SOME PROBLEMS OF LOW-DIMENSIONAL PHYSICS AND NANOPHYSICS

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Abstract. *Fermi and kinetic energy are usually calculated in periodic boundary conditions model, which is not self-consistent for low-dimensional problems, where particles are confined. Thus for confined particles the potential box model was used self-consistently to calculate Fermi and kinetic energies in 3-, 2-, and 1-dimensional cases. This approach is much more logical and self-consistent. Then the conditions for neglecting dimensions, that is conditions under which the movement of particles in the box could be considered as 2- and 1- dimensional, were derived. Some problems on electronic collective oscillations in Fullerene molecules and carbon nanotube were included also.*

1. FERMI AND KINETIC ENERGIES

To calculate Fermi and Kinetic energies the periodic boundary conditions model is used as a rule [1]. This model is rather adequate for a bulk solid. But when the motion of the particles is confined, the periodic boundary conditions model does not look like a proper one. More adequate in this case is the potential box model. When the potential box is infinitely deep, zero boundary conditions on the borders of the box are realized, thus leading to the zero boundary conditions model (ZBCM).

1.1. Fermi and kinetic energies in 3-d ZBCM

In ZBCM an ensemble of free particles, confined in an infinitely deep potential box, is considered [1]. The Schrodinger equation for the wave function $\psi(x,y,z)$ is as follows (provided the value of the potential in the box is zero):

$$-(\hbar^2/2m)\Delta\psi(x,y,z) = E\psi(x,y,z), \qquad (1)$$

where m is the mass of the particle and $\hbar$ is the Planck constant divided by 2π.

The wave functions are [1]:

$$\psi(x,y,z) = (8/abc)[\sin(\pi v_x x/a)][\sin(\pi v_y y/b)][\sin(\pi v_z z/c)]. \ v_i = 1, 2, 3, \ldots \qquad (2)$$

The components of the wave vectors are [1] $k_i = \pi v_i/a_i$; a, b and c are the sizes of the box and $i = x, y, z$; $a_x = a$, $a_y = b$, and $a_z = c$.

The energy levels are [1]:

$$E(v) = (\pi^2\hbar^2/2m)[(v_x/a)^2 + (v_y/b)^2 + (v_z/c)^2].\qquad(3)$$

The energy of the ground state is not zero: $E_0 = (\pi^2\hbar^2/2m)[(1/a^2) + (1/b^2) + (1/c^2)]$, but it is rather small when a, b, and c are quite large. The energy levels in ZBCM could be written as

$$E(v) = (\pi^2\hbar^2/2mV^{2/3})v^2,\qquad(4)$$

where $V = abc$ and $v^2 = [(V^{1/3}/a)v_x]^2 + [(V^{1/3}/b)v_y]^2 + [(V^{1/3}/c)v_z]^2$.

When $N = nV$ confined particles fill in the levels (for spin 1/2 each level is occupied by two particles), they reach in the process of filling the limiting value of v, v_F. As v_i are positive numbers only (see Eq. (2)), one has only 1/8 fraction of the incomplete sphere (in the v_i space, excluding planes corresponding to $v_i = 0$) of a radius v_F to be filled in. This yields the total number of the states filled being equal to $(\pi/3)v_F^3 - (\pi/2)v_F^2$ (as $v_i > 0$ only and $v_i = 0$ does not exist as was pointed out above). They are all occupied by the particles in consideration. For N much larger than unity (which is a regular case) one has

$$(\pi/3)v_F^3 = nV, \text{ or } v_F = (3nV/\pi)^{1/3}.\qquad(5)$$

Eqs. (4,5) yield for the Fermi energy following expression:

$$E_F = E(v_F) = (\hbar^2/2m)(3\pi^2 n)^{2/3}.\qquad(6)$$

Eq. (6) yields a well-known result [1].

When one has η particles in a unit volume, the Fermi energy of a system practically is $E_F = (\hbar^2/2m)(3\pi^2\eta)^{2/3}$. If $d\eta$ particles are added, the increase in the energy of a system is $(\hbar^2/2m)(3\pi^2\eta)^{2/3}d\eta$. As the potential energy in the box is zero, the kinetic energy of a system is equal to the total energy. The total energy (per unit volume) is the integral of the last expression on η from 0 to n. So we have:

$$T = 0.6NE_F.\qquad(7)$$

Eq. (7) also yields a well-known result [1].

1.2. Fermi and kinetic energies in 2-d ZBCM

In 2-d case Eq. (4) should be written as follows:

$$E(v) = (\pi^2\hbar^2/2mS)v^2,\qquad(8)$$

where $S = ab$ and $v^2 = [(S^{1/2}/a)v_x]^2 + [(S^{1/2}/b)v_y]^2$.

In 2-d case only 1/4 part of the disk (in the v_i space) is relevant because v_i are positive numbers only. Then, instead of $(\pi/3)v_F^3 = nV$, one has $(\pi/2)v_F^2 = N = n_sS = nV$ (n_s is a number of the confined particles per unit area). Instead of $v_F = (3nV/\pi)^{1/3}$ one has $v_F = (2n_sS/\pi)^{1/2}$. One should also take into account that the third (neglected) direction of a size $\delta \to 0$ yields (according to Eq. (3)) the following contribution to the energy of a system: $E(\delta) = (\pi\hbar)^2/2m\delta^2$. So the Fermi energy is as follows

$$E_F = E(v_F) + E(\delta) = (\hbar^2/2m)[2\pi n_s + (\pi/\delta)^2]. \tag{9}$$

Eq. (9) was also derived for the case of N being much larger than unity. The term π/δ^2 in Eq. (9) is a very essential one when δ is small.

The kinetic energy in 2-d case is as follows:

$$T = (\hbar^2/2m)[\pi N n_s + (\pi/\delta)^2 N]. \tag{10}$$

The last term (proportional to N/δ^2) in the right-hand part of Eq. (10), is very essential.

1.3. Fermi and kinetic energies in 1-d ZBCM

In 1-d case Eq. (4) should be written as follows:

$$E(v) = (\pi^2 \hbar^2/2ma^2)v^2. \tag{11}$$

In 1-d case only half of the double length (in the v space) is relevant because of the positive v numbers only. Then, instead of $(\pi/3)v_F^3 = nV$ one has $2v_F = N = n_l l$ (n_l is the number of the confined particles per unit length), so $v_F = 0.5 n_l l$, and

$$E_F = E(v_F) + E(\delta) + E(\delta_{max}) = (\hbar^2/2m)[(\pi n_l/2)^2 + (\pi/\delta)^2 + (\pi/\delta_{max})^2]. \tag{12}$$

Eq. (12) was also derived for the case of N being much larger than unity. Two last terms in the right-hand part of Eq. (12) represent the contribution of the neglected dimensions to the energy of a system (δ_{max} is the larger size of the neglected dimensions).

The kinetic energy in 1-d case is as follows:

$$T = (\pi^2\hbar^2/2m)N[(n_l^2/12) + (1/\delta^2) + (1/\delta_{max})^2]. \tag{13}$$

The contribution of the neglected dimensions is very essential.

1.4. In a potential well of a finite depth all the energy levels (including the Fermi energy) are lower than in the well of an infinite depth

The equations for the wave vectors k_i in a finite potential box is as follows [2]

$$k_i a_i + 2\arcsin[\hbar k_i/(2mU)^{1/2}] = v_i\pi, \; v_i = 1, 2, 3, \ldots, \tag{14}$$

where U is the potential depth.

As Eq. (14) has an additional positive term in the left-hand part of it, one can see that corresponding k_i and $E(v_i) = (\hbar k_i)^2/2m$ are smaller than in ZBCM. The model of a potential box of a finite depth yields lower (comparatively to ZBCM) energy levels, and the Fermi energy in this model is also lower.

It is worthwhile to note that the finite depth of a box leads to non-zero boundary conditions from which follows that the wavelength of each state is larger (comparative to the infinite depth model), and corresponding wave vector and energy are smaller.

2. CRITERIA FOR LOW-DIMENSIONAL MOVEMENT

2.1. A criterion for 2-d movement

Let one of the dimensions is small: $c = \delta \to 0$. The first excited energy level, corresponding to this direction in the ZBCM is $2\pi^2\hbar^2/m\delta^2$ (see Eq. (3)). When this quantity is larger than 2-d Fermi energy (Eq. (9)):

$$2\pi^2\hbar^2/m\delta^2 > (\hbar^2/2m)[(2\pi n_s) + (\pi/\delta)^2], \tag{15}$$

the movement could be considered as a 2-d one.

Using Eq. (15) and taking into account that the surface density of the particles $n_s = n\delta$, one could write

$$\delta < (3\pi/2n_s)^{1/2}, \text{ or } \delta < (3\pi/2n)^{1/3}. \tag{16}$$

For $n = (3\pi/2)\times10^{15}$ cm^{-3} we have $\delta < 10^{-5}$ cm. One should say that it is quite a considerable value.

2.2. A criterion for 1-d movement

When two dimensions are small, and the first excited energy level of the largest of the small dimensions δ_{max} is $2\pi^2\hbar^2/m\delta_{max}^2$, and it is larger than 1-d Fermi energy (see Eqs. (3,12):

$$2\pi^2\hbar^2/m\delta_{max}^2 > (\hbar^2/2m)[(\pi n_l/2)^2 + (\pi/\delta)^2 + (\pi/\delta_{max})^2], \tag{17}$$

then the movement could be considered as a 1-d one.

From Eq. (17) follows that

$$\delta_{max} < [12/(4 + \delta^2 n_l^2)]^{1/2}\delta. \tag{18}$$

Taking into account that the linear density of the particles $n_l = n\delta\delta_{max}$, one could write Eq. (18) for the case $\delta_{max} = \delta$ in the following form:

$$\delta < 2^{1/2}/n^{1/3}. \tag{19}$$

For $n = 2^{3/2}\times10^{15}$ cm^{-3} we have $\delta < 10^{-5}$ cm. That is a very considerable value.

3. FULLERENE MOLECULE

Nuclear liquid drop model was applied rather successfully to a series of nanoobjects. Metallic clusters and fullerene molecules were considered in [3,5]. Carbon nanotubes and carbon peapods were regarded in [4,5]. Here some problems in this field will be formulated. First of all a short introduction to the subject will be given.

Spherically shaped C_{60} (fullerene) molecule has a diameter of $2R_f = 0.7065$ nm at 110 K. The electronic configuration of the constituent carbon atoms is $1s^22s^22p^2$. In C_{60}, we can take the view that the two 1s electrons of each atom belong to the core (forming the ion itself), two 2s electrons form the molecular bonds, and two 2p electrons are collective or free. We model C_{60} molecule by assuming that $N = 60$ ions are situated on the sphere of radius R_f, their charge eZN ($e > 0$ is electron charge, $Z = 2$) being distributed homogeneously on the surface of the sphere. Neither the collective electrons nor the core ions could be found inside the sphere. The collective electrons cannot penetrate inside the

sphere as they repel each other. This feature distinguishes regular metallic clusters and fullerene molecules. We also assume that the charge of $N_f = 120$ collective electrons $-eN_f$ is distributed homogeneously in a spherical layer $R_f < r < R$. The electrostatic potential arising from the collective electrons can be obtained as a solution of the Poisson's equation:

$$\Delta\varphi(\mathbf{r}) = -4\pi\rho(\mathbf{r}), \tag{20}$$

where ρ is the charge density. It is related to the density of the collective electrons n given by

$$n = 3N_f/4\pi(R^3 - R_f^3). \tag{21}$$

Now let us formulate several problems in the topic.

3.1. Electrostatic energy during dipole oscillation
of the electronic cloud as a whole

Let us imagine that we fill the interior of the sphere with positive and negative electric charges of the same density as in the spherical layer. This does not change real electrostatic potential and the energy of the system considered. Total (real plus imaginary) negative charge produces, according to the Poisson's equation (Eq. (20)), the following potential inside the fullerene molecule:

$$\varphi(r) = \varphi(0) + [eN_f/2(R^3 - R_f^3)]\mathrm{r}^2. \tag{22}$$

Total (real plus imaginary) positive charge of the fullerene molecule is

$$q_p = eN_f R^3/(R^3 - R_f^3). \tag{23}$$

When total negative charge is shifted relative to the total positive charge by a distance s, the change in electrostatic energy is

$$W = e^2 N_f^2 [R^3/2(R^3 - R_f^3)^2]s^2. \tag{24}$$

During oscillations, when $s(t) = s_0 \sin \omega_f t$, the time-averaged value of W is

$$\langle W \rangle = e^2 N_f^2 [R^3/4(R^3 - R_f^3)^2]s_0^2. \tag{25}$$

3.2. The kinetic energy of the dipole oscillations
of the electronic cloud as a whole

Let us assume that the displacements inside the electronic cloud u are directed along the z-axis and:

$$u(r,t) = [(r - R_f)/(R - R_f)]s_0 \sin\omega_f t. \tag{26}$$

At $r = R_f$ we have $u = 0$, and at $r = R$ we have $u = s_0\sin\omega_f t$. The local velocity v is directed along the z-axis also and,

$$v(r,t) = \partial u(r,t)/\partial t = [(r - R_f)/(R - R_f)]\omega_f s_0 \cos\omega_f t. \tag{27}$$

Time-averaged value of kinetic energy is equal to the integral over the volume of the electronic cloud of half of the product of the density $3mN_f/4\pi(R^3 - R_f^3)$ and time averaged-value of v^2:

$$\langle T \rangle = 0.25mN_f\omega_f^2 s_0^2(0.6R^2 + 0.3RR_f + 0.1R_f^2)/(R^2 + RR_f + R_f^2). \tag{28}$$

3.3. The frequency of the dipole oscillations of the electronic cloud as a whole

According to the virial theorem, time-averaged values of kinetic (Eq. (28)) and potential (Eq. (25)) energies of the oscillations for a linear harmonic oscillator should be equal. This yields:

$$\omega_f = [e^2 N_f R^3 / m_f (R^3 - R_f^3)^2]^{1/2},$$
$$m_f = m \left[(0.6R^2 + 0.3RR_f + 0.1R_f^2)/(R^2 + RR_f + R_f^2)\right]. \tag{29}$$

Collective electrons can't move everyone with the same amplitude and velocity, because they can't penetrate inside the sphere on which the ions are situated and can't create neutral zones near the positively charged ions. That is why Eq. (26) was assumed. But consideration of the same movement of each electron would result in the same frequency as in Eq. (29), only with m instead of m_f. That is why m_f has a meaning of the effective mass for the regarded type of a dipole movement of the collective electrons in a fullerene molecule.

3.4. Calculation of the external radius
of the electronic cloud, assuming some value for ω_f

Let us take the value of $\omega_f = 20$ eV. Taking $N_f = 120$ and $\hbar\omega_f = 20$ eV, and using Eq. (29) we come to the following equation for R (in atomic units):

$$2220R^3 = (R - R_f)^2(R^2 + RR_f + R_f^2)(6R^2 + 3RR_f + R_f^2). \tag{30}$$

Numerical solution of Eq. (30) yeilds $R = 10.2\hbar^2/me^2 = 0.538$ nm for $R_f = 6.68\hbar^2/me^2 = 0.353$ nm.

3.5. The electric field inside a fullerene molecule arising
due to the dipole oscillations

Total negative charge creates inside a fullerene molecule electrostatic potential, described by Eq. (22). Total positive charge gives rise to the similar potential with the opposite sign. When the total negative charge is shifted by s relative to the ions along the z-axis, its potential is described by Eq. (22), but with $(z - s)$ instead of z. The potential of the positive charge remains unchanged. The sum of the two potentials is a total potential. The derivative of the total potential on z, taken with opposite sign, is the electrostatic field:

$$E = [eN_f/(R^3 - R_f^3)]s. \tag{31}$$

This homogeneous electrostatic field, proportional to the shift s acts inside a fullerene molecule.

4. CARBON NANOTUBE

Now we consider a metallic carbon nanotube of length l, which is much larger than its diameter. Let us assume that N ions per unit length of a carbon nanotube are situated on the surface of a cylinder of the radius R_n, their charge eZN ($Z = 2$) is distributed homogeneously on the surface of the cylinder. Neither the collective electrons nor the

core ions could be found inside the cylinder. Let us assume that the charge of N_n per unit length collective electrons $-eN_n$ is distributed homogeneously in a cylindrical layer $R_n < r < R_{ne}$ with a charge density $-en$ where the electron density n is given by

$$n = N_n/\pi(R_{ne}^2 - R_n^2). \tag{32}$$

4.1. The electrostatic energy during transverse dipole oscillation of the electronic cloud as a whole

Let us imagine that we fill the interior of the cylinder with positive and negative electric charges of the same density. This does not change real electrostatic potential and energy of the system considered. The total (real plus imaginary) negative charge produces (according to Eqs. (20) and (32)) the following potential inside the cylinder of radius R_{ne}:

$$\varphi(r) = \varphi(0) + [eN_n/(R_{ne}^2 - R_n^2)]r^2. \tag{33}$$

The total (real plus imaginary) positive charge per unit length of a carbon nanotube is $eN_n[R_{ne}^2/(R_{ne}^2 - R_n^2)]$. From this expression, Eq. (33), and cylindrical symmetry of the charge distribution on a carbon nanotube, it follows that when total positive charge is shifted relative to a total negative charge by distance h, electrostatic energy of the system per unit length changes by $e^2N_n^2[R_{ne}^2/(R_{ne}^2 - R_n^2)^2]h^2$.

Assuming $h = h_0\sin\omega_{nt}t$, we get the following expression for the time averaged value of the electrostatic energy of the oscillations per unit length:

$$\langle W_n\rangle = e^2N_n^2[R_{ne}^2/2(R_{ne}^2 - R_n^2)^2]h_0^2. \tag{34}$$

4.2. The kinetic energy of the transverse dipole oscillations of the electronic cloud as a whole

Let us assume that the displacements inside the electronic cloud u are directed along the x-axis and:

$$u(r,t) = [(r - R_n)/(R_{ne} - R_n)]h_0\sin\omega_{nt}t. \tag{35}$$

The local velocity v is directed along the x-axis also and

$$v(r,t) = \partial u(r,t)/\partial t = [(r - R_n)/(R_{ne} - R_n)]\omega_{nt}h_0\cos\omega_n t. \tag{36}$$

Kinetic energy per unit length is equal to the integral over the volume of the electronic cloud per unit length of half of the product of the density per unit length $mN_n/\pi(R_{ne}^2 - R_n^2)$ and time averaged-value of v^2:

$$\langle T\rangle = mN_n\omega_{nt}^2h_0^2(3R_{ne} + R_n)/24(R_{ne} + R_n). \tag{37}$$

4.3. The frequency of the transverse dipole oscillations of the electronic cloud as a whole

According to the virial theorem, time-averaged values of kinetic (Eq. (37)) and potential (Eq. (34)) energies of the oscillations for a linear harmonic oscillator should be equal. This yields:

$$\omega_{nt} = [2e^2N_nR_{ne}^2/m_n(R_{ne}^2 - R_n^2)^2]^{1/2},$$

$$m_n = [(3R_{ne} + R_n)/6(R_{ne} + R_n)]m. \tag{38}$$

Collective electrons can't move everyone with the same amplitude and velocity, because they can't penetrate inside the cylinder on which the ions are situated and can't create neutral zones near the positively charged ions. That is why Eq. (35) was assumed. But consideration of the same movement of each electron would result in the same frequency as in Eq. (38), only with m instead of m_n. That is why m_n has a meaning of the effective mass for the regarded type of a transverse dipole movement of the collective electrons in a carbon nanotube.

4.4. The electric field inside a carbon nanotube arising due to the transverse dipole oscillations

Total negative charge creates inside a carbon nanotube electrostatic potential, described by Eq. (33). Total positive charge gives rise to the similar potential with the opposite sign. When the total negative charge is shifted transversely by h relative to the ions along the x-axis, its potential is described by Eq. (22), but with $(x - h)$ instead of x. The potential of the positive charge remains unchanged. The sum of the two potentials is a total potential. The derivative of the total potential on x, taken with opposite sign, is the electrostatic field:

$$E = [2eN_n/(R_{ne}{}^2 - R_n{}^2)]h. \tag{39}$$

This homogeneous electrostatic field, proportional to the shift h acts inside a fullerene molecule.

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NEKI PROBLEMI FIZIKE MALOG BROJA DIMENZIJA I NANOFIZIKE

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Fermi i kinetička energija se obično izračunavaju u modelu sa periodičnim graničnim uslovima, koji nije konzistentan sa nisko-dimenzionalnim problemima, gde su čestice konfinirane. Zbog toga je za konfinirane čestice iskorišćen model potencijalne kutije za konzistentno izračunavanje Fermi i kinetičke energije u 3,2 i 1 dimenzionalnom slučaju. Ovaj prilaz je mnogo logičniji i samo-usaglašen. Onda su izvedeni uslovi za zanemarivanje dimenzija, odnosno uslovi pod kojima kretanje čestica u kutiji može biti razmatrano kao 2 i 1-dimenzionalno. Neki problemi elektronskih kolektivnih oscilacija kod molekula Fulerena i ugljenikovih nanotuba su takođe uključeni.