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Peculiarities of Electron-Electron Interaction in Quantum-Dimensional Objects

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In the Hartree-Fock approximation peculiarities of the effect of electron-electron interactions in a quantum-dimensional object are analyzed. It is established that a self-energy Σ_n has the sawtooth dependence on the Fermi level position or on the size of an object as a result of the size quantization effect. The smaller the size of nano-objects, the more pronounced oscillations of Σ_n. And secondly, the smaller the size of nano-objects, the less the electron-electron interaction.

Keywords: Nanoobject, Electron-electron interaction, Hartree-Fock approximation, Self-energy.

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1. INTRODUCTION

An electronic structure that is a solution of the stationary Schrödinger equation is the fundamental characteristic of problems of electronics. Sometimes it is enough to know such structure in the framework of the mean field approximation, ignoring an electron-electron interaction. But often the electron-electron interaction must be taken into account because it can essentially determine the behavior of physical properties of the materials. Recently, the effect of the electron-electron interaction became a subject of intense researches in so-called quantum-dimensional objects (see. e.g., [1]), in which the size at least in one of the crystallographic directions is of the same order as the wavelength of an electron. Such a spatial limitation causes a dimensional quantization of the electron spectrum. The easiest realization of a quantum-dimensional object is the spatial redistribution of charge on contact between two different media. If one of them is a solid and another is a liquid, charging of the metal surface is compensated by the charge of the opposite sign, which is concentrated in the nanosized region of the liquid medium. This redistribution of the charge is called a double electron layer.

A similar formation - the so-called inversion layer - occurs at the contact of two condensed matter. The inversion layer is a charged nanosized near-surface domain. As an example, in a MOS-structure (metal-oxide-semiconductor) (e.g. [2]), the carriers are localized in a potential well formed by the surface of the semiconductor barrier and the electrostatic potential of the bulk charge.

Such layers, as well as their created potentials, play an important role in the various physical phenomena. In particular, materials with them allow us to create entirely new, different from traditional, high-capacity energy storage system – supercapacitors [3]. There is a need to establish the role of electron-electron interaction in the nanoscale structures. This problem is particularly intensively studied in the transport phenomena, e.g. in transport through a nano-wire [4], through a nano-MOSFET [5], through a quasi-one-dimensional quantum dot [6] through a shuttling nanoisland [7] and others.

The theoretical description of the electron-electron interaction in nanoobjects uses different methods and approaches: different versions Greens functions techniques [5, 8], different versions of Hartree-Fock-method [9, 10] with various models of nano-objects: particles in the box [11], elliptical and bowl-like potentials [12] and others.

The above-mentioned double electron layers or inversion layers are spatially confined structures with dimensions commensurable with a de Broglie wavelength of the carriers, and as a result, an electron spectrum has sharply pronounced discrete character in contrast to the quasi-continuous spectrum in allowed zones of an ideal crystal. Taking into account the practical use such objects, the search for a deeper understanding of their physical properties are relevant.

Here we propose a model of such objects to study of the electron-electron interaction in them taking into account peculiarities of their one-electron spectrum. How, how much, and under what conditions such peculiarities are important is the goal of this paper.

2. MODEL

A model of infinitely deep potential is often used to describe different phenomena in real-space-confined structures. Thus, such a model was used to describe the ground and first excited levels in heterostructure InAs / AlSb [13]. Such a step was justified by the fact that in the 15 nm InAs layer the ground and first excited levels, measured from the bottom of its conduction band are ~ 60 and 200 meV respectively, while the distance between the conduction bands of the heterointerface is ~ 1.35 eV, that is considerably greater than in the discrete levels. This model is applicable to describe double layers [14] or inversion layers in semiconductors [15]. We use infinitely deep potential in this paper.

Figure 1 shown the real potential and the potential simulated by infinitely deep potential well for inversion layer. Analytical solutions of the problem of "particle in the infinitely deep well" are known [16], namely, the wave functions are

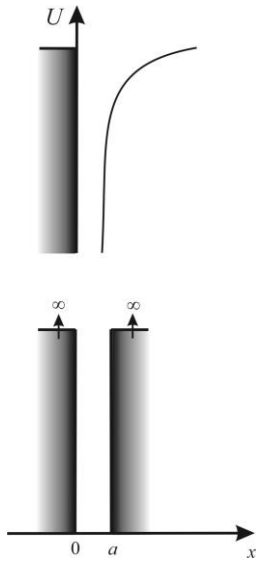

Fig. 1 – Diagrams of one-dimensional inversion potential: real (above) and simulated (below)

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x \tag{1}$$

and the eigenvalues are

$$E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2 , \tag{2}$$

where n is a number of the discrete levels $n = 1, 2, 3, \ldots$.

Solutions of the problem "particle in the infinitely deep well" can be also used in the case of the finite U_0 provided that $U_0 >> E_n$. This condition to a greater extent is performed on the ground and the lowest excited quantum states. On the other hand, at low surface (interfacial) concentration of carriers, electrons fill these states. From the viewpoint of applied problems, in particular, of the tunneling current calculation and optical properties of nanostructured systems, the distance between the ground and first excited states in the quantum well is important.

3. CALCULATIONS, RESULTS, AND DISCUSSIONS

Let's begin with the second-quantized form of the electron Hamiltonian with two-body interaction. The treatments will be similar to the widely used scheme in an ideal crystal. But in our task we choose, as basis wave functions, solutions of the problem of "particle in the infinitely deep well" (1). Then the Hamiltonian is

$$\hat{H} = \sum_n E_n a_n^+ a_n + \sum_{n_1 n_2 n_3 n_4} \Gamma_{n_1 n_2 n_3 n_4} a_{n_1}^+ a_{n_2}^+ a_{n_3} a_{n_4} ,$$

where E_n are the electron eigenvalues (2) in the well, a_n , a_n^+ are annihilation and creation operators of particles in the quantum state n, respectively, and $\Gamma_{n_1 n_2 n_3 n_4}$ is two-particle matrix element of interaction built on the potential

$$V(|x_1 - x_2|) = \frac{1}{4\pi\varepsilon_0} \frac{e^2}{|x_1 - x_2|} .$$

Using the method of the Green's function $\langle\langle a_n | a_{n'}^+ \rangle\rangle$, we obtain the expression for this function [17]

$$\langle\langle a_n | a_{n'}^+ \rangle\rangle = \frac{\hbar}{2\pi} \frac{1}{\hbar\omega - E_n - \Sigma_n} \delta_{nn'} .$$

The pole of this function describes the renormalized spectrum of the particle, namely, the shift of the energy state E_n of an isolated particle by the value of its self-energy Σ_n , which is a result of interactions between the particle and the system.

Possible and nowadays well-defined methods for the solution of the Schrodinger equation, which covers a many-particle problem, are Hartree-Fock and derived methods. They represent ab initio methods, which no empirical parameters. The only used parameters are the type and the number of the atoms, and the electron number. In the simplest Hartree-Fock approximation

$$\Sigma_n = \sum_{n_1} \left(\Gamma_{nn_1 nn_1} - \Gamma_{nn_1 n_1 n} \right) f(n_1) , \tag{3}$$

where

$$f(n_1) = \frac{1}{\exp\left(\frac{E_{n_1} - E_F}{kT} \right) + 1}$$

is the Fermi-Dirac distribution (E_F is the Fermi level; then under E_F we will understand $E_{F0}+eU$, that is a fixed position of the Fermi level E_{F0} with the potential bias U).

The first term in the sum (3),

$$\Gamma_{nn_1 nn_1} = \int_0^a dx_1 \int_0^a dx_2 \psi_n(x_1) \psi_{n_1}(x_2) V(|x_1 - x_2|) \psi_n(x_1) \psi_{n_1}(x_2)$$

describes the renormalization of the electron spectrum in the system due to some effective scattering potential. It is the essence of Hartree approximation. Taking into account the wave functions (1),

$$\Gamma_{nn_1 nn_1} = \int_0^a dx_1 \upsilon_{eff}(x_1) \left(\sin \frac{n\pi}{a} x_1 \right)^2 , \tag{4}$$

where

$$\upsilon_{eff}(x_1) = \frac{4}{a^2} \frac{e^2}{4\pi\varepsilon_0} \int_0^a dx_2 \frac{\left(\sin \frac{n_1 \pi}{a} x_2 \right)^2}{|x_1 - x_2|}$$

The second term in (3) describes the so-called exchange interaction:

$$\Gamma_{nn_1n_1n}=\int_0^a dx_1\int_0^a dx_2\psi_n(x_1)\psi_{n_1}(x_2)V(|x_1-x_2|)\psi_{n_1}(x_1)\psi_n(x_2)\Rightarrow\frac{4}{a^2}\frac{e^2}{4\pi\varepsilon_0}\int_0^a dx_1\int_0^a dx_2\frac{\sin\frac{n_1\pi}{a}x_1\cdot\sin\frac{n_1\pi}{a}x_2\cdot\sin\frac{n\pi}{a}x_1\cdot\sin\frac{n\pi}{a}x_2}{|x_1-x_2|}. \quad (5)$$

To establish a quality picture of renormalization of electron spectrum, it is sufficient to take advantage of the Hartree approximation (4). Below we show that result of the Hartree-Fock approximation differs only quantitatively.

We restrict our consideration to $T=0$ K. To eliminate divergence of the integral at $|x_1-x_2|=0$, we cut off this point by the change $|x_1-x_2|=0$ for $|x_1-x_2|+const=0$, where $const=10^{-4}$ nm, which is 10^{-5} of the width of the well at $a=10$ nm.

In the sum (3), n runs through the integer values which are defined by the equality $n_1=a\sqrt{\frac{E_F}{a}}$, where n_1 is the largest integer less than or equal to n; $a=\frac{\hbar^2\pi^2}{2m}$ (if in the expression of n_1 E_F is presented in eV and a in nm, then $a=0.37\text{eV}/\text{m}^2$).

Figure 2 presents self-energy dependence on the size of the well a at three fixed Fermi level E_F (0.2, 0.5, 0.8, eV) for the ground state.

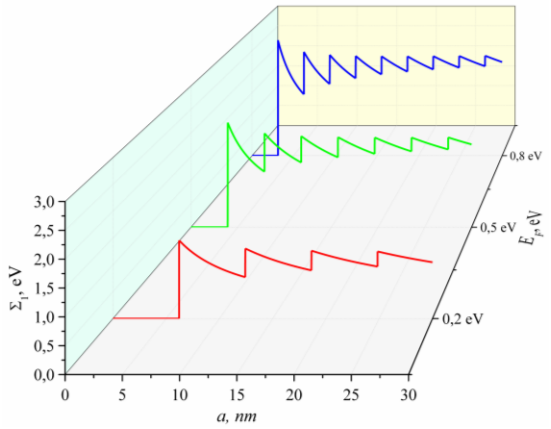

Fig. 2 – Dependence of the ground quantum state self-energy on the width a of the well at fixed Fermi level position E_F (0.2, 0.5, 0.8 eV)

Analysis of the curves indicates that they have saw-tooth dependence. Such dependence is a result of size quantization of electron spectrum. In the narrow wells, all curves Σ_1 are zero. It is those areas a, where the Fermi level E_F is below ground level. The growth of the width of the well a entails compression of the discrete levels. The first jump Σ_n occurs at coincidence the level of the ground state with fixed value E_F. The fastest overlap occurs for the highest value E_F, i.e. $E_F=0.8$ eV. The next jumps of emerge at every pass of the discrete levels through the Fermi level E_F. In the case when E_F is between the neighboring discrete levels, $\Sigma_n(a)$ decreases due to the normalizing factor $\sqrt{\frac{2}{a}}$ of the wave function. This fact is in compliance with the dependence of $\Sigma_1(a)$ on the Fermi level E_F at a fixed width of the well (in our case a = 10.0 nm), i.e. at fixed level positions (see Fig. 3).

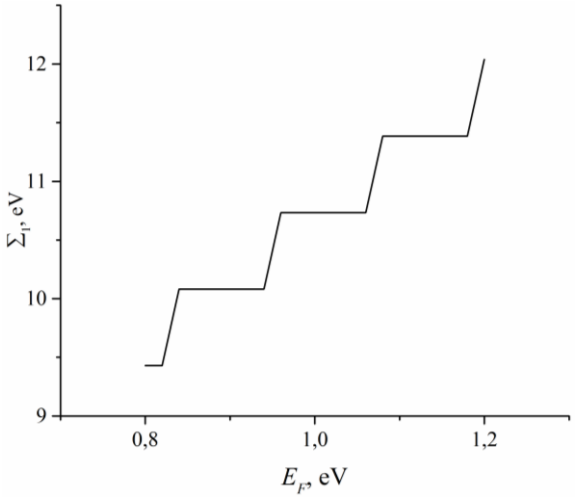

Fig. 3 – Dependence of the self-energy on the Fermi level position E_F at fixed width of the well (a = 10 nm)

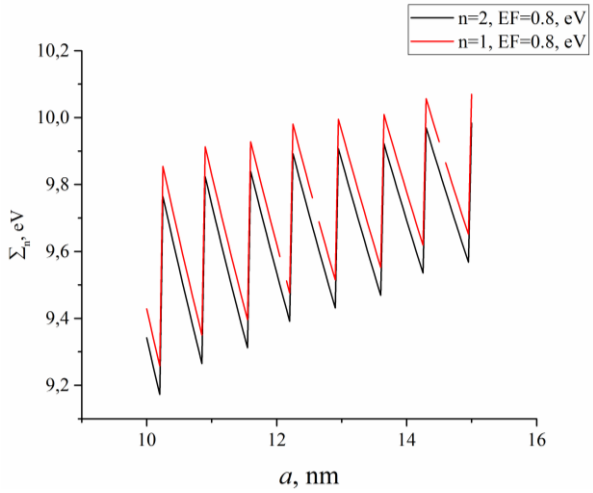

Fig. 4 – Dependence of the Coulomb self-energy on the width a of the well at fixed Fermi level position (E_F = 0.8 eV) for the ground and the first excited quantum states

Analysis of the curves in these figures indicates that

- the curves are parallel shifted relative to each other, and $\Sigma_1>\Sigma_2$;
- the value between two neighboring peaks $\Delta\Sigma_n$ decreases with increasing the size a of the well. Using the Lagrange interpolation polynomial of the 3rd order [18] for the state n = 1, namely

$$\Delta\Sigma_1(a) = \sum_{i=0}^{3} l_i(a)\cdot\Delta\Sigma_1(a_i) \Rightarrow \sum_{i=0}^{3}\prod_{j\neq i}\frac{a-a_j}{a_i-a_j}\Delta\Sigma_1(a_i)$$

at E_F = 0.8 eV ($\Delta\Sigma_1(a_i)$) in the points a_i are presented in Table 1, we can obtain the dependence $\Delta\Sigma_1(a)$, namely:

Table 1 – Parameters in the Lagrange interpolation polynomial

	0	1	2	3
a_i	10.95	11.60	12.80	14.00
$\Delta\Sigma_1(a_i)$	0.55563	0.52687	0.48086	0.44246

$$\Delta\Sigma_1(a) = -0.0002\,a^3 + 0.0096\,a^2 - 0.1911\,a + 1.7383.$$

It is seen that the dependence $\Delta\Sigma_1(a)$, taking into account small coefficients in nonlinear terms on a, has the pronounced linearly falling character.

From equation $\Delta\Sigma_1(a) = 0$, we can estimate the width of the well in which the jumps disappear. In this case, this width is 27.0 nm.

The analysis showed that $\Delta\Sigma_1 > \Delta\Sigma_2$. So, we can say that the range of the width of the wells, in which jumps are manifested, for the ground state is more than for the 1st excited state.

Let us analyze experimental manifestations the jumps of Σ_n. The cause of the jumps is a size quantization, therefore the value of smearing of the levels is important. It is known that such smearing may be a result of scattering by impurities, phonons and so on. The intensity of the scattering is characterized by half-width Γ of the level and is proportional to the relaxation time τ. In turn, τ is connected with mobility $\mu = \frac{e}{m}\tau$.

According to the Heisenberg uncertainty principle the finite τ generates energy uncertainty, namely:

$$\Delta E \geq \frac{\hbar}{2\tau} = \frac{e\hbar}{2\mu m}.$$

Therefore discreteness of the levels can manifest on condition

$$\Delta E_n = E_{n+1} - E_n \Rightarrow \frac{\hbar^2\pi^2}{2m}\frac{2n+1}{a^2} > \frac{e\hbar}{2\mu\, m}.$$

This condition is easily performed in crystals with high mobility that occurs in ideal crystals at low temperatures. Moreover, the temperature has another specific effect on the manifestation of size quantization it should satisfy the condition

$$\Delta E_n = \frac{\hbar^2\pi^2}{2m}\frac{2n+1}{a^2} > kT. \qquad (6)$$

In the case $a = 10$ nm ΔE_n between the ground and first excited state is equal to ~ $1\cdot10^{-2}$ eV that meets ~ 100 K, i.e. experimental observation of manifestations of the size quantization is possible at lower temperatures. If the condition (6) will not be executed, the occupancy of the levels will be almost the same and the observation of the quantization is impossible.

The extraordinary behavior of Σ_n also depends on the width a of the well. In the case of nanoplate, the only way to reduce its size is an axial compression along its normal. But this way is problematic. Indeed, let us use the formula for linear compressibility of an isotropic body [19]

$$\frac{1}{L}\frac{\Delta L}{\Delta p} \approx \frac{1}{3}\beta,$$

where ΔL is the change in the width of the plate under the pressure Δp; β is the coefficient of linear compressibility. According to Figure 4 in order to fix at least one jump Σ_n, the relative compression ΔL must be $\sim 10^{-2} L$. Then taking into account the fact that for most of the solids β is near 10^{-6} atm^{-1} [19], huge pressure of $\Delta p \sim 10^4$ atm is needed. However, the effects of jumps of the self-energy Σ_n can be achieved by changing of the Fermi level position or by the applied voltage bias U.

Finally, let us compare the obtained results with the results of the Hartree-Fock approximation, ie taking into account the exchange interaction (5). Figure 5 shows the Coulomb and exchange parts of the Hartree-Fock interaction and the resulting interactions. Both exchange and resulting interactions as the Coulomb interaction, have sawtooth nature with the same frequency and with the decreasing jumps with increasing of width a of the nanoplane. In other words, the Hartree-Fock results do not violate the qualitative conclusions of the Hartree ones. A similar dependence holds also for the 1st excited state, and, as in the Hartree case, $\Sigma_{1HF} > \Sigma_{2HF}$.

Thus, the ratio between the renormalized by electron-electron interaction ground state $\tilde{E}_1 = E_1 + \Sigma_{1HF}$ and first excited state $\tilde{E}_2 = E_2 + \Sigma_{2HF}$ levels may become $\tilde{\tilde{E}}_1 > \tilde{\tilde{E}}_2$, although in the absence of electron-electron interaction $E_2 > E_1$. A similar result passing of the normal ground state through the higher levels as a result of their different dependence on spatial confinement and electron concentration was obtained 1D quantum wires [20].

4. CONCLUSIONS

Renormalization of electron spectrum has been obtained in nanoobjects at $T = 0$ K in the Hartree-Fock approximation. The used "particle in the infinitely deep well" model is suitable for the qualitative description of the spectrum renormalization in the nanoplates and inversion layers. Analysis of the self-energy of the ground and the first excited states due to electron-electron interactions, depending on the width a of the nanoobject at the fixed Fermi level position, detects its sawtooth nature with jumps up to 6 %. It has been established that the

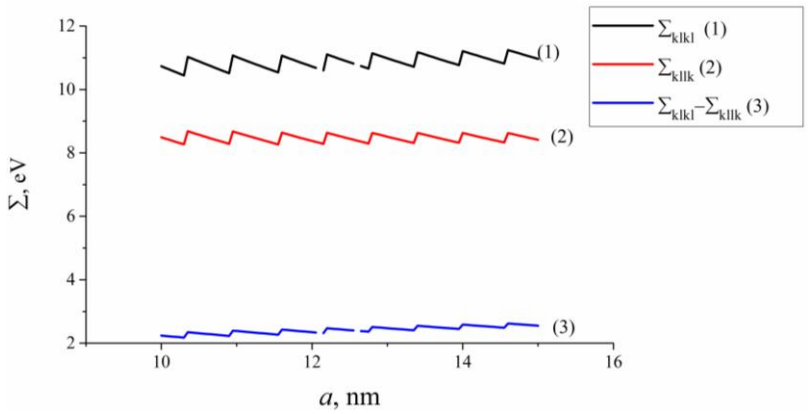

Fig. 5 – Dependence of the Coulomb, exchange and Hartree-Fock self-energy of the ground state on the width a of the well at the fixed Fermi level position (E_F = 1.0 eV)

amplitude of jumps decreases with growth of the width a, and the range of the width in which the jumps are observable for the ground state is greater than those for the excited ones. The only reason for such behavior, as well as analyzed correction depending on the Fermi level position at the fixed width a of the nanoobject, is the size quantization. The obtained renormalized non-trivial behavior of the electron spectrum can exhibit itself, in particular, in the optical properties of the nanoobjects.

Особливості електрон-електронної взаємодії в квантово-розмірних об'єктах

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В роботі проаналізовано особливості електрон-електронної взаємодії в квантово-розмірних об'єктах в наближенні Хартрі-Фока. Встановлено, що власна енергія Σ_n має пилоподібну залежність від положення рівня Фермі чи від розміру об'єкту, як прояв розмірного квантування. По-перше, чим менший розмір нанооб'єктів тим більш виразні осциляції Σ_n. І, по-друге, чим менший розмір нанооб'єктів, тим менша електрон-електронна взаємодія.

Ключові слова: Нанооб'єкт, Електрон-електронна взаємодія, Наближення Хартрі-Фока, Власна енергія.

Особенности электрон-электронного взаимодействия в квантово-размерных объектах

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В работе проанализировано особенности электрон-электронного взаимодействия в квантово-размерных объектах в приближении Хартри-Фока. Установлено, что собственная энергия Σ_n имеет пилообразную зависимость от положения уровня Ферми или от размера объекта как проявление размерного квантования. Во-первых, чем меньший размер нанообъектов тем более виражные осцилляции Σ_n. И во-вторых, чем меньший размер нанообъектов, тем меньше электрон-электронное взаимодействие.

Ключевые слова: Нанообъект, Электрон-электронное взаимодействие, Приближение Хартри-Фока, Собственная энергия.

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