / m_0$, where m_0 is the mass of the first component. The energy is calculated in units of 1 Ry $= e^2 / 2\epsilon a_0$. For optical plasmons we get in the limit $Q \to 0$

$$\omega_{pl}^2 = \frac{4\pi e^2}{c} \sin^2\theta \left(\frac{n_1}{m_1} + \frac{n_2}{m_2} \right) + O(Q^2), \tag{14}$$

which is the same as in Ref. 3.

When θ goes from 0 to $\pi/2$ the energies obtained from the equations above form two bands. These results hold when the excitations are considered as a function of the total momentum Q of the associated electric field. When plotting the dispersion as a function of the in-plane wave vector q, one gets two acoustic plasmon bands as in Ref. 2. Ignoring the second term in Eq. (12) leads exactly to the excitation energies of Ref. 2. On the other hand, keeping this term will give the correct single-particle dispersion in the large wave-vector limit.

For a finite number of layers we can express the pressure as a function of the structure factor matrices:

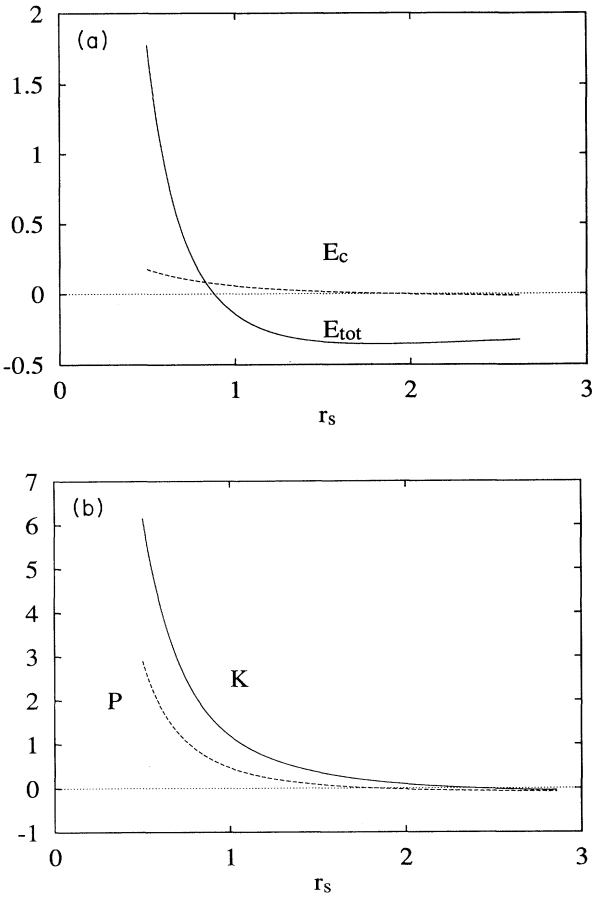

FIG. 2. (a) The total energy and the correlation energy (in Ry) as a function of r_s for a two-electron-layer system with the layer separation $0.5 r_s a_0$. (b) The pressure P and compressibility K for the same system. The pressure is in units of Ry/ρ and the compressibility is in units of Ry/ρ^2, where ρ is the total density of the system.

$$P = E_{\mathrm{tot}} + \frac{1}{r_s^2} - \frac{\hbar^2}{8} \frac{1}{(2\pi)^2} \int k^2 \mathrm{tr}[3M^{-1}S^{-1} - S^{-1}M^{-1}S^{-1} + S_F^{-1}M^{-1}S_F^{-1}S - 4M^{-1}S_F^{-1} + S_F^{-1}M^{-1}S_F^{-1}] d\mathbf{k} - \frac{\hbar^2}{4} \frac{1}{(2\pi)^2} \bar{\rho} \int k^2 \mathrm{tr} \left\{ [SM^{-1}S_F^{-3} - S_F^{-1}M^{-1}S_F^{-1}] \frac{\partial S_F}{\partial \rho} \right\} d\mathbf{k}, \tag{15}$$

where the total energy is

$$E_{\mathrm{tot}} = \frac{1}{r_s^2} - \frac{\hbar^2 \rho}{2} \sum_\alpha \frac{x_\alpha}{m_\alpha} R_{\alpha\alpha}(0) - \frac{\hbar^2}{4} \frac{1}{(2\pi)^2} \int \mathrm{tr}[(S-1)M^{-1}R + (S-1)RM^{-1}] d\mathbf{k} + \frac{\hbar^2}{8} \frac{1}{(2\pi)^2} \int k^2 \mathrm{tr}[(S-1)M^{-1}(S-1) + (S-1)M^{-1}S_F^{-1} - (S-1)M^{-1}S^{-1} - S_F^{-1}SS_F^{-1}M^{-1}(S_F - 1) + S_F^{-1}M^{-1}(S_F - 1)] d\mathbf{k} + \frac{1}{2} \frac{1}{(2\pi)^2} \int \mathrm{tr}[(S-1)V] d\mathbf{k}. \tag{16}$$

The matrix R is composed of the pair-distribution functions and their derivatives.[8] In Fig. 2(a) we have plotted the total energy and the correlation energy $E_c = E_{\rm tot} - 1/r_s^2 + 8\sqrt{2}/3\pi r_s$ as a function of r_s for a system of two electron layers with the interlayer separation $c = 0.5 r_s a_0$. The first and second derivatives of the total energy correspond to pressure and compressibility, respectively. These are plotted in Fig. 2(b). As in the experiment of Eisenstein, Pfeiffer, and West[4] for a two-dimensional layer, the compressibility becomes negative when r_s reaches a certain value. According to the Monte Carlo calculations of Tanatar and Ceperley,[11] the compressibility approaches zero at $r_s = 2.03$ in the single-layer case. In the two-layer system of Fig. 2 it becomes negative at $r_s = 2.4$. The stability of the system is therefore enhanced by introducing one extra layer.

In conclusion, we have developed a method for calculating the collective excitations in semiconductor superlattices. This method has the advantage of being computationally simple and is capable of describing most of the physically relevant quantities. The Fermi correction is taken into account already in the uniform limit approximation, which corresponds closely to the random-phase approximation (RPA) at the intermediate densities. At lower densities the correlations become more important, and the uniform limit (or RPA) is not sufficient. It is, however, straightforward to go beyond the RPA and take the correlations into account by solving numerically the Euler-Lagrange equations (5). At large wave-vector limit the Fermi correction in Eq. (12) has the effect of increasing the slope of the dispersion curve by the amount which is roughly proportional to the total volume density of the charge carriers. Although at the values of the parameters used in Fig. 1 this increment is negligible ($\approx 1\%$), it will be appreciable at higher areal densities or at smaller interlayer separations. Details including the compressibility as a function of the interlayer separation for the electron-electron and electron-hole double-layer systems will be presented elsewhere.[12]

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