ELECTRONIC STRUCTURE OF SINGLE ULTRASMALL ELECTRON DEVICES AND DEVICE ARRAYS

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(Received 17 August 1986)

Several questions must be addressed to develop the theory of the electronic structure of single ultrasmall (submicrometer) electron devices and the band structures of device arrays. The effects of intradevice Coulomb interactions and correlations on the electronic structure of individual devices have been studied by use of the multi-electron effective-mass Schrodinger equation for interacting few-electron systems confined in a single ultrasmall device. The band structures for noninteracting electrons in device arrays have been studied by performing augmented plane wave calculations for two-dimensional arrays of two-dimensional circular quantum wells and quantum barriers. Results are presented and the impact on the understanding of the electronic structure of devices and arrays is discussed.

The electronic structure of a crystal can be fully understood only if the electronic structure of the constituent atoms is known and if the banding of the atomic bound states, which occurs when the atoms are in a lattice, is accurately determined. Similarly, the electronic structure of an array of ultrasmall (submicrometer dimensions) devices[1-3] can be fully understood only if the electronic structure of the carriers localized to a single device and the band structure can be determined.

For typical surface- or inversion-layer charge densities ($\sim 10^{10}$-10^{12} cm^{-2}), a single ultrasmall device structure traps only a few carriers. Thus the electronic structure of a single ultrasmall device is that of an interacting, few-electron (atomic-like) system, rather than that of a nearly free electron gas, and therefore consideration of intradevice Coulomb interactions and correlation is essential. In an array of devices, the band structure is determined by the size, shape, and separation of the device elements and by the geometry of the lattice. In the fabrication process, all of these parameters, including the lattice geometry, could, in principle, be controlled. Thus there should be tremendous freedom to control the array band structure; in principle, more freedom should be allowed for the array than for other artificially structured materials because the lattice geometry can be controlled.

Here we report on initial efforts to understand the electronic structure of devices and arrays. To keep the calculations tractable, we have modeled the single ultrasmall devices as two-dimensional quantum wells and the arrays as two-dimensional lattices formed from two-dimensional quantum wells (dot arrays) or quantum barriers (bump lattices); thus the results we present will illustrate the possibilities for tailoring the electronic structure of a two-dimensional electron gas. The electronic structure of single devices and the band structure of arrays will be treated separately. The electronic structure of single ultrasmall devices will be considered first.

Single ultrasmall devices can trap only a few carriers. For example, if the inversion-layer charge density were 10^{11} cm^{-2}, then a two-dimensional uniform gas in a square structure 0.1 μm wide would contain 10 carriers; in a structure 0.05 μm wide, 2.5 carriers; and in a structure 0.01 μm wide, less than one carrier. These structures must be treated as finite-particle systems. Few-particle ($N \leq 6$) systems have been studied by solving the multiparticle effective-mass Schrodinger equation for a two-dimensional interacting-particle-in-a-box model. In this approach the device is modeled as a strictly-two-dimensional quantum well. No effects of inversion layer width are included. The well has infinite barriers and is rectangular. Thus a basis set of wave functions which are separable in the two directions

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that define the well can be employed. The one-dimensional (1D)-basis functions are the exact single-particle 1D-states (sines and cosines) for the noninteracting system. The well is described with material parameters for GaAs (effective mass $m = 0.067\ m_0$ and dielectric constant $\varepsilon = 13.1$).

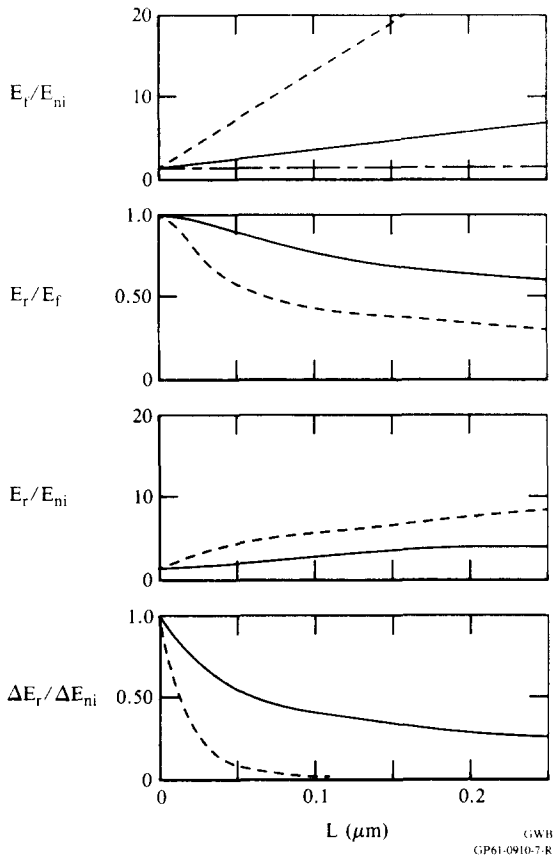
The particle interaction is the Coulomb interaction screened by the background dielectric constant. The correlations are included by use of a configuration interaction approach. The multiparticle wave function is expanded in terms of Slater determinants constructed from the single-particle noninteracting eigenstates. The kinetic energy and interaction matrix elements are found by use of the Slater determinant basis and the Hamiltonian is diagonalized to find the eigenstates. Because an infinite barrier model is used, all kinetic-energy matrix elements scale as $1/L^2$, and all interaction matrix elements scale as $1/L$ when the dimension L of the well is changed without changing the well's shape. In all cases the matrix elements were calculated for one well size and scaled to obtain results for other well sizes. The evaluation of Coulomb matrix elements is straightforward.[4]

The effects of the Coulomb interaction and correlation on the ground-state energies and charge densities are shown in Figs. 1 and 2 for two-particle systems with even x and y parity (the two directions that define the rectangle) and zero spin. The effect of the Coulomb interaction is evident when the energies of the noninteracting ground state, E_{ni}, and the state frozen into the noninteracting configuration but with Coulomb interactions included, E_f, are compared with the fully relaxed state, E_r. The Coulomb energy scales as $1/L$ and the kinetic energy scales as $1/L^2$, therefore E_f/E_{ni} scales linearly with L. When the carriers relax, correlating their positions to minimize their interaction, the ground state energies are reduced substantially, indicating the importance of correlation. Even after the energy has been reduced by correlation effects, E_r is still very different from E_{ni}.

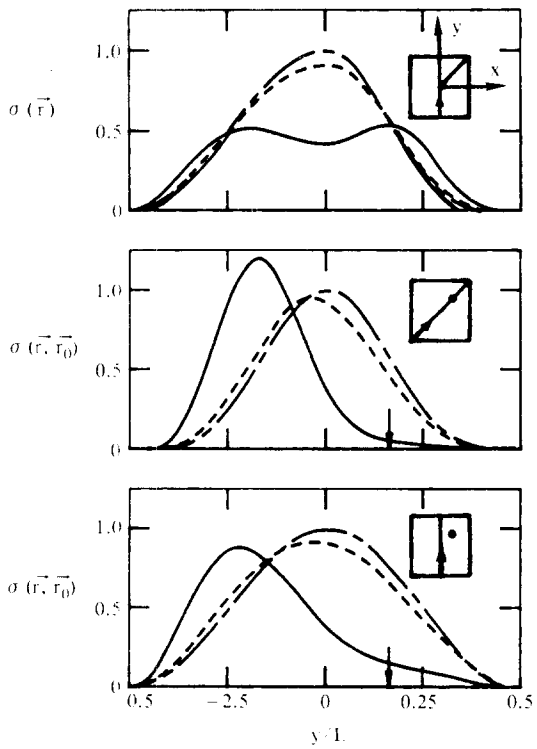
When the interaction effects are dominant, the particles move as far apart as allowed by the confining potential. In square structures they move apart along diagonals with the carrier density $\sigma(r)$ peaking nearly half way from the center when $L = 0.1$ μm. For structures in which the confining potential dominates, the density approaches the free-particle density.

The extent of correlation is shown by the conditional carrier density, $\sigma(r,r_0)$ (the density at r of one particle when the other is fixed at r_0). When interactions dominate, the particle motions are not independent, and the particles stay as far away from each other as possible.

Since Coulomb effects can be significant, single ultrasmall devices should exhibit the same rich variety of electronic structure as



1. Effect of the Coulomb interaction and correlation on the ground state and excitation energies of two particles in an ultrasmall structure. E_f/E_{ni} is the ratio of the energy of the interacting system when frozen into the lowest noninteracting state to the energy of the noninteracting ground state. E_r is the energy of the fully relaxed state. ΔE_r and ΔE_{ni} are the excitation energies of the relaxed and noninteracting systems. The solid curves are for square structures with dimension L. The long-short dashed curve is for a quasi-one-dimensional channel ($L_y = 10L_x = L$). The short dashed curves are for the narrow channel after the large kinetic energy contribution from confinement in the x-direction is eliminated from the energies.



2. Effect of the Coulomb interaction and correlation on the single-particle density, $\sigma(r)$, and the two-particle conditional density, $\sigma(r,r_0)$ for two particles in a square structure. The broken curves are for noninteracting particles, the dashed curves for a structure of width L = 0.01 μm and the solid curves for L = 0.1 μm. The paths in the inserts define the contours on which the densities are determined. The dot in the insert and the arrow on the x-axis indicate the position r_0. The densities are scaled for each L so that the densities of the noninteracting state are independent of L.

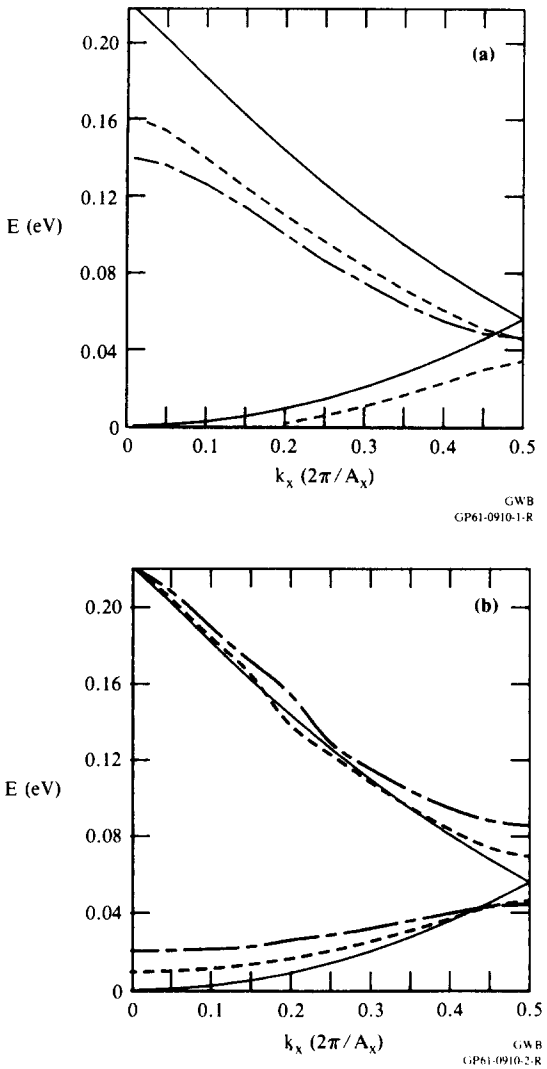
displayed by atoms. There are devices which, analogous to light atoms, display single particle effects, while other devices, analogous to heavy atoms, are highly correlated. For example, in a device with N = 3 and $L_x = L_y$ = 0.01 μm, Coulomb effects are weak; the eigenstates are formed by filling the single-particle states. The symmetries (x and y parity and spin) of the interacting and noninteracting ground states are the same. The ground state has a filled core, the lowest excited states have one particle excited from the core. The most probable configuration in the interacting state is the configuration of the analogous noninteracting state. When the same device has a width $L_x = L_y$ = 0.2 μm, the Coulomb effects are strong, the energy is minimized by separating particles, the core level of the ground state is singly occupied, and the interacting and noninteracting ground states have different symmetry and spin. The interacting ground state has odd x and y parity and spin 3/2, while the noninteracting ground state is degenerate with spin 1/2, even parity in one direction and odd in the other. The most probable configuration in the interacting state is still the configuration of the analogous noninteracting state, but many other configurations contribute as well. Results for devices with N = 4,5 and 6 are similar, with Coulomb effects sensitive to device dimensions.[5]

Although intradevice Coulomb effects can be significant, we have chosen to first perform simple band structure calculations in which the carriers are noninteracting. Previously, Iafrate, Ferry and Reich[1] used a tight-binding approach to study the band structure of an array of devices and Carlsson and Ashcroft[3] used a tight-binding approach to study disorder effects in such an array. We use the augmented-plane-wave (APW) approach[6] within the effective-mass approximation to determine the array band structure. The APW approach should be much more reliable for nearly free states; moreover, use of the APW allows us to treat the quantum bump array.

This study considers two-dimensional square lattices of quantum devices. In the quantum dot case, the devices are circular, two-dimensional wells of GaAs surrounded by $Ga_{1-x}Al_xAs$. In the quantum-bump case, the devices are circular, two-dimensional barrier regions of $Ga_{1-x}Al_xAs$ surrounded by GaAs. The material parameters used are $m_{GaAs} = 0.067\ m_0$, $m_{GaAlAs} = (0.067 + 0.083x)\ m_0$ and conduction band discontinuity, V = 0.75 x eV (as derived using the 60-40 rule).

The band structures of dot and bump arrays are shown in Figs. 3a and 3b. In each case the lattice constants are $A_x = A_y$ = 10 nm, the alloy composition is x = 0.2; and three well (barrier) sizes are considered: R = 0 (free electrons), 1 nm and 2 nm. The isolated well has s-bound states at -0.000005 eV when R = 1 nm and at -0.012 eV when R = 2 nm. No bound states occur for higher angular momentum. Only results for nearly free electrons with wave vectors in the first Brillouin zone in the (10)-direction are shown.

As R increases, the free-electron bands become substantially distorted. In the dot array, the bands flatten out and the lowest free-electron band is pulled into the band of states localized to the wells. For R = 1 nm,



3. The band structure of the nearly free states in the first Brillouin zone along the (10) direction of quantum dot (a) and bump (b) arrays. The lattice constants are $A_x = A_y = 10$ nm; while R = 0 nm for free electrons (solid curves), R = 1 nm (dashed curves), and R = 2 nm (dash-dot curves). The alloy composition is x = 0.2. The zero of energy is the bottom of the conduction band of $Ga_{1-x}Al_xAs$ (GaAs) for the dot (bump) array.

states with k along the (1,0) and (1,1) directions have similar dispersion. For R = 2 nm, all states in the lowest band, except those in pockets around the (1,1) directions and near the Brillouin zone edge, are localized to the wells. For larger R, even more severe distortions of the bands occur. Iafrate[1] studied the banding of the isolated well bound states. Those states remained well localized when the wells were placed in an array. Iafrate's results complement our results for the nearly free states.

In the bump array, the lowest band of states has energies below the bump barrier; therefore the states are resonantly trapped between the bumps. Significant flattening of the lowest band also occurs in the bump arrays even though the states are not truly localized. However, this flattening does not occur in all directions. States with wave vectors along directions where the bumps are widely spaced [for example, (1,3)] have much greater dispersion than states for k along (1,0) and (1,1). Other arrays with different dimensions show similar trends but on different length and energy scales.[7]

In summary, Coulomb interactions and correlations are important in our theory of single ultrasmall devices. Such devices exhibit a wide range of electronic structures--nearly free-electron or highly correlated, filled or unfilled (magnetic) cores--just as atoms do. In fact, the importance of Coulomb interactions, especially for very small structures, is underestimated in our theory, because the infinite barrier model overestimates the competing kinetic energy effects. Carriers in real devices with dimensions $L \lesssim 0.01$ μm are expected to be much less like noninteracting electrons than electrons in infinite barrier devices of the same size are. Difficulty is expected in pairing electrons in very small real structures because of the presence of Coulomb repulsion and the finiteness of confining barriers.

The results for the band structures of quantum dot and bump arrays indicate that the free-electron band structure can be severely modified, even for noninteracting electrons, by the presence of the array potential. Calculations of the band structure for interacting systems will be much more difficult. Intradevice interaction effects will have to be included in the calculations when devices are so small (L ~ 1-10 nm) that real barriers must be used to realistically model the intradevice interaction effects. Interdevice interactions will also have to be included in the calculations. Just as the electrons in single devices (L ~0.1-1 μm) can be highly correlated, device arrays that have an active area with dimensions L ~ 0.1-1 μm can be highly correlated. The possibility of charge instabilities in quantum well arrays has been previously explored[1,8] by use of a dielectric response approach. Our complementary approach suggests the same possibility and re-emphasizes that the electronic structure of ultrasmall quantum arrays will not be simple to model.

Acknowledgements--Research conducted in part under the McDonnell Douglas Independent Research and Development program.

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