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COLLECTIVE EXCITATIONS IN CARBON NANOTUBES

The effective action functional has been built by a functional integral method for nanotubes. The closed, self-consistent system of equations of the system is built on the basis of the variational differentiation the effective action on collective variables of an electron-phonon subsystem. A general expression for a polarization function and spectrum of the system are considered.

1.   Introduction

The atomic and electron structure of carbon nanotubes can be represented as, a two-dimensional carbon hexagonal structure rolling along a given direction and reconnecting the carbon bonds. Systems of carbon atoms can exist in several modifications: laminated graphite with a hexagonal structure, nite carbon, crystal diamond, the fullerenes C_{60}, C_{70}, C_{78}, C_8, and carbon nanotubes—two-dimensional extended structures rolled up in a single- or multiwall tube [1,2]. Carbon nanotubes were synthesized simultaneously with fullerenes and are more interesting structures because they model a one-dimensional system. Soliton states are known to be formed in such systems.

The property of nanotubes to absorb liquid metal, hydrogen, oxygen, methane, and other gases opens a prospect for constructing strong thin conducting lines of fuel elements and creating new types of fuel. The discovery of superconductivity in metal-doped C_{60} [3] feeds the hope to find the same phenomenon in nanotubes filled with metal or to modify the superconductivity of known superconductors by injecting them in a nanotube.

Electron spectrum of such structure is characterized by quantum numbers including the number of radial (n), azimuthal (m) and longitudinal (k) modes [4,5]. Its physical properties are considerably related to collective electron-phonon excitations and oscillations of electron density (plasmons or plasma oscillations).

The equations, describing such excitations, can be obtained on the basis the functional integral method with help of the variational derivatives of the expression for the effective action integral. We assume that a such approach allows most precisely to calculate polarizing function of the carbon nanotube in view of all features of its atomic structure.

2.   The effective action function of the system

The researched system consists of ions with charge Ze and degenerate electrons. Then the functional integral of the system in terms of spatial coordinates (x, y, z) and imaginary time (τ) can be represented as [4,5]

$$Z = \int D\psi^+ D\psi \exp\left(S[\psi]\right), \tag{1}$$

where the action $S[\psi]$ is determined by the expression

$$S[\psi] = \int_0^\beta dr \int dx \sum_s \psi_s^+(x,r) K(x,r) \psi_s(x,r) -$$

$$-\frac{e^2}{2} \int_0^\beta dr \int dx dy \rho(x,r) V(x-y) \rho(y,r) + \qquad (2)$$

$$+ \int_0^\beta dr \sum_{l_a} \left[i p_{l_a}(r) \partial_r q_{l_a}(r) - \frac{p_{l_a}(r)}{2M_C} \right], \qquad a = \alpha, \beta.$$

Here s is an electron spin, $\psi_s(x,r)$ is the two-component wave function of the nanotube lattice (a, b)

$$\psi_s(x,\tau) = \begin{pmatrix} \psi_{as}(x,\tau) \\ \psi_{as}(x,\tau) \end{pmatrix},$$

p_{l_a}, q_{l_a} and $2M_C$ are a moment, a coordinate and the mass of an ion in l_a sublattice cite, $V(x-y) = 1/|x-y|$ is the operator of the Coulomb interaction. Beside, $K(x,r)$ is the operator of kinetic energy of the form

$$K(x,r) = \begin{pmatrix} K_a(x,r) & 0 \\ 0 & K_b(x,r) \end{pmatrix}, K_{a,b}(x,r) = -\partial_r + \frac{\Delta_{a,b}}{2m_\varepsilon} + \mu_{a,b},$$

where $\partial_r = \partial/\partial_r$, $\Delta_a/(2m)$ is the kinetic energy for the a th sublattice, μ_a a chemical potential of the a th sublattice.

The charge density $\rho(x,r)$ is composed of ion ($\rho^q(x,r)$) and electron ($\rho^e(x,r)$) parts and equals $\rho(x,r) = \rho^q(x,r) - \rho^e(x,r)$, where

$$\rho^q(x,r) = \sum_{\alpha,\gamma} \rho_{\alpha\gamma}^q(x,r) \delta_{\alpha,\gamma}, \quad \rho^e(x,r) = \sum_{\alpha,\gamma} \rho_{\alpha\gamma}^e(x,r).$$

The summation on α and γ is carried out over all lattice sites a and b.

In the representation of the functional integral (1) can be rewritten as

$$Z[\psi,\varphi] = \int D\psi^+ D\psi \int D\varphi \exp\left(S[\psi,\varphi] \right), \qquad (3)$$

where the action function $S[\psi,\varphi]$, which contains an electron influence, the field φ and its interaction, has the form

$$S[\psi] = -\frac{1}{2} \int_0^\beta dr \int dx dy \varphi(x,\tau) V^{-1}(x-y) \varphi(y,\tau) +$$

$$+ \int_0^\beta d\tau \int dx \sum_s \psi_s^+(x,r) K'(x,r) \psi_s(x,r) + ie \int_0^\beta dr \int dx \rho^q(x,\tau) \varphi(x,\tau) +$$

$$+ \int_0^\beta dr \sum_{l_a} \left[i p_{l_a}(r) \partial_r q_{l_a}(r) - \frac{p_l^2(r)}{2M_C} \right], \quad a = \alpha, \beta.$$

Here

$$K'(x,r) = \begin{pmatrix} K_a(x,r) - ie\varphi(x,\tau) & -ie\varphi(x,\tau) \\ ie\varphi(x,\tau) & K_b(x,r) - ie\varphi(x,\tau) \end{pmatrix}.$$

Integrating in (3) on Fermi fields [4] and using the known Liouville formulae, $(\lg \det A)' = \mathrm{Sp}((\ln A)')$, where A is matrix, a prime denotes a first derivative, we can transform (3) to the form $Z = \int D\varphi \exp(S_{eff}[\varphi])$. Here the effective action

$$S_{eff}[\varphi] = -\frac{1}{2}\int_0^\beta dr \int dx dy \varphi(x,\tau) V^{-1}(x-y)\varphi(y,\tau) +$$

$$+2\mathrm{Spln}K'(x,\tau) + ie\int_0^\beta d\tau \int dx \rho^q(x,\tau)\varphi(x,\tau) +$$

$$+\int_0^\beta dr \sum_{l_a}\left[ip_{l_a}(r)\partial_r q_{l_a}(r) - \frac{p_l^2(r)}{2M_C} \right], \quad a = \alpha, \beta,$$

(4)

allows to describe the system in collective variables.

The matrix Green function, $G = \| G_{\alpha,\beta} \|$ of the system is determined by the equation

$$K'(x,\tau)G(x,\tau_x; y,\tau_y) = \delta(x-y)\delta(\tau_x - \tau_y) \qquad (5)$$

At presence only the effective field, V_{eff}, of single-electron model potential of carbon nanotube (see [Ah]) the Green function, $G_0 \| G_{0,\alpha\beta} \|$, is determined by the equation

$$K_0'(x,\tau)G_0(x,\tau_x; y,\tau_y) = \delta(x-y)\delta(\tau_x - \tau_y),$$

where $K_0(x,\tau_x) = K'(x,\tau_x)|_{\varphi=iV_{eff}}$.

Using the representation $K'(x,\tau_x) = K_0(x,\tau_x) + K_1(x,\tau_x)$, where the function $K_0(x,\tau_x) = (-ie\varphi(x,\tau_x) + eV_{eff}(x)) \| c_{ik} \|, c_{ik} = 1, (i,k = 1,2)$ (5) can be rewritten in the form

$$G(x,\tau_x; y,\tau_y) = G_0(x,\tau_x; y,\tau_y) -$$

$$-\int_0^\beta d\tau_z \int dz G_0(x,\tau_x; z,\tau_z)K_1(z,\tau_z)G(z,\tau_z; y,\tau_y).$$

(6)

The obtained expressions for the effective action function together with the equation (6) for the Green function permit build the equations determining the field $\varphi(x,\tau_x)$.

3. The equations for field functions

The equations describing states of the system are obtained by equating to zero the variational derivation of the effective action function (4) with respect to generalized coordinates $\varphi(x,\tau_x)$, q_{l_a}, p_{l_a} that give the system

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$$\frac{\delta S_{eff}[\varphi]}{\delta(\varphi(x,\tau))}=0,\ \frac{\delta S_{eff}[\varphi]}{\delta(q_{l_\alpha}(\tau))}=0,\ \frac{\delta S_{eff}[\varphi]}{\delta(p_{l_\alpha}(\tau))}=0.$$

These three equality result in the system of the three equations

$$-\int dy V^{-1}(x-y)\varphi(y,\tau)+ie\rho^q(x,\tau)-$$

$$-2e\lim_{\substack{y\to k\\ \tau_y\to\tau_x-0}}\mathrm{Sp}\left\{G(x,\tau_x;y,\tau_y)\begin{pmatrix}1&1\\1&1\end{pmatrix}\right\}=0,$$

$$i\partial_\tau p_{l_\alpha}(\tau)-ieZ\int d^3x\varphi(x,\tau)\nabla\delta(x-q_{l_\alpha})=0,$$

$$i\partial_\tau q_{l_\alpha}(\tau)-\frac{p_{l_\alpha}(\tau)}{M_C}=0.$$

(7)

From the first equation of the system (7) follows that the field function

$$\varphi(z,\tau)=ie\int dx V(z-x)\rho^q(x,\tau)-4ie\int dx V(z-x)\times$$

$$\times\lim_{\substack{y\to k\\ \tau_y\to\tau_x-0}}\left(G_1(x,\tau_x;y,\tau_y)+G_2(x,\tau_x;y,\tau_y)\right),$$

(8)

means the electrical field of the electrical potential of ions and electrons. This quantity completely determines the interaction in the system and its collective excitations. Taking into account that $\Delta V(x-y)=-4\pi\delta(x-y)$, the equation (8) can be transformed to the form

$$\Delta\varphi(z,\tau)=4\pi e\rho^q(x,\tau)-$$

$$-16\pi e\lim_{\tau_y\to\tau_x-0}\left(G_1(x,\tau_x;y,\tau_y)+G_2(x,\tau_x;y,\tau_y)\right),$$

(9)

that together with the equation (6) consists the closed system. For solving this system we introduce the new notations the $G=G_1+G_2$ and $G_0=G_{01}+G_{02}$. Then taking into account that for statical ions

$$iV_{eff}=ie\int dz V(x-z)\rho^q(z,\tau)-4ie\int dx V(z-x)\lim_{\substack{z_1\to z\\ \tau_{z_1}\to\tau_z-0}}\left(G_0(z,\tau_z;z_1,\tau_{z_1})\right)$$

and

$$G=G_0+2ieG_0(\varphi-iV)G\approx G_0+2ieG_0(\varphi-iV)G_0+...,$$

we can obtain the expression

$$\varphi(z,\tau)-iV_{eff}=8e^2\int dzdz_1d\tau_{z_1}\,V(x-z)G_0(z,\tau;z_1,\tau_1)\times$$

$$\times\left(\varphi(z_1-iV_{eff}(z_1))\right)G_0(z,\tau;z_1,\tau_1)G_0(z_1,\tau_1;z,\tau)+...,\quad \tau_z\to\tau,$$

which describes plasma oscillations.

The second and third equations of the system (7) determine motion of carbon ions. The obtained self-consistent close system of equations describes the electron and vibrational subsystems via collective variations.

For calculation the electron density fluctuation induced by plasma vibration relative to the stationary ion lattice we will enter into (8) the polarization operator $P(x, \tau; z_1, \tau_1)$ which is determined by equality

$$\int dz_1 d\tau_1 V(x - z_1)\delta(\tau - \tau_1)G(z_1, \tau_1; z', \tau') -$$

$$-\int dz_1 d\tau_1 P(x, \tau; z_1, \tau_1)\delta(\tau - \tau_1)G_0(z_1, \tau_1; z', \tau').$$

Then the field function can represent in terms of the effective potential V_{eff} and polarization operator P in the form

$$\varphi(z, \tau) = iV_{eff}(z, \tau) - 4ie\int dz_1 d\tau_1 \left(P(x, \tau; z_1, \tau_1) - \right.$$
$$\left. -V(x - z_1)\delta(\tau - \tau_1) \ \right)G_0(z_1, \tau_1; z', \tau')$$

The Green function obeys the matrix equation

$$G = G_0 + 8e^2 G_0 \left(P - V \right) G_0 G \quad,$$

whence applying the relation $VG = PG_0$ we can obtain the equation

$$P = V - 8e^2 V G_0 P, \qquad (10)$$

determining in the linear approximation the polarization P. The poles of the Fourier transform of the polarization function P determine plasma oscillations of the density relative to a ground stationary state.

Applying the Fourier transform to (10) we can obtain in the approximation of the second order in V the expression

$$P(q, \omega; q', \omega') = -\frac{4\pi}{q^2}\delta(q - q')\delta(\omega - \omega') \times$$

$$\times \left(1 + \frac{e^2}{2}\frac{4\pi}{q^2} \sum_{\substack{n,m,k; \\ n_1, m_1, k_1}} \int dx G_{nmk}(x) G_{n_1 m_1 k_1}(-x) e^{-iqx}\delta(\omega - E_{nmk} + E_{n_1 m_1 k_1}) \right),$$

where q and ω are coordinate and frequency components of the Fourier transform; Energy levels of stationary states of the electron subsystem are denoted as E_{nmk} (see [1]). The spectrum and intensity of the collective excitations are described by the diagonal part of $P(q, \omega; q', \omega')$.

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ОЗНАЧЕННЯ ТА ВИКОРИСТАННЯ МНОЖИНИ СТРОГО РАЦІОНАЛЬНИХ СТРАТЕГІЙ У ДЕЯКИХ АНТАГОНІСТИЧНИХ ІГРАХ

There has been defined the set of strictly rational strategies and the set of nonstrictly rational strategies of a player in the antagonistic game. On the example it has been shown what advantage a player obtains if it applies the set of strictly rational strategies by the other player swerve from the set of its optimal strategies.

Означено множину строго раціональних стратегій та множину нестрого раціональних стратегій гравця в антагоністичній грі. За допомогою прикладу показано, яку вигоду отримує гравець, якщо він використовує множину строго раціональних стратегій при відступі іншого гравця від множини своїх оптимальних стратегій.

Передмова та формулювання задач дослідження

Прийняття оптимальних рішень в умовах конфліктних ситуацій є актуальною та практично значущою задачею сучасної прикладної математики [1]. Багато таких задач формалізуються та моделюються за допомогою апарату теорії антагоністичних ігор [2]. Методика розв'язування антагоністичних ігор заснована на класичному принципі оптимальності, де центральною категорією є концепція рівноваги, звідки і знаходяться сідлові точки у чистих, чи, взагалі кажучи, змішаних стратегіях [3, 4]. Очевидно, що ця концепція не суперечить інтуїтивним уявленням про вигідність, стійкість та справедливість. Проте відомо, а у роботах [5 — 10] звернуто увагу на ту обставину, що не всі елементи множини оптимальних стратегій гравця в певній антагоністичній грі є рівноправними з точки зору однакових наслідків їх використання. Так, у роботі [8] означено множину строго раціональних чистих стратегій та множину нестрого раціональних чистих стратегій гравця в антагоністичній грі, де показано, яку вигоду отримує гравець, якщо він використовує множину строго або нестрого раціональних чистих стратегій при відступі іншого гравця від множини своїх оптимальних чистих стратегій. Зокрема, якщо антагоністична гра є матричною та її ядром є матриця [8]