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CONDUCTIVE AND SUPERCONDUCTIVE PROPERTIES OF NANORODS

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Abstract
An analysis of the electron and phonon spectra in a metallic nanorod is discussed. It is found that the phonon energy gap can shift the critical temperature of the system. It is also shown that an autoreduction effect occurs as a consequence of the fact that the momentum space has a smaller number of degrees of freedom than the configurational space.

1. Introduction

Nanorods are structures with rectangular cross section of nanodimension and macroscopic length. Nanodimensions in two directions require the introduction of boundary conditions, which noticeably change the physical characteristics of the system compared to those corresponding to the bulk structure. These changes are antiproportional to the thickness of the structures. The mentioned effect is expectable on the basis of the Heisenberg uncertainty relations, which are a fundamental quantum mechanical principle. In this work we are going to present an analysis of the dependence of the physical characteristics on the boundary conditions. A special attention will be given to the electron subsystem of the quantum rod. Some consequences of the phonon excitations will be also discussed.

The existence of the phonons in the nanorod is essential for a proper determination of the superconductive properties[1] of the system. In the papers[2, 3] it was shown that the phonon excitations require an energy larger than the zero activation energy. This energy gap (expressed here in temperature units) shows that the temperature $T_g = \frac{E_{act}}{k_B}$ plays the role of the absolute

zero for the resistance of the metallic nanoconductors, i.e. $R = R_0\left(1 + \frac{t}{273\,°C}\right)$ [illegible]. Besides this shift in the zero activation energy caused by nanodimensions, virtual exchange of phonons (BCS theory) and extreme transitivity (Abrikosov's idea) [4] can also occur, all these effects contributing to a possible increasing of the critical temperature of the system. The last two effects are also present in bulk structures.

2. Electron subsystem of nanorod

We shall investigate nanorods whose numbers of layers are denoted with integers $n_x \in [0, N_x]$, $n_y \in [0, N_y]$ and $n_z \in \left[-\frac{N_z}{2}, \frac{N_z}{2}\right]$, where n_x and n_y are of the order 10 while n_z is of the order 10^8. We shall apply the Green's function method. As it is well known, this is the unique method which allows a systematic determination of the dynamic and thermodynamic characteristics of the system. Here we will use the Hubbard model of the electronic Hamiltonian[5]. We will use the approximation of the nearest neighbors and we shall assume that the nanorod has a simple cubic structure. In this case, the Hamiltonian in the Hubbard model can be written as follows:

$$H = -\sum_{\vec n} \Big([illegible] \Big) - \sum_{\vec n} \Big([illegible] \Big) \quad (1)$$

where A^+ and A are Fermi creation and annihilation operators for the electrons and

$$W_{\vec n;\vec n_x} = W_{n_x n_y n_z;\, n_x+1\, n_y n_z} = W_x$$

$$W_{\vec n;\vec n_y} = W_{n_x n_y n_z;\, n_x\, n_y+1\, n_z} = W_y$$

$$W_{\vec n;\vec n_z} = W_{n_x n_y n_z;\, n_x n_y\, n_z+1} = W$$

(2)

Since the Hamiltonian (1) is composed from fermionic operators, we shall use the anticommutator Green's function:

$$G_{n_x,n_y,n_z;m_x,m_y,m_z}(t) \equiv << A_{n_x,n_y,n_z}(t) \mid A^{+}_{m_x,m_y,m_z}(0) >>= \Theta(t) < \left\{ A_{n_x,n_y,n_z}(t), A^{+}_{m_x,m_y,m_z}(0) \right\} > \quad (3)$$

where $\Theta(t)$ is Heaviside step function.

We start with the basic observation that the translational symmetry of nanorod is broken in *x* and *y* direction. These boundary conditions have to be specified in these directions. Our boundary conditions are based on the simple fact that there is no interaction with the absent layers, and thus:

(4)

Due to the disturbed symmetry in *x* and *y* directions, the equation for the Green's function (3) leads to a system of nine differential equations. The resulting expressions are quite long and we will not write them explicitly here[5]. In order to indicate the construction of these nine equations, we will give a graphical scheme. It represents the cross section of nanorod, which is shown in fig. 1.

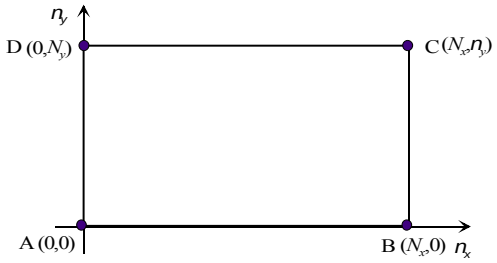

Figure 1. The scheme for the construction of the equations that define the Green's functions of the rod.

According to this scheme, all points inside of rectangle ABCD determine the complete equation for the Green's function. This equation has the following form:

(5)

Note that along the sides of rectangle one layer does not exist, so in accordance with the boundary conditions (4) the corresponding interactions must be set equal to zero. The missing sides with the corresponding layer index are as follows: the side AB with the layer $n_x = -1$, the side CD with the layer $n_x = N_x + 1$, the side AC with $n_y = -1$, and the side BD with $n_y = N_y + 1$. It is clear that the identities (5) that include these indexes should be modified in order to incorporate these zero interactions.

In order to simplify the resulting equations, we shall use the fact that the system is invariant to translations along the z direction, which suggests us to introduce the Fourier transform :

(6)

The system of nine equations can be reduced to only one equation (valid for all n_x and n_y) using the substitution

(7)

$$\varphi_\nu = \frac{\nu\pi}{N_x+1};\ \nu = 1,2,..N_x \qquad \psi_\mu = \frac{\mu\pi}{N_y+1};\ \mu = 1,2,..N_y$$

(8)

From this equation it is easy to derive the final expression for the Green's function, i.e.:

(9)

The coefficients $L^x_{\nu\nu'}$ and $L^y_{\mu\mu'}$ can be determined from the equations

(10)

(11)

The dispersion law is given by:

(12)

We can now discuss the effects that appear due to the broken translational symmetry. A first observation is that standing waves form along the x and y directions. This means that in these directions the electron currents will not propagate. Another observation is that the momentum space (ν, μ, k_z) is narrower than the configurational space (n_x, n_y, n_z). This means that an anisomorphism of the type $(n) \to (n-1 n 1)$ will occur. This effect is called autoreduction[6] and appears because for $\nu = 0$, $\mu = N_x + 1$, $\mu = 0$ and $\mu = N_y + 1$ the transformation (7) leads to a null value of the Green's function.

Note also that in the electron spectrum there is also an energy gap equal to

It should be recalled that in the Hubbard model applied to the *bulk* structure the energy gap does *not* exist.

We can now use the spectral intensity of the Green's function

(13)

in order to determine the electron concentrations. In the chemical potential representation these concentrations are:

(14)

Note that in the above formula the functions F and Φ are expressed in terms of coefficients *L*. For the case of a 3x3 nanorod the parameter μ_0 is just the chemical potential defined as the electron energy of the Fermi boundary, i.e.

(15)

We shall now establish the electron concentrations in the vicinity of the Fermi boundary for the 3x3 nanorod. This nanorod contains nine atoms in the cross section, but due to the autoreduction effect only four of them will have a non-zero concentration. The antiisomorphism  in this case goes over to 3x3 $\rightarrow$ 2x2. Using the standard procedure for the calculation of the concentrations near the Fermi boundary, we have found that the values of the concentrations are as follows (see fig. 2).

Note that the concentrations at boundary atoms are higher than those of the internal atoms. This means that a skin-type effect can appear in the rod.

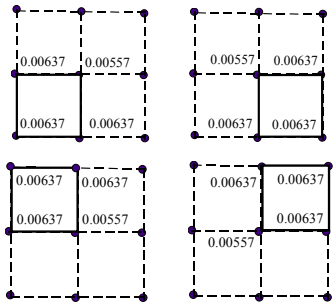

Figure 2. Electron concentrations for a square nanorod 3x3.

3. Mechanical oscillations in the nanorod

The analysis of the phonon subsystem requires the use of two types of Green's function. These are the displacement-displacement and the momentum-momentum Green's functions. We will state here only the final conclusions. One finds that the autoreduction effect does not appear in the phonon subsystem and that the acoustical branches of the phonon spectra, which are usually present in bulk structures, do not exist in the nanostructure. One also finds that every phonon branch possesses a lower or higher energy gap. These energy gaps decrease with the increase of thickness of the nanostructure.

The phonon energies of nanorod are given by:

(16)

where *C* is Hook's constant, M is mass of atom and the integers ν and μ take the values

$$\nu \in [1, N_x - 1], \mu \in [1, N_y - 1] \tag{17}$$

The minimal phonon energy is different from zero:

(18)

The presence of this gap practically means a shift of the absolute zero to the value $T_g = \frac{E_{\min}}{k_B} > 0$. Other processes, such as the virtual exchange of phonons and high transparency, can also add to the temperature T_g a few kelvins. Our results concerning the potential increase of the critical temperature with respect to that corresponding to the bulk structure are summarized in the two tables.Table 1 shows the temperatures T_g corresponding to the phonon energy gap and Table 2 shows the critical temperatures for the bulk structure.

Table 1. The potential temperatures T_g for the phonon energy gap.

Element	T_g **(K)**			
	$N_x = 2$	$N_x = 3$	$N_x = 5$	$N_x = 10$
Lead Pb	9,9371	8,0242	5,7782	3,3893
Tantalum Ta	42,4587	34,2854	24,6887	14,4819
Niobium Nb	43,5895	35,1985	25,3462	14,8676
Aluminium Al	51,0370	41,2124	29,6767	17,4078
Tungsten W	56,1160	45,3137	32,6300	19,1401
Vanadium V	62,4129	50,3984	36,2915	21,2879
Molybdenum Mo	70,8597	57,2192	41,2032	24,1689

Table 2. The critical temperature and relevant parameters for the bulk superconductors.

Element	**ρ (g/cm^J)**	**C(m/s)**	**Atomic mass**	**Lattice const. (m)**	**T_C(K)**
Aluminium Al	2,70	5000	26,982	4,050E-10	1,140
Vanadium V	6,00	4560	50,942	3,020E-10	5,380
Niobium Nb	8,57	3480	92,906	3,300E-10	9,500
Molybdenum Mo	10,28	5400	95,940	3,150E-10	0,900
Tantalum Ta	16,69	3400	180,948	3,310E-10	4,483
Tungsten W	19,25	4290	183,840	3,160E-10	0,012
Lead Pb	11,34	1190	207,200	4,950E-10	7,193

Conclusion

The main goal of this work was to point out that in nanorods an increase of the critical temperatures can be expected. We have determined the electron and phonon dispersion laws in the nanorod, with the conclusion that the energy gap for the phonon excitations is sufficiently large in order to cause a shift in the critical temperature. This gap is maximal for 3x3 nanorods and decreases with the increase of surface of nanorod cross section. Our conclusion seems to be supported by the data in[7]. For the electron subsystem in the nanorod, we have found that a skin effect can occur, and that the electron spectrum contains an energy gap, although in the bulk structure the energy gap is absent.

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