

Electronic properties of quantum points

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The Coulomb interaction is taken into account in a calculation of the spectra of two- and three-electron quasi-zero-dimensional systems: quantum points. The density distribution is derived analytically in the Thomas-Fermi model for a multielectron system. In agreement with experiment, the resonant IR absorption frequency depends very weakly on the number of electrons in the quantum point.

Recent progress in submicron technology has made it possible to fabricate and study quasi-zero-dimensional semiconductor systems or “quantum points” (or “quantum-well boxes”), in which the motion of two-dimensional electrons is restricted along both directions in the plane of an interface. The typical geometric size of a quantum point is a few thousand angstroms, but the size of the region actually occupied by electrons may be much smaller, because of the lateral potential. Under these conditions, quantization in the plane of the interface becomes important for semiconductors with a small effective mass (GaAs and InSb, so we are actually dealing with an artificial atom in which the number of electrons can be controllably varied from a few to a few tens. The conditions under which quantum points are produced are of such a nature that the lateral potential of the “empty atom” (i.e., the initial shape of the potential well, not occupied by mobile carriers) can be regarded as parabolic,

$V = m\Omega^2\rho^2/2$, where m is the effective mass, Ω is the characteristic frequency of the parabola, and $\rho = \sqrt{x^2 + y^2}$ is the distance from the center of the quantum point in the plane. Motion along the z axis corresponds, as usual, to the ultraquantum limit; i.e., the atom is planar.

The absorption of IR light by a quantum-point system has been measured in experiments by Sikorski and Merkt.¹ The number of electrons in a point, N varied from 3 ± 1 to about 20. The position of the absorption peak was independent of N within the experimental error (in contrast with the situation for ordinary atoms, in which a change in the atomic number of the element results in a substantial change in the resonant frequency).

In this letter we are reporting Hartree-Fock calculations of the spectra of helium-like and lithium-like quantum points ($N = 2, 3$). We have also derived an (analytic) solution of the Thomas-Fermi model for the case $N \gg 1$. In particular, it can be seen from the latter solution that as the number of electrons in a quantum point increases, the radius of the quantum point varies in such a way that the frequency of collective vibrations (standing plasma waves) depends extremely weakly on N . If the IR absorption peak observed in Ref. 1 is interpreted as absorption by a natural mode of a plasma disk, we see why the resonant frequency is independent of the number of electrons in the quantum point. The parabolic approximation of the potential of an "empty" point also receives indirect support.

1. The role of exchange-correlation effects in the spectrum of a quantum point is determined by the ratio of the Coulomb interaction energy of two particles over a characteristic distance $(\hbar/m\Omega)^{1/2}$ to the distance between oscillator levels, $\hbar\Omega$. This parameter can be written in the form $(Ry^*/\hbar\Omega)^{1/2}$, where the effective Rydberg energy includes the renormalized charge $\tilde{e}^2 = 2e^2/\epsilon_1 + \epsilon_2$, where $\epsilon_{1,2}$ are the dielectric constants of the media on the two sides of the interface at which the two-dimensional electrons are located. In more-complex situations (a three-layer system or a metal-insulator-semiconductor structure) the interaction would not be purely Coulombic, so \tilde{e}^2 would depend on the momentum transfer q in the Fourier representation. With increasing number of electrons, there is also an increase in the index of the last filled level, $n_{\max} \sim \sqrt{N}$. Correspondingly, the contribution of exchange and correlation to the energy of the outer electrons falls off as $(Ry^*/\hbar\Omega)^{1/2} N^{-1/4}$. It turns out that for electrons in a parabolic two-dimensional potential well (for an arbitrary interaction law!) the frequency of an allowed optical transition between the ground and first excited states of this system is equal to its "one-electron value" Ω . By calculating the Coulomb integral W_C and the exchange integral W_A with the wave functions of the first excited state of a two-dimensional isotropic oscillator in the standard way, we thus find that for an arbitrary $\tilde{e}^2(q)$ the shift of the singlet ground state, ΔE_0 , is equal to the sum $W_A + W_C$, while the energy of the lowest-lying triplet level is $\hbar\Omega + W_C - W_A - \Delta E_0 = \hbar\Omega - \partial\Delta E_0/\partial\Omega$. The energies are reckoned from the ground state. The frequency of a resonant singlet-singlet transition thus does not change when the interelectron interaction is taken into account, at least in first-order perturbation theory (by way of comparison, this change is $\approx 50\%$ in a helium atom).

In a three-electron quantum point, the interaction of particles leads, even in first order, to a shift and a splitting of the resonant line, but small numerical coefficients

make the effect fairly weak. The state closest to the ground state, with a spin of 3/2 (a forbidden transition), has an energy of $\hbar\Omega - (11/16)\Delta$, where $\Delta \equiv \tilde{\epsilon}^2 (\pi m \Omega / 2 \hbar)^{1/2}$. This result refers to a heterojunction, where $\tilde{e}^2(q) = \text{const}$. The closest doublet excited states, which are optically coupled with the ground state, form a quartet with energies $\hbar\Omega - \gamma_i \Delta$, $i = 1-4$; $\gamma_1 = 13/32$, $\gamma_2 = 3/16$, $\gamma_3 = 7/64$, $\gamma_4 = 3/32$. In contrast with ordinary atoms with a spectrum which becomes thicker, the resonant line in this case is associated with the transition of an electron from the last, completely filled shell to the nearest unfilled shell (as in the model of a quantum point with a square-well potential²).

2. At $N \gg 1$ we can use the Thomas-Fermi model, which leads to the following equation in the case of a heterojunction:

$$\Delta(e, \varphi) = - \frac{4}{a_0^*} [E_F - e\varphi(\rho, z) - V(\rho)] \delta(z) \sigma(R - \rho) \quad (1)$$

$$\sigma(x > 0) = 1, \quad \sigma(x < 0) = 0.$$

Here $e\varphi + V$ is the total potential energy of the electron, $V(\rho)$ is its parabolic part, E_F is the Fermi level, $a_0^* = \hbar^2 / m \tilde{e}^2$ is the effective Bohr radius, and R is the radius of the quantum point. The surface charge density $n_s(\rho) = (m / \pi \hbar^2) [E_F - e\varphi(\rho, 0) - V(\rho)]$ vanishes at $\rho = R$; i.e., in this case we should solve Eq. (1) as an equation with a moving boundary. Specifically, we should find $n(\rho)$ which is regular at the origin and which vanishes at an arbitrary point R , and we should then determine R from the condition $\int n_s(\rho) d\rho = N$.

This solution can be found through a Fourier-Bessel expansion:

$$e\varphi(\rho, z) = \sum_{j=1}^{\infty} A_j(z) J_0(k_j \rho); \quad J_0(k_j R) = 0, \quad (2)$$

where J_0 is the Bessel function of index zero, and $k_j R \equiv \lambda_j$ is its j -th root (numbered in order of increasing value). For the coefficients $A_j(z)$ we find the equation

$$A_j''(z) - k_j^2 A_j = B_j + A_j(0) \delta(z), \quad (3)$$

where B_j are the coefficients of the expansion of the constant $\Delta V(\rho)$ in the set $J_0(k_j \rho)$. Solving Eq. (3) and then calculating $\int n_s(\rho) d\rho$, we find the implicit dependence of the radius of the quantum point on the number of electrons in it:

$$N = 8(m\Omega / \hbar)^2 R^3 a_0^* \sum_{j=1}^{\infty} R / \lambda_j^3 (2R + \lambda_j a_0^*). \quad (4)$$

Let us consider two limiting cases.

a) $R \ll a_0^*$. This is the case of noninteracting electrons. We have $\sum_j \lambda_j^{-4} = 1/32$ and $N = (m\Omega / 2\hbar^2)^2 R^4$ here. Such a limit exists if $1 \ll N \ll (\hbar\Omega / R^*)^2 R^4$. The depolarization shift Δ_p of the resonant frequency $\omega_{res} = \sqrt{\Omega^2 + \Delta_p^2}$ is estimated as the fre-

quency of a natural mode of a two-dimensional plasma disk: $\Delta_p^2 \sim \bar{n}_s \tilde{e}^2 / mR$, $\bar{n}_s = N / \pi R^2$. In other words, we find $\Delta_p \sim N^{1/8}$.

b) $R \gg a_0^*$; $N \approx 0.3 (m\Omega / \hbar)^2 R^3 a_0^*$. In this case we must impose the condition $N \gg (\hbar\Omega / Ry^*)^2$. We then have $R \approx N^{1/3}$ and $\Delta_p \sim N^0 = \text{const}$. In other words, the resonant frequency becomes independent of the number of particles in the quantum point. In the experiments of Ref. 1, the value $\hbar\Omega / Ry^* \approx 2$ prevailed. In other words, case b) prevails at $N \gg 4$.

A corresponding calculation for one-dimensional channels in the parabolic model leads to the following relationship between the linear particle density and the “electron width” of the channel, d which is determined by the equation $n_s (\pm d/2) = 0$:

$$N_L = \frac{8}{\pi^4} \left(\frac{m\Omega}{\hbar} \right)^2 d^3 a_0^* \sum_{j=0}^{\infty} (2j+1)^{-3} [2d + (2j+1)\pi a_0^*]^{-1} .$$

In the limit $d \gg a_0^*$ we have $N_L = (7/2\pi^4)\zeta(3)(m\Omega/\hbar)^2 d^2 a_0^*$, and the depolarization shift $\Delta_p \sim (N_L \tilde{e}^2 / md^2)^{1/2}$ is again independent of N_L .

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¹C. Sikorski and U. Merkt, Phys. Rev. Lett. in press, 1989.

²G. W. Bryant, Phys. Rev. Lett. **59**, 1140 (1987).