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Energy Spectrum and Optical Absorption Spectrum of Fullerene C_{26} within the Hubbard Model

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Anticommutator Green's functions and energy spectra of fullerene C_{26} and endohedral fullerene U@C_{26} with the D_{3h} symmetry groups have been obtained in an analytical form within the Hubbard model in the approximation of static fluctuations. The energy states have been classified using the methods of group theory, and the allowed transitions in the energy spectra of molecules C_{26} and U@C_{26} with the D_{3h} symmetry groups have been determined.

Keywords: Hubbard model, Green's functions, energy spectrum, nanosystems, fullerene C_{26}.

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1. Introduction

An intensive study of carbon clusters started in 1985 after the discovery of fullerene C_{60} [1] led to the discovery of a whole series of fullerenes C_n and endohedral fullerenes A@C_n, as with $n < 60$, and $n > 60$. Fullerenes C_n with $n < 60$ belong to the so-called class of small fullerenes. Currently a large number of studies are devoted to the study of small fullerene properties: C_{20} [2,3], C_{24} [4,5], C_{28} [6,7], C_{36} [8,9]. One of the small fullerenes is the fullerene C_{26}, the existence of which was experimentally confirmed in a number of studies [10,11]. Quite a lot of studies [12–15] are devoted to the study of physical and chemical properties of fullerene C_{26}.

Fullerene C_{26} consists of 12 pentagons and 3 hexagons, as shown in Fig. 1, and has a symmetry group D_{3h}. From the Schlegel diagram shown in Fig. 1 we can see, that this fullerene contains five nonequivalent bonds and four groups of nonequivalent carbon atoms: $G_1 = \{1, 4, 9, 15, 21, 25\}$, $G_2 = \{2, 3, 5, 6, 8, 10, 14, 16, 20, 22, 24, 26\}$, $G_3 = \{7, 11, 13, 17, 19, 23\}$, $G_4 = \{12, 18\}$. The set G_1 includes the atoms, which are at the vertices of the junction of one hexagon and two pentagons, the common border of which connects two hexagons. The set G_2 includes the atoms, which are at the vertices of the junction of one hexagon and two pentagons, the common boundary of which connects the hexagon and the pentagon. The set G_3 includes the atoms, which are at the vertices of the junction of three pentagons, the common boundary of which connects the pentagon and the hexagon. The set G_4 includes the atoms, which are at the vertices of the junction of three pentagons, the common boundary of which connects two pentagons.

The Hubbard model [16] is widely used to describe the electronic properties of carbon nanosystems. Within the framework of this model, the electronic and optical properties of both fullerenes [17–22], and nanotubes [23] were studied. So, for example, within the framework of the Hubbard model in the approximation of static fluctuations, the energy spectra and optical absorption spectra of fullerene C_{60} [17], fullerene C_{70} [18], fullerene C_{36} with symmetry group D_{6h} [19], fullerene C_{28} with symmetry group T_d [20], fullerene C_{24} with symmetry groups O_h, D_6 and D_{6d} [21] and fullerene C_{20} with symmetry groups I_h, D_{5d} and D_{3d} [22] were obtained. The results obtained in the studies [17,18] are in good agreement with the experimental data.

The purpose of this study is to study the energy spectrum of fullerene C_{26} with symmetry group D_{3h} in the framework of the Hubbard model in the static fluctuation approximation.

2. Energy spectrum of fullerene C_{26}

To describe π-electronic system of the fullerene C_{26}, we will use the Hubbard model [16]:

$$H = \sum_{\sigma,i} \varepsilon_i n_{i\sigma} + \sum_{\sigma,i\neq j} t_{ij} c^+_{i\sigma} c_{j\sigma} + \frac{1}{2}\sum_{\sigma,i} U_i n_{i\sigma} n_{i\bar{\sigma}}, \tag{1}$$

where $c^+_{i\sigma}$ and $c_{i\sigma}$ are the creation and annihilation operators of electrons with spin σ at site i; $n_{i\sigma}$ is the operator of the number of particles with spin σ at site i; ε_i is the energy of the one-electron atomic state at site i; t_{ij} is the transfer integral describing the hopping of electrons from site i to site j; U_i is the Coulomb repulsion energy of two electrons located at site i; and $\bar{\sigma} = -\sigma$.

From the Schlegel diagram shown in Fig. 1, we can be see, that the fullerene C_{26} has five types of nonequivalent bonds. Therefore, within the Hubbard model, five transfer

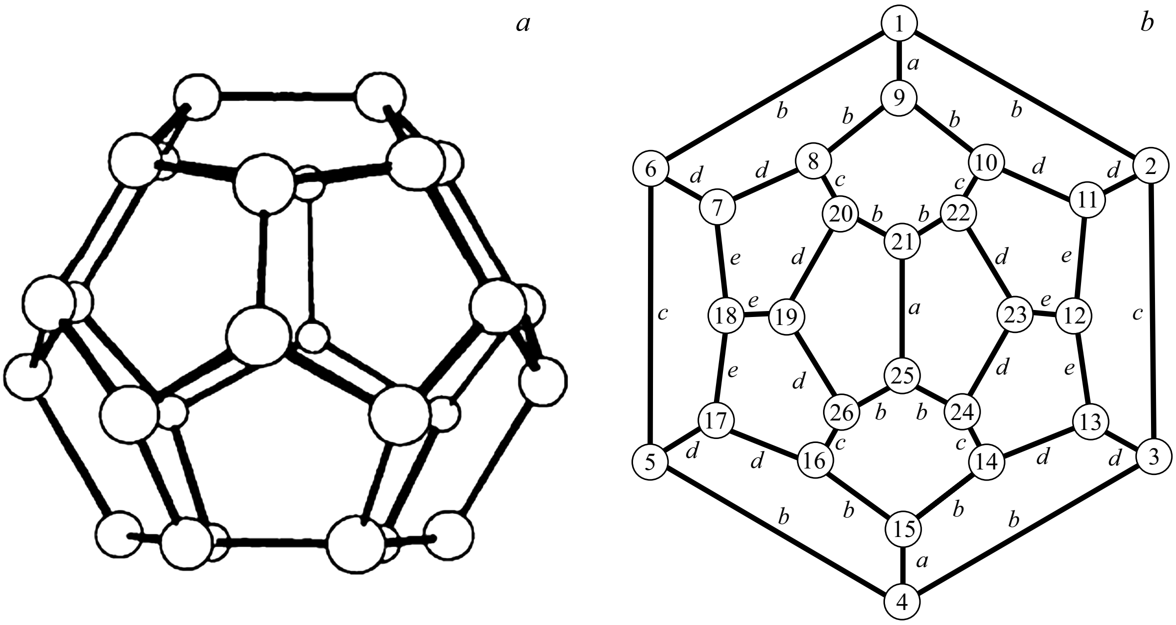

Figure 1. Fullerene C_{26} with the symmetry group D_{3h} and its Schlegel diagram showing the position of carbon atoms and bonds between carbon atoms.

integrals correspond to these bonds:

$$t_{1,9} = t_{4,15} = t_{21,25} = t_a,$$

$$t_{1,2} = t_{1,6} = t_{3,4} = t_{4,5} = t_{8,9} = t_{9,10} = t_{14,15} = t_{15,16}$$

$$= t_{20,21} = t_{21,22} = t_{24,25} = t_{25,26} = t_b,$$

$$t_{2,3} = t_{5,6} = t_{8,20} = t_{10,22} = t_{14,24} = t_{16,26} = t_c,$$

$$t_{2,11} = t_{3,13} = t_{5,17} = t_{6,7} = t_{7,8} = t_{10,11} = t_{13,14} = t_{16,17}$$

$$= t_{19,20} = t_{19,26} = t_{22,23} = t_{23,24} = t_d,$$

$$t_{7,18} = t_{11,12} = t_{12,13} = t_{12,23} = t_{17,18} = t_{18,19} = t_e. \qquad (2)$$

Using Hamiltonian (1), relations (2), and also the Schlegel diagram shown in Fig. 1, we write down the equations of motion for all creation operators $c^{+}_{f\sigma}(\tau)$ given in the Heisenberg representation

$$\begin{cases} \dfrac{dc^{+}_{1\sigma}}{d\tau} = \varepsilon_\sigma c^{+}_{1\sigma} + t_b(c^{+}_{2\sigma} + c^{+}_{6\sigma}) + t_a c^{+}_{9\sigma} + U c^{+}_{1\sigma} n_{1\bar{\sigma}}, \\ \dfrac{d(c^{+}_{1\sigma} n_{1\bar{\sigma}})}{d\tau} = (\varepsilon_\sigma + U) c^{+}_{1\sigma} n_{1\bar{\sigma}} + t_b(c^{+}_{2\sigma} n_{2\bar{\sigma}} + c^{+}_{6\sigma} n_{6\bar{\sigma}}) \\ \qquad + t_a c^{+}_{9\sigma} n_{9\bar{\sigma}}, \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \dfrac{dc^{+}_{26\sigma}}{d\tau} = \varepsilon_\sigma c^{+}_{26\sigma} + t_b c^{+}_{25\sigma} + t_c c^{+}_{16\sigma} + t_d c^{+}_{19\sigma} + U c^{+}_{26\sigma} n_{26\bar{\sigma}}, \\ \dfrac{d(c^{+}_{26\sigma} n_{26\bar{\sigma}})}{d\tau} = (\varepsilon_\sigma + U) c^{+}_{26\sigma} n_{26\bar{\sigma}} + t_b c^{+}_{25\sigma} n_{25\bar{\sigma}} \\ \qquad + t_c c^{+}_{16\sigma} n_{16\bar{\sigma}} + t_d c^{+}_{19\sigma}. \end{cases} \qquad (3)$$

The system of equations (3) is a closed system. Using the solution of this system of equations, we can calculate the Fourier transforms of the anticommutator Green's functions for all sites of the fullerene C_{26}:

$$\langle\langle c^{+}_{j\sigma}/c_{j\sigma}\rangle\rangle = \frac{i}{2\pi}\sum_{m=1}^{36}\frac{F_{j,m}}{E - E_m + ih},$$

$$E_k = \varepsilon + e_k, \quad E_{k+18} = E_k + U, \quad F_{j,m} = q_m Q_{j,m},$$

$$Q_{j,k+18} = Q_{j,k}, \quad k = 1\ldots 18, \qquad (4)$$

$$q_m = \begin{cases} 1 - \dfrac{n}{2}, & m = 1\ldots 18 \\ \dfrac{n}{2}, & m = 19\ldots 36 \end{cases}$$

where

$$Q_{x,1} = Q_{x,4} = Q_{x,5} = Q_{x,6} = Q_{x,7} = Q_{x,8} = Q_{x,9} = Q_{p,1}$$

$$= Q_{p,2} = Q_{p,3} = Q_{s,1} = Q_{s,2} = Q_{s,3} = Q_{s,4} = Q_{s,5}$$

$$= Q_{s,6} = Q_{s,14} = Q_{s,15} = Q_{s,16} = Q_{s,17} = Q_{s,18} = 0;$$

$$Q_{x,2} = \frac{\sqrt{(t_a - t_c)^2 + 8t_b^2} + t_c - t_a}{12\sqrt{(t_a - t_c)^2 + 8t_b^2}},$$

$$Q_{x,3} = \frac{\sqrt{(t_a - t_c)^2 + 8t_b^2} - t_c + t_a}{12\sqrt{(t_a - t_c)^2 + 8t_b^2}},$$

$$Q_{x,k} = \frac{1}{6}\,\frac{e_k^3 - e_k^2 t_c - e_k(2t_d^2 + 3t_e^2) + 3t_c t_e^2}{\begin{gathered}4e_k^3 - 3e_k^2(t_a + t_c) + 2(t_c t_a - 3t_e^2 - 2t_b^2 - 2t_d^2)e_k + \\ + 3t_e^2(t_a + t_c) + 2t_d^2 t_a\end{gathered}},$$

$$k = 10,\ 11,\ 12,\ 13;$$

$$Q_{x,k} = \frac{2}{3}\,\frac{e_k^4 - e_k^2(2t_d^2 + 2t_b^2 + t_c^2) + e_k t_c t_d^2 + 2t_d^2 t_b^2}{\begin{array}{c}5e_k^4 - 3e_k^2(2t_d^2 + t_c^2 + t_a^2 + 4t_b^2) + 2t_c t_d^2 e_k + t_c^2 t_a^2 + \\ + 4t_b^2 t_d^2 + 2t_a^2 t_d^2 + 2t_b^2 t_a t_c + 4t_b^4\end{array}},$$

$$k = 14,\ 15,\ 16,\ 17,\ 18;$$

$$Q_{y,1} = \frac{1}{12},$$

$$Q_{y,2} = \frac{\sqrt{(t_a - t_c)^2 + 8t_b^2} - t_c + t_a}{24\sqrt{(t_a - t_c)^2 + 8t_b^2}},$$

$$Q_{y,3} = \frac{\sqrt{(t_a - t_c)^2 + 8t_b^2} + t_c - t_a}{24\sqrt{(t_a - t_c)^2 + 8t_b^2}},$$

$$Q_{y,k} = \frac{1}{3}\,\frac{e_k^2 - t_d^2}{3e_k^2 - t_c^2 - 2t_d^2},\ \ k = 4,\ 5,\ 6,$$

$$Q_{y,k} = \frac{1}{12}\,\frac{e_k^2 - 3t_e^2}{3e_k^2 - 2t_c e_k - 3t_e^2 - 2t_d^2},\ \ k = 7,\ 8,\ 9,$$

$$Q_{y,k} = \frac{1}{12}\,\frac{(e_k^2 - 3t_e^2)(e_k - t_a)}{\begin{array}{c}4e_k^3 - 3e_k^2(t_a + t_c) + 2(t_c t_a - 3t_e^2 - 2t_b^2 - 2t_d^2)e_k + \\ + 3t_e^2(t_a + t_c) + 2t_d^2 t_a\end{array}},$$

$$k = 10,\ 11,\ 12,\ 13;$$

$$Q_{y,k} = \frac{2}{3}\,\frac{e_k^4 - e_k^2(2t_b^2 + t_a^2 + t_d^2) + t_d^2 t_a^2}{\begin{array}{c}5e_k^4 - 3e_k^2(2t_d^2 + t_c^2 + t_a^2 + 4t_b^2) + 2t_c t_d^2 e_k + t_c^2 t_a^2 + \\ + 4t_b^2 t_d^2 + 2t_a^2 t_d^2 + 2t_b^2 t_a t_c + 4t_b^4\end{array}},$$

$$k = 14,\ 15,\ 16,\ 17,\ 18;$$

$$Q_{p,k} = \frac{1}{3}\,\frac{e_k^2 - t_c^2}{3e_k^2 - t_c^2 - 2t_d^2},\ \ k = 4,\ 5,\ 6,$$

$$Q_{p,k} = \frac{1}{6}\,\frac{e_k(e_k - t_c)}{3e_k^2 - 2t_c e_k - 3t_e^2 - 2t_d^2},\ \ k = 7,\ 8,\ 9,$$

$$Q_{p,k} = \frac{1}{6}\,\frac{e_k(e_k^2 - (t_a + t_c)e_k + t_a t_c - 2t_b^2)}{\begin{array}{c}4e_k^3 - 3e_k^2(t_a + t_c) + 2(t_c t_a - 3t_e^2 - 2t_b^2 - 2t_d^2)e_k + \\ + 3t_e^2(t_a + t_c) + 2t_d^2 t_a\end{array}},$$

$$k = 10,\ 11,\ 12,\ 13;$$

$$Q_{p,k} = \frac{1}{3}\,\frac{e_k^4 - e_k^2(4t_b^2 + t_a^2 + t_c^2) + t_c^2 t_a^2 + 4t_b^4 - 2t_b^2 t_a t_c}{\begin{array}{c}5e_k^4 - 3e_k^2(2t_d^2 + t_c^2 + t_a^2 + 4t_b^2) + 2t_c t_d^2 e_k + t_c^2 t_a^2 + \\ + 4t_b^2 t_d^2 + 2t_a^2 t_d^2 + 2t_b^2 t_a t_c + 4t_b^4\end{array}},$$

$$k = 14,\ 15,\ 16,\ 17,\ 18;$$

$$Q_{s,k} = \frac{1}{2}\,\frac{e_k^2 - e_k t_c - 2t_d^2}{3e_k^2 - 2t_c e_k - 3t_e^2 - 2t_d^2},\ \ k = 7,\ 8,\ 9,$$

$$Q_{s,k} = \frac{1}{2}\,\frac{e_k^3 - e_k^2(t_a + t_c) + e_k(t_a t_c - 2t_b^2 - 2t_d^2) + 2t_a t_d^2}{\begin{array}{c}4e_k^3 - 3e_k^2(t_a + t_c) + 2(t_c t_a - 3t_e^2 - 2t_b^2 - 2t_d^2)e_k + \\ + 3t_e^2(t_a + t_c) + 2t_d^2 t_a\end{array}},$$

$$k = 10,\ 11,\ 12,\ 13;$$

$$x \in G_1,\ \ y \in G_2,\ \ p \in G_3,\ \ s \in G_4,$$

$$e_1 = t_c,$$

$$e_2 = -\frac{t_a + t_c}{2} + \frac{1}{2}\sqrt{(t_a - t_c)^2 + 8t_b^2},$$

$$e_3 = -\frac{t_a + t_c}{2} - \frac{1}{2}\sqrt{(t_a - t_c)^2 + 8t_b^2},$$

$$e_4 = \frac{2}{\sqrt{3}}\sqrt{t_c^2 + 2t_d^2}\,\sin\left(\frac{\pi}{6} + \frac{\varphi_3}{3}\right),$$

$$e_5 = \frac{2}{\sqrt{3}}\sqrt{t_c^2 + 2t_d^2}\,\cos\left(\frac{\varphi_3 + \pi}{3}\right),$$

$$e_6 = -\frac{2}{\sqrt{3}}\sqrt{t_c^2 + 2t_d^2}\,\cos\left(\frac{\varphi_3}{3}\right),$$

$$e_7 = \frac{t_c}{3} + \frac{2}{3}\sqrt{t_c^2 + 6t_d^2 + 9t_e^2}\,\cos\left(\frac{\varphi_2}{3}\right),$$

$$e_8 = \frac{t_c}{3} - \frac{2}{3}\sqrt{t_c^2 + 6t_d^2 + 9t_e^2}\,\cos\left(\frac{\varphi_2 + \pi}{3}\right),$$

$$e_9 = \frac{t_c}{3} - \frac{2}{3}\sqrt{t_c^2 + 6t_d^2 + 9t_e^2}\,\cos\left(\frac{\pi}{6} + \frac{\varphi_2}{3}\right),$$

$$e_{10} = \frac{1}{4}\Bigg(t_c + t_a + 2\sqrt{A}$$

$$+\sqrt{8A + \frac{(t_c + t_a)((t_c - t_a)^2 + 8t_b^2 - 12t_e^2) + 8t_d^2(t_c - t_a)}{\sqrt{A}} - 12z}\Bigg),$$

$$e_{11} = \frac{1}{4}\Bigg(t_c + t_a + 2\sqrt{A}$$

$$-\sqrt{8A + \frac{(t_c + t_a)((t_c - t_a)^2 + 8t_b^2 - 12t_e^2) + 8t_d^2(t_c - t_a)}{\sqrt{A}} - 12z}\Bigg),$$

$$e_{12} = \frac{1}{4}\Bigg(t_c + t_a - 2\sqrt{A}$$

$$+\sqrt{8A - \frac{(t_c + t_a)((t_c - t_a)^2 + 8t_b^2 - 12t_e^2) + 8t_d^2(t_c - t_a)}{\sqrt{A}} - 12z}\Bigg),$$

$$e_{13} = \frac{1}{4}\Bigg(t_c + t_a - 2\sqrt{A}$$

$$-\sqrt{8A - \frac{(t_c + t_a)((t_c - t_a)^2 + 8t_b^2 - 12t_e^2) + 8t_d^2(t_c - t_a)}{\sqrt{A}} - 12z}\Bigg),$$

$$e_{14} = x_1,$$

$$e_{15} = x_2,$$

$$e_{16} = x_3,$$

$$e_{17} = x_4,$$

$$e_{18} = x_5,$$

$$A = \frac{t_a^2}{4} - \frac{t_a t_c}{6} + \frac{t_c^2}{4} + \frac{4t_d^2}{3} + \frac{4t_b^2}{3} + 2t_e^2 + z,$$

$$z = \frac{2}{3}\,\big[4(t_d^2 + t_b^2 + 3t_e^2)(t_d^2 + t_b^2 - t_c t_a)$$

$$+ t_a\big(6t_d^2(t_c + t_a) + t_a t_c^2\big) + 3t_e^2\big(24t_b^2 + 2t_c t_a + 3t_e^2$$

$$+ 3(t_c - t_a)^2\big)\big]^{1/2}\cos\left(\frac{\pi}{3} - \frac{\varphi_1}{3}\right),$$

$$\begin{aligned}\varphi_1 = \arccos\Big\{\frac{1}{2}\big[\big(2(2t_d^2+2t_b^2-t_ct_a+3t_e^2)^2\\ +27\big((t_c+t_a)^2+8t_ct_a-16t_b^2\big)t_e^2+18(t_c+t_a)t_d^2t_a\big)\\ \times(2t_d^2+2t_b^2-t_ct_a+3t_e^2)-27\big(3(t_c+t_a)t_e^2+2t_d^2t_a\big)^2\\ +81t_e^2(t_ct_a-2t_b^2)(t_c+t_a)^2\big]\big[6t_a(t_c+t_a)t_d^2\\ +(2t_d^2+2t_b^2-t_ct_a+3t_e^2)^2\\ +9t_e^2\big(8t_b^2+(t_c-t_a)^2\big)\big]^{(-3/2)}\Big\},\end{aligned}$$

$$\varphi_2 = \arccos\left(\frac{t_c(t_c^2+9t_d^2-27t_e^2)}{(t_c^2+6t_d^2+9t_e^2)^{3/2}}\right),$$

$$\varphi_3 = \arccos\left(\frac{3^{3/2}t_d^2t_c}{2(t_c^2+2t_d^2)^{3/2}}\right),$$

where x_1, x_2, x_3, x_4, x_5 are the roots of the following equation

$$\begin{aligned}x^5-(t_a^2+4t_b^2+t_c^2+2t_d^2)x^3+t_d^2t_cx^2+(4t_d^2t_b^2+4t_b^4\\ +t_a^2t_c^2+2t_a^2t_d^2+2t_b^2t_ct_a)x-4t_d^2t_b^2t_a-t_a^2t_d^2t_c=0. \quad (6)\end{aligned}$$

The values E_m, which are included into relation (4) are the poles of the Fourier transform of the anticommutator Green's function, which, as it is known [24], correspond to the energy states of a quantum system. Consequently the values E_m, which are included into the Green's function (4), determine the energy spectrum of the fullerene C_{26} with the symmetry group D_{3h}.

The energy states of the fullerene C_{26} with the symmetry group D_{3h} can be classified according to the irreducible representations of the group D_{3h}, which, as it is known [25], has four one-dimensional irreducible representations a_1', a_1'', a_2', a_2'' and two two-dimensional irreducible representations e', e''. It can be shown that the energy states of fullerene C_{26}, determined by the poles of the Green's function (4), are related to the irreducible representations of the group D_{3h} in the following way:

$E_1(a_1'')$, $E_2(a_2')$, $E_3(a_2')$, $E_4(e'')$, $E_5(e'')$, $E_6(e'')$, $E_7(a_2'')$, $E_8(a_2'')$, $E_9(a_2'')$, $E_{10}(a_1')$, $E_{11}(a_1')$, $E_{12}(a_1')$, $E_{13}(a_1')$, $E_{14}(e')$, $E_{15}(e')$, $E_{16}(e')$, $E_{17}(e')$, $E_{18}(e')$, $E_{19}(a_1'')$, $E_{20}(a_2')$, $E_{21}(a_2')$, $E_{22}(e'')$, $E_{23}(e'')$, $E_{24}(e'')$, $E_{25}(a_2'')$, $E_{26}(a_2'')$, $E_{27}(a_2'')$, $E_{28}(a_1')$, $E_{29}(a_1')$, $E_{30}(a_1')$, $E_{31}(a_1')$, $E_{32}(e')$, $E_{33}(e')$, $E_{34}(e')$, $E_{35}(e')$, $E_{36}(e')$.

As it is known, the energy levels of a quantum system, in addition to the energy value, are also characterized by the degree of degeneracy, which can be found using the following relation [17,18]:

$$g_i = \sum_{j=1}^{N} Q_{j,i}, \quad (7)$$

where N — the number of sites in the nanosystem.

In order to obtain numerical values for the degrees of degeneracy of the energy levels of the fullerene C_{26}, we substitute into formula (7) the values $Q_{j,i}$, which are included into the Green's function (4):

$$\begin{aligned}g_1 = g_2 = g_3 = g_7 = g_8 = g_9 = g_{10} = g_{11}\\ = g_{12} = g_{13} = g_{19} = g_{20} = g_{21} = g_{25} = g_{26}\\ = g_{27} = g_{28} = g_{29} = g_{30} = g_{31} = 1,\\ g_4 = g_5 = g_6 = g_{14} = g_{15} = g_{16} = g_{17} = g_{18} = g_{22}\\ = g_{23} = g_{24} = g_{32} = g_{33} = g_{34} = g_{35} = g_{36} = 2. \quad (8)\end{aligned}$$

Thus, the quantities E_m, which are included into the Green's function (4) and the quantities g_m from (8) describe the energy spectrum of the fullerene C_{26} with the symmetry group D_{3h} in Hubbard model in the static fluctuation approximation. It follows from these relations that the energy spectrum of fullerene C_{26} with the symmetry group D_{3h} consists of 36 energy states, among which 20 energy states are not degenerate, and 16 energy states are doubly degenerate.

3. Results discussion

The studies carried out in the study [15] have shown, that the distances between carbon atoms in fullerene C_{26} with the symmetry group D_{3h} have the following values:

$$\begin{aligned}x_a = 1.540\,\text{Å},\ x_b = 1.428\,\text{Å},\ x_c = 1.450\,\text{Å},\\ x_d = 1.473\,\text{Å}, \quad x_e = 1.410\,\text{Å}. \quad (9)\end{aligned}$$

In order to obtain numerical values for the energy spectrum of the fullerene C_{26}, it is necessary to find the numerical values for the transfer integrals, which correspond to this fullerene. For this we will use the following relation [18,21]:

$$t_s = -8.17065\exp(-1.69521x_s). \quad (10)$$

Substituting (9) into relation (10), we obtain the numerical values for the transport integrals for the fullerene C_{26} with the symmetry group D_{3h}:

$$\begin{aligned}t_a = -0.60045\,\text{eV},\ t_b = -0.72600\,\text{eV},\ t_c = -0.69942\,\text{eV},\\ t_d = -0.67268\,\text{eV}, \quad t_e = -0.74849\,\text{eV}. \quad (11)\end{aligned}$$

As can be seen from the Green's function (4), the relation describing the energy spectrum of the fullerene C_{26} can be written as follows:

$$E_k = \varepsilon + \frac{U}{2} + \bar{e}_k, \quad (12)$$

Table 1. Energy spectrum of fullerene C_{26} with symmetry group D_{3h}: values of levels energy, multiplicity of their degeneracy and irreducible representations of the group D_{3h}, to which they belong

№	e_j, eV	E_j, eV	g_j	$E(\Gamma_j)$	№	e_j, eV	E_j, eV	g_j	$E(\Gamma_j)$
1	−4.930	−9.923	1	$E_{13}(a_1')$	19	0.732	−4.261	1	$E_{31}(a_1')$
2	−4.612	−9.605	1	$E_9(a_2'')$	20	1.050	−3.943	1	$E_{27}(a_2'')$
3	−4.479	−9.472	2	$E_{18}(e')$	21	1.183	−3.810	2	$E_{36}(e')$
4	−3.906	−8.899	1	$E_{12}(a_1')$	22	1.756	−3.237	1	$E_{30}(a_1')$
6	−3.876	−8.869	2	$E_6(e'')$	23	1.786	−3.207	2	$E_{24}(e'')$
5	−3.752	−8.745	2	$E_{17}(e')$	24	1.910	−3.083	2	$E_{35}(e')$
8	−3.266	−8.259	1	$E_8(a_2'')$	25	2.396	−2.597	1	$E_{26}(a_2'')$
7	−3.209	−8.202	1	$E_3(a_2')$	26	2.453	−2.540	1	$E_{21}(a_2')$
9	−3.071	−8.064	2	$E_{16}(e')$	27	2.591	−2.402	2	$E_{34}(e')$
10	−3.067	−8.060	2	$E_5(e'')$	28	2.595	−2.398	2	$E_{23}(e'')$
11	−2.531	−7.524	1	$E_{11}(a_1')$	29	3.131	−1.862	1	$E_{29}(a_1')$
12	−2.132	−7.125	1	$E_1(a_1'')$	30	3.530	−1.463	1	$E_{19}(a_1'')$
13	−1.712	−6.705	2	$E_{14}(e')$	31	3.950	−1.043	2	$E_{32}(e')$
14	−1.550	−6.543	2	$E_4(e'')$	32	4.112	−0.881	2	$E_{22}(e'')$
16	−1.314	−6.307	1	$E_7(a_2'')$	33	4.348	−0.645	1	$E_{25}(a_2'')$
15	−1.257	−6.250	1	$E_{10}(a_1')$	34	4.405	−0.588	1	$E_{28}(a_1')$
17	−1.153	−6.146	1	$E_2(a_2')$	35	4.509	−0.484	1	$E_{20}(a_2')$
18	−1.142	−6.135	2	$E_{15}(e')$	36	4.520	−0.473	2	$E_{33}(e')$

Table 2. Energy spectrum of endofullerene $U@C_{26}$ with symmetry group D_{3h}: values of levels energy, multiplicity of their degeneracy and irreducible representations of the group D_{3h}, to which they belong

№	e_j, eV	E_j, eV	g_j	$E(\Gamma_j)$	№	e_j, eV	E_j, eV	g_j	$E(\Gamma_j)$
1	−4.803	−9.796	1	$E_{13}(a_1')$	19	0.859	−4.134	1	$E_{31}(a_1')$
2	−4.518	−9.511	1	$E_9(a_2'')$	20	1.144	−3.849	1	$E_{27}(a_2'')$
3	−4.370	−9.363	2	$E_{18}(e')$	21	1.292	−3.701	2	$E_{36}(e')$
4	−3.867	−8.860	1	$E_{12}(a_1')$	22	1.795	−3.198	1	$E_{30}(a_1')$
6	−3.808	−8.801	2	$E_6(e'')$	23	1.854	−3.139	2	$E_{24}(e'')$
5	−3.676	−8.669	2	$E_{17}(e')$	24	1.986	−3.007	2	$E_{35}(e')$
8	−3.250	−8.243	1	$E_8(a_2'')$	25	2.412	−2.581	1	$E_{26}(a_2'')$
7	−3.138	−8.131	1	$E_3(a_2')$	26	2.524	−2.469	1	$E_{21}(a_2')$
9	−3.073	−8.066	2	$E_{16}(e')$	27	2.589	−2.404	2	$E_{34}(e')$
10	−3.052	−8.045	2	$E_5(e'')$	28	2.610	−2.383	2	$E_{23}(e'')$
11	−2.585	−7.578	1	$E_{11}(a_1')$	29	3.077	−1.916	1	$E_{29}(a_1')$
12	−2.173	−7.166	1	$E_1(a_1'')$	30	3.489	−1.504	1	$E_{19}(a_1'')$
13	−1.774	−6.767	2	$E_{14}(e')$	31	3.888	−1.105	2	$E_{32}(e')$
14	−1.632	−6.625	2	$E_4(e'')$	32	4.030	−0.963	2	$E_{22}(e'')$
16	−1.383	−6.376	1	$E_7(a_2'')$	33	4.279	−0.714	1	$E_{25}(a_2'')$
15	−1.336	−6.329	1	$E_{10}(a_1')$	34	4.326	−0.667	1	$E_{28}(a_1')$
17	−1.262	−6.255	2	$E_{15}(e')$	35	4.400	−0.593	2	$E_{33}(e')$
18	−1.257	−6.250	1	$E_2(a_2')$	36	4.405	−0.588	1	$E_{20}(a_2')$

where $\bar{e}_k$ — energy of the k- energy level relative to the energy $\varepsilon + U/2$:

$$\bar{e}_k = \begin{cases} e_k - \frac{U}{2}, & k = 1 \ldots 18, \\ e_{k-18} + \frac{U}{2}, & k = 19 \ldots 36. \end{cases} \tag{13}$$

Using relations (13), (5) and (11), as well as $U = 5.662\,\text{eV}$ [17], we will obtain the numerical values for the values $\bar{e}_k$, which are given in Table 1. Substituting $\bar{e}_k$ from Table 1, as well as $\varepsilon = -7.824\,\text{eV}$, $U = 5.662\,\text{eV}$ [17] into relation (12) we obtain the energy spectrum of the fullerene C_{26} with the symmetry group D_{3h}. The calculation results are given in Table 1, as well as in Fig. 2. As can be seen from relations (12), (13) and Fig. 2, the energy states of fullerene C_{26} form two Hubbard subbands. The energy states forming the lower Hubbard subband are concentrated near the energy ε, and the energy states forming the upper Hubbard subband are concentrated near the energy $\varepsilon + U$.

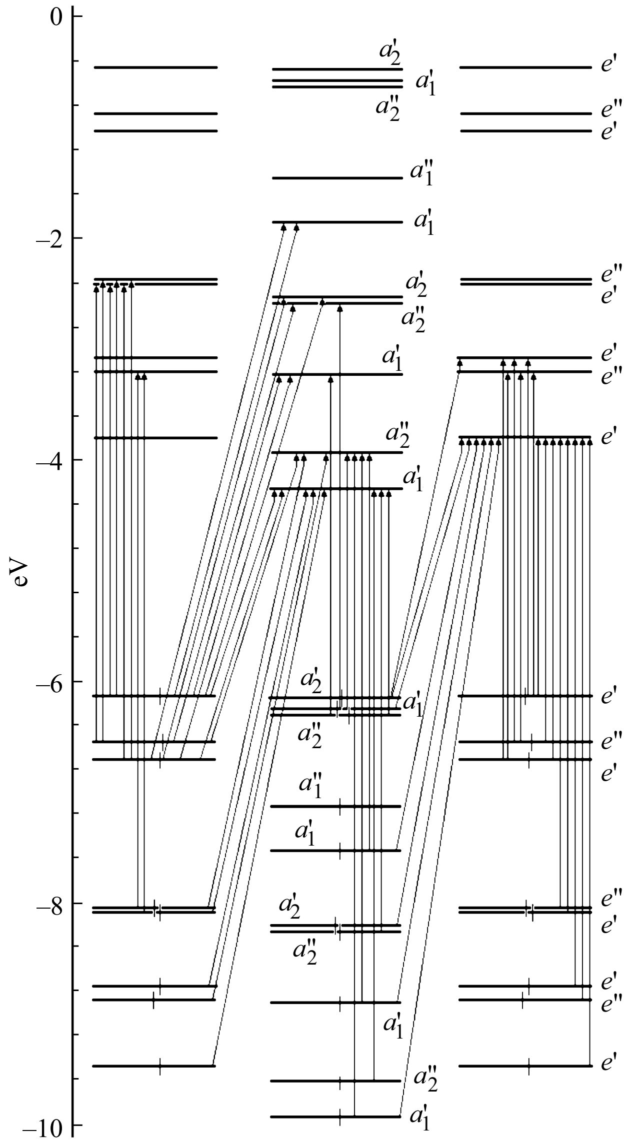

Figure 2. Energy spectrum of fullerene C_{26} with symmetry group D_{3h}.

Let us now consider an endohedral fullerene U@C_{26}. The studies have shown [15], that the endohedral fullerene U@C_{26} has a symmetry group D_{3h}, and the distances between carbon atoms in this molecule have the following values:

$$x_a = 1.531\,\text{Å},\ x_b = 1.480\,\text{Å},\ x_c = 1.486\,\text{Å},$$
$$x_d = 1.514\,\text{Å},\quad x_e = 1.433\,\text{Å}. \tag{14}$$

Now, in order to obtain numerical values for the transfer integrals for the molecule U@C_{26}, we substitute (14) into relation (10):

$$t_a = -0.60968\,\text{eV},\ t_b = -0.66474\,\text{eV},\ t_c = -0.65801\,\text{eV},$$
$$t_d = -0.62751\,\text{eV},\quad t_e = -0.71987\,\text{eV}. \tag{15}$$

Substituting the numerical values for ε, U and the transfer integrals (15) into relations (5), (13) and (12), we obtain for the molecule U@C_{26} numerical values for the quantities $\bar{e}_k$ and E_k, which are given in Table 2. In Fig. 2, Fig. 3, Table 1 and Table 2 we can see, that the energy spectra of molecules C_{26} and U@C_{26} differ from each other in the relative position of the energy states $E_2(a_2')$, $E_{15}(e')$ and $E_{20}(a_2')$, $E_{33}(e')$. It is believed that when a metal atom is introduced into the fullerene, no significant change in its energy levels occurs. In this case, in the first approximation, it is assumed that upon the implantation of a metal atom, the valence electrons of this atom are transferred to the core of fullerene [26]. When the endohedral fullerene U@C_{26} is formed, four valence electrons of the Uranium atom pass into the shell of the fullerene C_{26} and, as can be seen from Fig. 3, occupy levels $E_{31}(a_1')$, $E_{27}(a_2'')$ and $E_{36}(e')$.

One of the most important characteristics of a quantum system is its optical absorption spectrum. Let us find the transitions that determine the optical spectra of the fullerene C_{26} and the endohedral fullerene U@C_{26} with the symmetry group D_{3h}. To do this, we will use the energy spectra of these molecules, and using the group theory [27], we will find, which transitions from the point of view of

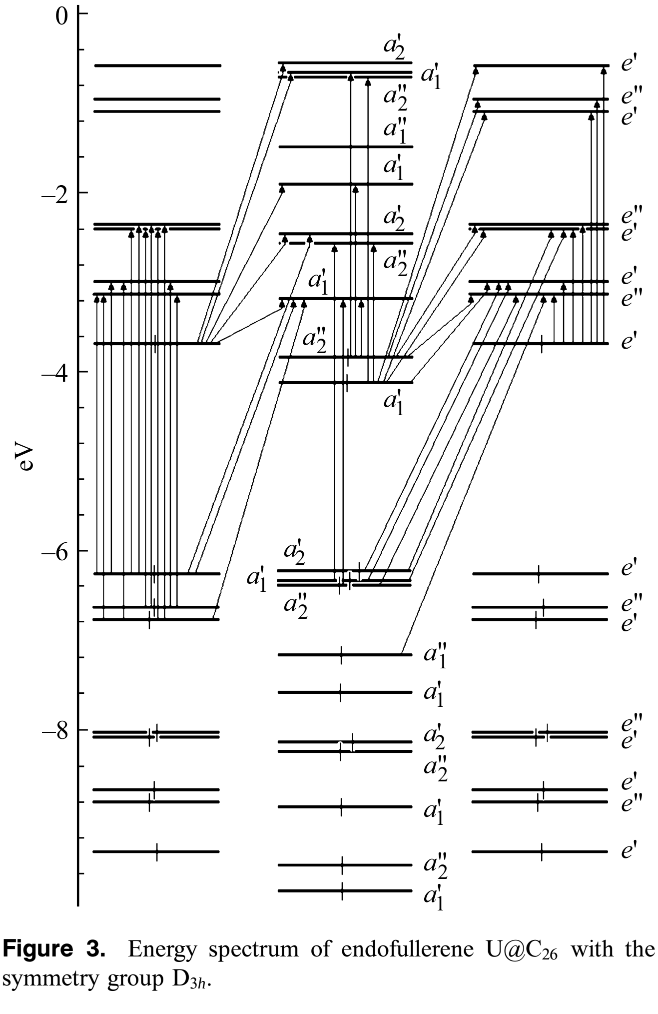

Figure 3. Energy spectrum of endofullerene U@C_{26} with the symmetry group D_{3h}.

Table 3. Allowed transitions in the energy spectrum of fullerene C_{26}

№	ΔE	ΔE, eV	№	ΔE	ΔE, eV	№	ΔE	ΔE, eV	№	ΔE	ΔE, eV
1	$E_{31}-E_{15}$	1.874	45	$E_{36}-E_{3}$	4.392	89	$E_{35}-E_{17}$	5.662	133	$E_{32}-E_{5}$	7.018
2	$E_{31}-E_{7}$	2.046	46	$E_{35}-E_{11}$	4.441	90	$E_{32}-E_{14}$	5.662	134	$E_{32}-E_{16}$	7.021
3	$E_{27}-E_{10}$	2.307	47	$E_{29}-E_{7}$	4.446	91	$E_{23}-E_{5}$	5.662	135	$E_{33}-E_{11}$	7.051
4	$E_{36}-E_{15}$	2.325	48	$E_{31}-E_{17}$	4.483	92	$E_{36}-E_{18}$	5.662	136	$E_{34}-E_{18}$	7.071
5	$E_{36}-E_{2}$	2.336	49	$E_{21}-E_{1}$	4.585	93	$E_{23}-E_{16}$	5.665	137	$E_{23}-E_{18}$	7.074
6	$E_{24}-E_{4}$	3.336	50	$E_{19}-E_{2}$	4.684	94	$E_{33}-E_{2}$	5.673	138	$E_{32}-E_{3}$	7.159
7	$E_{36}-E_{10}$	2.440	51	$E_{23}-E_{1}$	4.726	95	$E_{28}-E_{7}$	5.719	139	$E_{22}-E_{5}$	7.180
8	$E_{31}-E_{14}$	2.443	52	$E_{30}-E_{16}$	4.827	96	$E_{33}-E_{10}$	5.777	140	$E_{22}-E_{16}$	7.183
9	$E_{27}-E_{4}$	2.600	53	$E_{29}-E_{14}$	4.843	97	$E_{35}-E_{6}$	5.786	141	$E_{23}-E_{9}$	7.206
10	$E_{36}-E_{4}$	2.733	54	$E_{24}-E_{5}$	4.854	98	$E_{34}-E_{3}$	5.800	142	$E_{26}-E_{13}$	7.326
11	$E_{36}-E_{14}$	2.895	55	$E_{24}-E_{16}$	4.857	99	$E_{35}-E_{12}$	5.816	143	$E_{22}-E_{8}$	7.378
12	$E_{30}-E_{15}$	2.899	56	$E_{27}-E_{6}$	4.926	100	$E_{22}-E_{14}$	5.824	144	$E_{19}-E_{6}$	7.406
13	$E_{24}-E_{15}$	2.929	57	$E_{26}-E_{11}$	4.927	101	$E_{23}-E_{8}$	5.861	145	$E_{25}-E_{5}$	7.415
14	$E_{35}-E_{15}$	3.052	58	$E_{36}-E_{17}$	4.935	102	$E_{25}-E_{4}$	5.898	146	$E_{28}-E_{16}$	7.475
15	$E_{35}-E_{2}$	3.064	59	$E_{27}-E_{12}$	4.956	103	$E_{27}-E_{13}$	5.981	147	$E_{34}-E_{13}$	7.522
16	$E_{30}-E_{7}$	3.071	60	$E_{35}-E_{5}$	4.978	104	$E_{33}-E_{4}$	6.070	148	$E_{20}-E_{16}$	7.579
17	$E_{24}-E_{7}$	3.101	61	$E_{35}-E_{16}$	4.981	105	$E_{36}-E_{13}$	6.113	149	$E_{33}-E_{5}$	7.587
18	$E_{35}-E_{10}$	3.167	62	$E_{30}-E_{8}$	5.023	106	$E_{28}-E_{14}$	6.117	150	$E_{33}-E_{16}$	7.590
19	$E_{35}-E_{4}$	3.460	63	$E_{24}-E_{8}$	5.053	107	$E_{29}-E_{16}$	6.202	151	$E_{29}-E_{18}$	7.610
20	$E_{30}-E_{14}$	3.468	64	$E_{36}-E_{6}$	5.059	108	$E_{21}-E_{17}$	6.205	152	$E_{28}-E_{8}$	7.671
21	$E_{24}-E_{14}$	3.498	65	$E_{19}-E_{4}$	5.080	109	$E_{20}-E_{14}$	6.221	153	$E_{32}-E_{17}$	7.702
22	$E_{27}-E_{11}$	3.581	66	$E_{36}-E_{12}$	5.089	110	$E_{33}-E_{14}$	6.232	154	$E_{33}-E_{3}$	7.729
23	$E_{21}-E_{15}$	3.595	67	$E_{32}-E_{15}$	5.092	111	$E_{30}-E_{18}$	6.235	155	$E_{29}-E_{9}$	7.743
24	$E_{35}-E_{14}$	3.622	68	$E_{32}-E_{2}$	5.103	112	$E_{22}-E_{1}$	6.244	156	$E_{32}-E_{6}$	7.826
25	$E_{26}-E_{10}$	3.653	69	$E_{35}-E_{3}$	5.119	113	$E_{24}-E_{18}$	6.265	157	$E_{32}-E_{12}$	7.856
26	$E_{36}-E_{11}$	3.714	70	$E_{34}-E_{11}$	5.122	114	$E_{26}-E_{6}$	6.271	158	$E_{22}-E_{17}$	7.864
27	$E_{34}-E_{15}$	3.734	71	$E_{32}-E_{10}$	5.207	115	$E_{26}-E_{12}$	6.301	159	$E_{22}-E_{6}$	7.988
28	$E_{23}-E_{15}$	3.737	72	$E_{31}-E_{18}$	5.211	116	$E_{34}-E_{17}$	6.343	160	$E_{28}-E_{17}$	8.157
29	$E_{34}-E_{2}$	3.745	73	$E_{22}-E_{15}$	5.254	117	$E_{23}-E_{17}$	6.346	161	$E_{25}-E_{6}$	8.223
30	$E_{34}-E_{10}$	3.849	74	$E_{31}-E_{9}$	5.343	118	$E_{30}-E_{9}$	6.368	162	$E_{25}-E_{12}$	8.253
31	$E_{31}-E_{16}$	3.802	75	$E_{22}-E_{7}$	5.426	119	$E_{35}-E_{18}$	6.389	163	$E_{20}-E_{17}$	8.260
32	$E_{23}-E_{7}$	3.909	76	$E_{26}-E_{5}$	5.463	120	$E_{29}-E_{8}$	6.397	164	$E_{33}-E_{17}$	8.272
33	$E_{24}-E_{1}$	3.918	77	$E_{32}-E_{4}$	5.500	121	$E_{24}-E_{9}$	6.398	165	$E_{33}-E_{6}$	8.395
34	$E_{26}-E_{4}$	3.946	78	$E_{30}-E_{17}$	5.508	122	$E_{34}-E_{6}$	6.467	166	$E_{33}-E_{12}$	8.425
35	$E_{31}-E_{8}$	3.998	79	$E_{21}-E_{16}$	5.524	123	$E_{23}-E_{6}$	6.470	167	$E_{32}-E_{18}$	8.429
36	$E_{27}-E_{5}$	4.118	80	$E_{24}-E_{17}$	5.538	124	$E_{32}-E_{11}$	6.481	168	$E_{22}-E_{18}$	8.591
37	$E_{34}-E_{4}$	4.141	81	$E_{28}-E_{15}$	5.547	125	$E_{34}-E_{12}$	6.497	169	$E_{22}-E_{9}$	8.724
38	$E_{23}-E_{4}$	4.144	82	$E_{25}-E_{10}$	5.605	126	$E_{20}-E_{1}$	6.540	170	$E_{32}-E_{13}$	8.881
39	$E_{21}-E_{14}$	4.165	83	$E_{20}-E_{15}$	5.651	127	$E_{19}-E_{5}$	6.598	171	$E_{28}-E_{18}$	8.884
40	$E_{36}-E_{5}$	4.250	84	$E_{34}-E_{5}$	5.659	128	$E_{19}-E_{3}$	6.739	172	$E_{20}-E_{18}$	8.988
41	$E_{36}-E_{16}$	4.253	85	$E_{24}-E_{6}$	5.662	129	$E_{35}-E_{13}$	6.841	173	$E_{33}-E_{18}$	8.999
42	$E_{29}-E_{15}$	4.273	86	$E_{34}-E_{16}$	5.662	130	$E_{25}-E_{11}$	6.878	174	$E_{28}-E_{9}$	9.017
43	$E_{34}-E_{14}$	4.303	87	$E_{22}-E_{4}$	5.662	131	$E_{29}-E_{17}$	6.883	175	$E_{25}-E_{13}$	9.278
44	$E_{2}3-E_{14}$	4.306	88	$E_{33}-E_{15}$	5.662	132	$E_{21}-E_{18}$	6.932	176	$E_{33}-E_{13}$	9.450

symmetry in molecules C_{26} and $U@C_{26}$ are allowed and which are prohibited. It can be shown, that the following transitions are allowed in the energy spectrum of a molecule with the symmetry group D_{3h}:

$$a'_1 \leftrightarrow e',\ a'_2 \leftrightarrow e',\ e' \leftrightarrow e',$$

$$a''_1 \leftrightarrow e'',\ a''_2 \leftrightarrow e'',\ e'' \leftrightarrow e'',$$

$$a'_1 \leftrightarrow a''_2,\ a'_2 \leftrightarrow a''_1,\ e' \leftrightarrow e''. \qquad (16)$$

From the Green's function (4), Fig. 2, Fig. 3 and selection rules (16) it follows that fullerene C_{26} has 176 allowed transitions, and the endohedral fullerene $U@C_{26}$ has 171 allowed transitions, which are presented in Table 3 and Table 4. The remaining transitions are considered prohibited. The different number of allowed C_{26} and $U@C_{26}$ transitions is due to the fact that, as can be seen from Fig. 2 and Fig. 3, when an uranium atom is inserted into fullerene C_{26} four valence electrons are transferred from the uranium atom to the fullerene C_{26} and fill four lower free

Table 4. Allowed transitions in the energy spectrum of endofullerene $U@C_{26}$

№	ΔE	ΔE, eV	№	ΔE	ΔE, eV	№	ΔE	ΔE, eV	№	ΔE	ΔE, eV
1	$E_{30} - E_{36}$	0.503	44	$E_{24} - E_{1}$	4.027	87	$E_{22} - E_{4}$	5.662	130	$E_{34} - E_{18}$	6.960
2	$E_{24} - E_{36}$	0.562	45	$E_{26} - E_{4}$	4.045	88	$E_{32} - E_{14}$	5662	131	$E_{23} - E_{18}$	6.980
3	$E_{30} - E_{27}$	0.651	46	$E_{34} - E_{4}$	4.222	89	$E_{33} - E_{15}$	5.662	132	$E_{33} - E_{11}$	6.985
4	$E_{35} - E_{36}$	0.695	47	$E_{23} - E_{4}$	4.242	90	$E_{24} - E_{6}$	5.662	133	$E_{32} - E_{3}$	7.025
5	$E_{24} - E_{27}$	0.709	48	$E_{21} - E_{14}$	4.299	91	$E_{20} - E_{15}$	5.667	134	$E_{22} - E_{5}$	7.082
6	$E_{35} - E_{31}$	1.128	49	$E_{29} - E_{15}$	4.339	92	$E_{23} - E_{16}$	5.682	135	$E_{22} - E_{16}$	7.102
7	$E_{21} - E_{36}$	1.233	50	$E_{34} - E_{14}$	4.364	93	$E_{28} - E_{7}$	5.709	136	$E_{23} - E_{9}$	7.128
8	$E_{34} - E_{36}$	1.298	51	$E_{23} - E_{14}$	4.384	94	$E_{34} - E_{3}$	5.727	137	$E_{26} - E_{13}$	7.215
9	$E_{23} - E_{36}$	1.318	52	$E_{29} - E_{7}$	4.460	95	$E_{33} - E_{10}$	5.736	138	$E_{22} - E_{8}$	7.279
10	$E_{23} - E_{27}$	1.466	53	$E_{35} - E_{11}$	4.572	96	$E_{35} - E_{6}$	5.795	139	$E_{19} - E_{6}$	7.297
11	$E_{26} - E_{31}$	1.553	54	$E_{21} - E_{1}$	4.697	97	$E_{22} - E_{14}$	5.804	140	$E_{25} - E_{5}$	7.331
12	$E_{34} - E_{31}$	1.730	55	$E_{19} - E_{2}$	4.746	98	$E_{35} - E_{12}$	5.853	141	$E_{34} - E_{13}$	7.392
13	$E_{29} - E_{36}$	1.785	56	$E_{23} - E_{1}$	4.783	99	$E_{25} - E_{4}$	5.911	142	$E_{28} - E_{16}$	7.398
14	$E_{29} - E_{27}$	1.933	57	$E_{29} - E_{14}$	4.851	100	$E_{33} - E_{4}$	6.032	143	$E_{29} - E_{18}$	7.447
15	$E_{32} - E_{36}$	2.596	58	$E_{30} - E_{16}$	4.868	101	$E_{28} - E_{14}$	6.100	144	$E_{33} - E_{5}$	7.452
16	$E_{22} - E_{36}$	2.738	59	$E_{24} - E_{5}$	4.906	102	$E_{29} - E_{16}$	6.149	145	$E_{33} - E_{16}$	7.473
17	$E_{22} - E_{27}$	2.886	60	$E_{24} - E_{16}$	4.926	103	$E_{30} - E_{18}$	6.165	146	$E_{20} - E_{16}$	7.478
18	$E_{32} - E_{31}$	3.029	61	$E_{26} - E_{11}$	4.997	104	$E_{20} - E_{14}$	6.180	147	$E_{33} - E_{3}$	7.538
19	$E_{28} - E_{36}$	3.034	62	$E_{35} - E_{5}$	5.039	105	$E_{33} - E_{14}$	6.174	148	$E_{32} - E_{17}$	7.563
20	$E_{30} - E_{15}$	3.057	63	$E_{30} - E_{8}$	5.045	106	$E_{21} - E_{17}$	6.200	149	$E_{28} - E_{8}$	7.576
21	$E_{33} - E_{36}$	3.108	64	$E_{35} - E_{16}$	5.059	107	$E_{22} - E_{1}$	6.203	150	$E_{29} - E_{9}$	7.595
22	$E_{20} - E_{36}$	3.114	65	$E_{24} - E_{8}$	5.103	108	$E_{26} - E_{6}$	6.221	151	$E_{32} - E_{6}$	7.696
23	$E_{24} - E_{15}$	3.116	66	$E_{19} - E_{4}$	5.121	109	$E_{24} - E_{18}$	6.224	152	$E_{22} - E_{17}$	7.705
24	$E_{30} - E_{7}$	3.178	67	$E_{35} - E_{3}$	5.124	110	$E_{34} - E_{17}$	6.265	153	$E_{32} - E_{12}$	7.755
25	$E_{28} - E_{27}$	3.182	68	$E_{32} - E_{2}$	5.144	111	$E_{26} - E_{12}$	6.279	154	$E_{22} - E_{6}$	7.838
26	$E_{24} - E_{7}$	3.237	69	$E_{32} - E_{15}$	5.150	112	$E_{23} - E_{17}$	6.285	155	$E_{28} - E_{17}$	8.00
27	$E_{35} - E_{2}$	3.243	70	$E_{34} - E_{11}$	5.175	113	$E_{30} - E_{9}$	6.313	156	$E_{33} - E_{17}$	8.076
28	$E_{35} - E_{15}$	3.248	71	$E_{32} - E_{4}$	5.520	114	$E_{29} - E_{8}$	6.327	157	$E_{20} - E_{17}$	8.081
29	$E_{35} - E_{10}$	3.323	72	$E_{32} - E_{10}$	5.224	115	$E_{35} - E_{18}$	6.357	158	$E_{25} - E_{6}$	8.087
30	$E_{25} - E_{31}$	3.420	73	$E_{22} - E_{15}$	5.292	116	$E_{24} - E_{9}$	6.371	159	$E_{25} - E_{12}$	8.146
31	$E_{24} - E_{4}$	3.486	74	$E_{22} - E_{7}$	5.413	117	$E_{34} - E_{6}$	6.398	160	$E_{33} - E_{6}$	8.208
32	$E_{33} - E_{31}$	3.541	75	$E_{26} - E_{5}$	5.464	118	$E_{23} - E_{6}$	6.418	161	$E_{32} - E_{18}$	8.258
33	$E_{30} - E_{14}$	3.569	76	$E_{30} - E_{17}$	5.471	119	$E_{34} - E_{12}$	6.456	162	$E_{33} - E_{12}$	8.267
34	$E_{35} - E_{4}$	3.619	77	$E_{24} - E_{17}$	5.529	120	$E_{32} - E_{11}$	6.473	163	$E_{22} - E_{18}$	8.400
35	$E_{24} - E_{14}$	3.628	78	$E_{28} - E_{15}$	5.588	121	$E_{19} - E_{5}$	6.541	164	$E_{22} - E_{9}$	8.548
36	$E_{26} - E_{10}$	3.748	79	$E_{21} - E_{16}$	5.597	122	$E_{20} - E_{1}$	6.578	165	$E_{32} - E_{13}$	8.691
37	$E_{35} - E_{14}$	3.761	80	$E_{23} - E_{8}$	5.860	123	$E_{19} - E_{3}$	6.627	166	$E_{28} - E_{18}$	8.696
38	$E_{21} - E_{15}$	3.786	81	$E_{25} - E_{10}$	5.615	124	$E_{29} - E_{17}$	6.752	167	$E_{33} - E_{18}$	8.770
39	$E_{34} - E_{2}$	3.846	82	$E_{34} - E_{5}$	5.642	125	$E_{35} - E_{13}$	6.790	168	$E_{20} - E_{18}$	8.776
40	$E_{34} - E_{15}$	3.851	83	$E_{33} - E_{2}$	5.657	126	$E_{25} - E_{11}$	6.864	169	$E_{28} - E_{9}$	8.844
41	$E_{23} - E_{15}$	3.872	84	$E_{34} - E_{16}$	5.662	127	$E_{21} - E_{18}$	6.895	170	$E_{33} - E_{13}$	9.203
42	$E_{34} - E_{10}$	3.926	85	$E_{35} - E_{17}$	5.662	128	$E_{32} - E_{5}$	6.940	171	$E_{25} - E_{13}$	9.082
43	$E_{23} - E_{7}$	3.993	86	$E_{23} - E_{5}$	5.662	129	$E_{32} - E_{16}$	6.960			

energy states in the upper Hubbard subband. As a result of the filling of four energy states in the upper Hubbard subband, twenty-nine allowed transitions from the lower Hubbard subband to the upper Hubbard subband, which are present in the fullerene C_{26}, disappear, but at the same time in the endohedral fullerene $U@C_{26}$ twenty-four new allowed transitions appear in the upper Hubbard subband, which are absent in the molecule C_{26}. Thus, the allowed transitions from the lower Hubbard subband to the upper Hubbard subband participate in the formation of the optical spectrum of the fullerene C_{26}, and in the formation of the optical spectrum of the endohedral fullerene $U@C_{26}$ both allowed transitions from the lower Hubbard subband to the upper Hubbard subband, and allowed transitions within the upper Hubbard subband participate. As you can see from the Table 4 allowed transitions for the endohedral fullerene $U@C_{26}$ within the upper Hubbard subband form mainly the optical spectrum in the infrared and visible areas of the spectrum, and allowed transitions from the lower Hubbard subband to the upper Hubbard subband, as for the fullerene

C_{26}, form mainly the optical spectrum in the ultraviolet area of the spectrum.

4. Conclusion

The study of the fullerene C_{26} with the symmetry group D_{3h} within the Hubbard model in the static fluctuation approximation showed that in this molecule the lower Hubbard subband is completely occupied, while the upper Hubbard subband is free. The study of the endohedral fullerene $U@C_{26}$, which, like the fullerene C_{26} has the symmetry group D_{3h}, showed, that in this molecule the lower Hubbard subband is completely busy, and there are four electrons in the upper Hubbard subband. In addition, these studies have shown that allowed transitions 176 and 171 are involved in the formation of optical spectra of absorption of molecules C_{26} and $U@C_{26}$. We also note that studies of the optical properties of fullerenes C_{60} and C_{70}, carried out within the Hubbard model in the studies [17,18], have shown good agreement between the experimental data and theoretical results. This allows us to consider, that the Hubbard model in the static fluctuation approximation describes the electronic properties of carbon nanosystems quite well.

Conflict of interest

The author declares that they he has no conflict of interest.

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