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THE SHIFT OF THE CONSTANT ENERGY LEVEL AFTER THE INTERACTION OF PARTICLES WITH THE POLARIZING PHONONS

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Abstract: The shift of the electron energy level due to its interaction with the polarizing phonons is investigated here for the particles whose energy does not depend on the wave vector. We also analyze the influence of the value of the constant of electron - phonon interaction and other parameters of the problem on the electron energy change. The methods of Green's functions, presented by the the Feynman diagrams and using the double permutations, are present here. The paper contains the analysis of the columns of the corresponding double permutations, the analytical expressions of which form the mass operator presented by the chain fractions. We received the expressions for admissibles and inadmissibles columns for phonon components of double permutations. The numerical calculations allow to conclude about the energy shift and how it depends on the parameters.

Keywords: Energy shift in multiparticle interaction, double permutation method for determining Green's function for multiparticle interaction

1. Motivation

During last years the applications of quantum dots are widely used in different electronic devices. The most important physical parameter in this problems is energy level, which can be changed by interaction of electron with the phonons, denoting the temperature vibrations of the atoms or ions of the environment. This is an significant question, because you cannot remove the temperature influence on the spectrum of electron in quatum dots [1,2]. Here the energy level is constant: it does not depend on the wave vector of the particle. The similar problem appears if you consider the layered crystals, including the intercalated atoms in the Van der Waals slit or if people investigate the energies of electron on the local impurity level. The constant energy level allows to simplify the energy shift calculation using the Green function method, because here we do not need to integrate over all possible wave vectors of virtual electron and we do not consider the Feynman diagrams with the crossing lines, as it is shown in [1]. In this work we also used the double permutations, introduced in [3] for electron phonon interaction. The results of this work are in good agreement with the results obtained in [4] for the similar problem with the essentially different parameters (constant of electron – phonon interaction).

2. Analytical equation to determine the energy

The electron – phonon interaction is described by the Froehlich Hamiltonian [5],

$$H = \sum_{a\vec{k}} E_{a\vec{k}} a^{+}_{a\vec{k}} a_{a\vec{k}} + \sum_{b\vec{q}\nu} W_{b\vec{q}\nu} b^{+}_{b\vec{q}\nu} b_{b\vec{q}\nu} + \\ + \sum_{a,b,\vec{k},\vec{q}} V_b(\vec{q}) a^{+}_{a\vec{k}-\vec{q}} a_{a\vec{k}} \left(b_{b,-\vec{q}\nu} + b^{+}_{b\vec{q}\nu} \right), \quad (1)$$

In (1) α i β are quantum numbers corresponding to the states of the particles (electrons and phonons), $\vec{k}, \vec{q}$ denote the wave vectors of particles, $W_{b\vec{q}}$ - energy of β – level of phonon spectrum, $V_b(\vec{q})$ - electron - phonon interaction function.

The energy shift is determined from the Fourier image of the Green's function

$$G_a(w) = \{w - E_a - M_a(w)\}^{-1}, \quad (2)$$

which can be presented by the infinitesimal equations after normalizing over the phonon frequency [1]. We define the mass operator ($M_\alpha(\omega)$ from (2)), which contains the average possible interactions between electrons and phonons. We adde it to the energy of a particle in denominator of the Fourier image of the Green's function (2). Then we determine the energy of the particles is from the poles of this Green's function (2). In our case, the energies from (2) and the interaction function are independed on the wave vectors of the particles.

The expressions, forming the mass operator are represented by Feynman diagrams [6], or by means of the double permutations introduced in [7] for the electron - phonon interaction and in [8] for the electron - electron interaction.

2. Mass operator in formalism of Feynman diagrams and double permutations

The virtual interactions of electrons with phonons, are presented by Feynman diagrams and corresponding

double permutations, where the pairwise averaging of phonon and electron operators are reflecting. These expressions contain selection rules derived from the conservation of energy and momentum. In particular, the element of the Feynman diagram shown in Fig.1 corresponds to the column of the double permutation (3) and denotes the conservation laws (4).

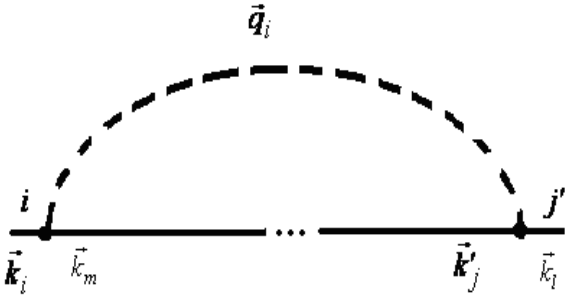


Fig.1. Element of Feynman diagram and corresponding column of double permutation in (3)

$$\begin{pmatrix} i & \dots \\ \dots & m \\ \dots & j' \\ \dots & l \end{pmatrix} \cdot V(\vec{q}_i)V(\vec{q}_j')\left\langle Tb^{+}_{\vec{q}_i} b_{\vec{q}_j'}\right\rangle \times \left\langle Ta^{+}_{\vec{k}_i - \vec{q}_i} a_{\vec{k}_m}\right\rangle \times \left\langle Ta^{+}_{\vec{k}_j' + \vec{q}_j'} a_{\vec{k}_i}\right\rangle, \quad (3)$$

$$\begin{aligned} \vec{k}_i + \vec{k}_j' &= \vec{k}_m + \vec{k}_l, \\ \vec{q}_i = q_j' &= \vec{k}_i - \vec{k}_m = \vec{k}_l - \vec{k}_j'. \end{aligned} \quad (4)$$

On the left side of (3) we can see the pairwise averaging procedure of phonon and electron operators. The first expression in (4) denotes the corresponding conservation of momentum, which can be derived from the column (3), as well as from diagram in Fig.1.

To determine the mass operator, we consider diagrams described by the phonon permutations corresponding to Young scheme with one line: these are permutations denoted by one cycle. In order to avoid the repeating expressions that differ on the renumbering of dots, we number the dots denoting the beginnings of phonon lines sequentially with ordinary numbers, and the endings of these lines sequentially with dashed numbers. Let us assume that within this cycle there are *t* groups containing ordinary and dashed numbers

$$\begin{aligned} &\left(1 \le k_i - 1 \; l_i' \le l_{(i+1)} - 1\right)' \\ &k_i \le k_{(i+1)} - 1 \; l_{(i+1)}' \le n'\Big) \end{aligned}, \quad (5)$$

Therefore, we can put down the expressions for admissible and inadmissible columns as follows:

Admissible columns Inadmissible columns

$$\sum_{i=1}^{t+1} \sum_{j=k_i}^{k_{i+1}-1} \sum_{s=l_i}^{n} \begin{pmatrix} j \\ s' \end{pmatrix} \quad \sum_{i=1}^{t+1} \sum_{j=k_i}^{k_{i+1}-1} \sum_{s\le(l_{i+1}-1)} \begin{pmatrix} j \\ s' \end{pmatrix}, \quad (6)$$

In particular, for cycles showing the pairwise averaging procedure for electronic operators in Table 1 in the phonon permutation missing expressions containing columns will appear:

$$\begin{aligned} &\text{DP4.2}: \begin{pmatrix} 4 \\ 1' \end{pmatrix}; \quad \text{DP4.3}: \begin{pmatrix} 3 & 4 \\ 1' & 1' \end{pmatrix} \\ &\text{DP5.1}: \begin{pmatrix} 3 & 4 & 4 & 5 & 5 & 5 \\ 1' & 1' & 2' & 1' & 2' & 3' \end{pmatrix} \\ &\text{DP5.2}: \begin{pmatrix} 3 & 4 & 5 & 5 & 5 \\ 1' & 1' & 1' & 2' & 3' \end{pmatrix} \\ &\text{DP5.3}: \begin{pmatrix} 4 & 4 & 5 & 5 \\ 1' & 2' & 1' & 2' \end{pmatrix}; \quad \text{DP5.4}: \begin{pmatrix} 5 \\ 1' \end{pmatrix}; \\ &\text{DP5.5}: \begin{pmatrix} 3 & 4 & 5 \\ 1' & 1' & 1' \end{pmatrix}; \quad \text{DP5.6}: \begin{pmatrix} 4 & 5 & 5 \\ 1' & 1' & 2' \end{pmatrix} \\ &\text{DP5.7}: \begin{pmatrix} 4 & 5 \\ 1' & 1' \end{pmatrix} \end{aligned} \quad (7)$$

Diagrams with nonintersecting phonon lines are considered in this work. They are shown in Table 1 together with the corresponding double permutation and factor denoting the number of such expressions for the first (1), the second (2), the third (3.1, 3.2), the fourth (4.1 - 4.4) and the fifth (5.1 - 5.8) orders of the perturbation theory.

In fact, the corresponding double permutation is very easy to obtain from the diagram, in which all the dots with coming out phonon lines should be numbered successively in ordinary numbers and the dots with coming in phonon lines numbered successively with dashed numbers. In the double permutation, the first and third lines represent the one-particle phonon Green's functions, and the digits of the first and second, third, and fourth lines represent the one-particle electronic Green's functions. The intersection of phonon lines leads to the appearance of a non-degenerate row in the double permutation, particularly, one containing 3 independent variables. For diagrams without the intersection of phonon lines, the double permutations (DPs) with following features are considered:

i) degenerate columns - when they contain two identical digits. They are: column 1 in DP 1); columns 1 and 2 in DP 2); columns 1 - 3 in DP 3.1); columns 1,3 in DP 3.2); columns 1 - 4 in DP 4.1); columns 1,3,4 in DP 4.2); columns 1,2,4 in DP 4.3); columns 1,4 in PP 4.4); columns 1 - 5 in DP 5.1); 1,2,4,5 in DP 5.2); columns 1,3,5 in DP 5.3); columns 1,4,5 in DP 5.4); columns

1,2,5 in DP 5.5; columns 1,3 - 5 in DP 5.6); columns 1, 3,5 in DP 5.7); columns 1,5 in DP 5.8)

ii) quasi-degenerate columns - containing a pair of digits, which is included in the degenerate column. They are: column 2 in DP 3.2); column 2 in DP 4.2); column 3 in DP 4.3); columns 2,3 in DP 4.4); column 3 in DP 5.2); columns 2,4 in DP 5.3); column 2 in DP 5.4); column 4 in DP5.5; column 2 in DP5.6; columns 2, 4 in DP 5.7); columns 2,4 in DP 5.4);

iii) strongly degenerate columns - a) contain a pair of digits, both of which are included in the degenerate columns together with other common digits in these columns. It is column 3 in DP 5.4); or b) containing a pair of digits included in the quasi-degenerate column. They are: column 3 in DP 5.5); columns 3 in DP5.8).

Only these columns are included in the double permutations from Table 1.

2.1. Mass operator as chain fraction

In [1,3,4], the analytical expressions corresponding all diagrams and double permutations introduced in Table 1 were calculated. The results were compared with the numerical results of partial summation, which allow finding a mass operator in a chain fraction. For this purpose, we consider the interaction of the particle with a certain number of virtual phonons. So, for the mass operator in the second approximation, we consider the infinite number of diagrams which contain no more than two phonon lines above the base line. They are: 1), 2), 3.1), 4.1), 5.1) diagrams from Table 1. To describe the three phonon processes, we choose diagrams that do not contain more than 3 lines above the base line. They are expressions 3.2), 4.2), 4.3), 5.2), 5.3), 5.6) in Table 1. Partial summing for two and three phonon processes allows us to denote the mass operator as the chain fraction

$$MF(x,a)=\cfrac{a_1}{1+\cfrac{a_2}{1+\cfrac{a_3}{1+\cfrac{a_4}{1+\cfrac{a_5}{1-..}}}}}, \qquad (8)$$

where

$$a_1=\frac{a}{(x-1)}, \qquad a_n=\frac{-na}{(x-n+1)\times(x-n)}, \qquad (9)$$

With the dimensionless variables [1]:

$$x=\frac{w-E}{W};a=\sum_q\frac{|V^2|}{W^2};MF=\frac{M}{W}, \qquad (10)$$

where E is an electron energy level, Ω is phonon energy, V is the coupling function which is also supposed to be independent on quasi momentum, MF is a dimensionless mass operator (the mass operator is divided by the phonon energy). In [6], we also performed the direct calculation for mass operator for some particular cases and showed that up to the fifth order of perturbation theory the numerical results for (8) and direct calculations coinside.

2.2. Calculation

The renormalized energy of the particles was obtained from the equation:

$$x-MF(x)=0, \qquad (11)$$

Fig.2. illustrates solving for α = 0.01; 0.05; 0.08; 0.3; 0.5; 0.8. In Fig.2. The crossing points of solid and dash lines denote the energy shift (6), where the solid lines depict $M(\xi)$ and dash lines – ξ. Our calculations were made for n = 100.

3. Results and discussions

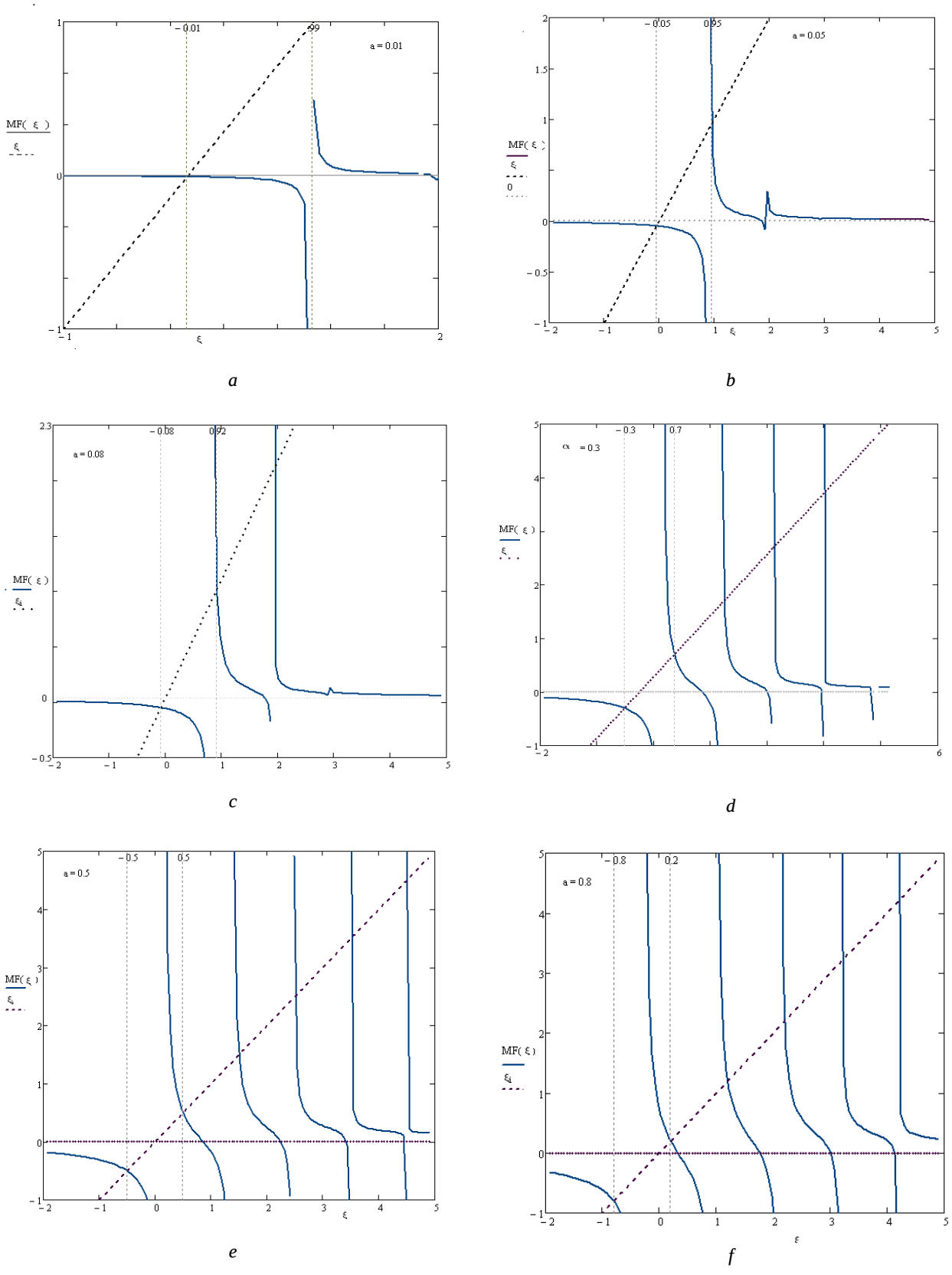
As we can see from Fig.2, an energy shift (the first crossing point between solid and dash lines) corresponds to $\xi = -\alpha$ for all cases presented in Fig.2. It means that energy shift depends on an electron-phonon coupling constant and phonon frequencies. It does not depend on any parameter of particle as far as we can suggest that the coupling constant and phonon frequency are independent of these parameters.

For small α we can see only one solution of (10), that is, the level shift without any phonon repetition (Fig.2 a)). Increasing absolute value of α allows more solutions of (10). Every solution differs from the previous by the same value (phonon frequency) and means phonon repetitions. As we can see, for $\xi < 5$ and $\alpha = 0.01$ we have only one solution of (10) – Fig.2 a); for $\alpha = 0.05$ we obtain two solutions – Fig.2b); three solutions for $\alpha = 0.08$ - Fig.2c); five solutions for $\alpha = 0.3$ – Fig.2d); six solutions for $\alpha = 0.5$ and $\alpha = 0.8$ – Fig. 2 c) and Fig – 2 d).

So we can conclude that increasing the absolute value of α means

i) the decrease of energy level, because of electron-phonon interaction

ii) the increase of the number of phonon repetitions.

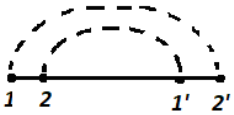
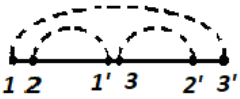
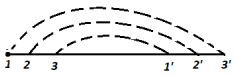
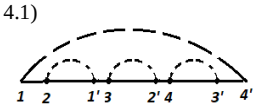
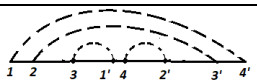
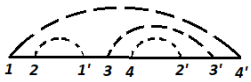
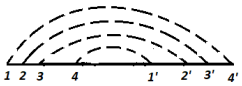
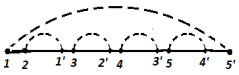
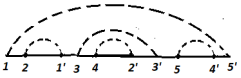
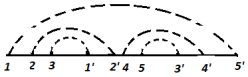
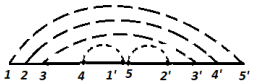
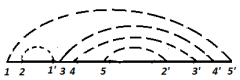
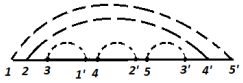
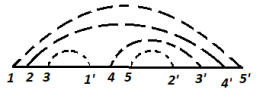
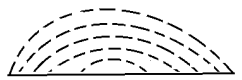


a *b* *c* *d* *e* *f*

Fig. 2. The crossing points define the energy shift for the different values of α at n = 100

Table 1

Some expressions representing the virtual interaction of particles with the constant energy levels

The first order		The second order	
1) 	æ1 ö ç ÷ ç1' ÷ ç ÷ ç1' ÷ ç ÷ è1 ø	2) 	æ1 2 ö ç ÷ ç2 1' ÷ ç ÷ ç2' 1' ÷ ç ÷ è1 2' ø
The third order			
3.1) 	æ1 2 3 ö ç ÷ ç2 1' 2' ÷ ç ÷ ç3' 1' 2' ÷ ç ÷ è1 3 3' ø $2!\times 2$	3.2) 	æ1 2 3 ö ç ÷ ç2 3 1' ÷ ç ÷ ç3' 2' 1' ÷ ç ÷ è1 3' 2' ø $3!$
The fourth order			
4.1) 	æ1 2 3 4 ö ç ÷ ç2 1' 2' 3' ÷ ç ÷ ç4' 1' 2' 3' ÷ ç ÷ è1 3 4 4' ø $2!\times 2^2$	4.2) 	æ1 2 3 4 ö ç ÷ ç2 3 1' 2' ÷ ç ÷ ç4' 3' 1' 2' ÷ ç ÷ è1 4' 4 3' ø 2×3^2
4.3) 	æ1 2 3 4 ö ç ÷ ç2 1' 4 2' ÷ ç ÷ ç4' 1' 3' 2' ÷ ç ÷ è1 3 4' 3' ø $3!\times 2^2$	4.4) 	æ1 2 3 4 ö ç ÷ ç2 3 4 1' ÷ ç ÷ ç4' 3' 2' 1' ÷ ç ÷ è1 4' 3' 2' ø $4!$
The fifth order			
5.1) 	æ1 2 3 4 5 ö ç ÷ ç2 1' 2' 3' 4' ÷ ç ÷ ç5' 1' 2' 3' 4' ÷ ç ÷ è1 3 4 5 5' ø $2!\times 2^3$	5.2) 	æ1 2 3 4 5 ö ç ÷ ç2 1' 4 2' 4' ÷ ç ÷ ç5' 1' 3' 2' 4' ÷ ç ÷ è1 3 5 3' 5' ø $3!\times 3\times 2^2$
5.3) 	æ1 2 3 4 5 ö ç ÷ ç2 3 1' 5 3' ÷ ç ÷ ç5' 2' 1' 4' 3' ÷ ç ÷ è1 4 2' 5' 4' ø $3!\times 2\times 3^2$	5.4) 	æ1 2 3 4 5 ö ç ÷ ç2 3 4 1' 2' ÷ ç ÷ ç5' 4' 3' 1' 2' ÷ ç ÷ è1 5' 4' 5 3' ø $4!\times 4$
5.5) 	æ1 2 3 4 5 ö ç ÷ ç2 1' 4 5 2' ÷ ç ÷ ç5' 1' 4' 3' 2' ÷ ç ÷ è1 3 5' 4' 3' ø $4!\times 2^2$	5.6) 	æ1 2 3 4 5 ö ç ÷ ç2 3 1' 2' 3' ÷ ç ÷ ç5' 4' 1' 2' 3' ÷ ç ÷ è1 5' 4 5 4' ø $3!\times 3^2$
5.7) 	æ1 2 3 4 5 ö ç ÷ ç2 3 1' 5 2' ÷ ç ÷ ç5' 4' 1' 3' 2' ÷ ç ÷ è1 5' 4 4' 3' ø $4!\times 2\times 3$	5.8) 	æ1 2 3 4 5 ö ç ÷ ç2 3 4 5 1' ÷ ç ÷ ç5' 4' 3' 2' 1' ÷ ç ÷ è1 5' 4' 3' 2' ø $5!$

4. Results and discussions

As we can see from Fig.2, an energy shift (the first crossing point between solid and dash lines) corresponds to $\xi = -\alpha$ for all cases presented in Fig.2. It means that energy shift depends on an electron-phonon coupling constant and phonon frequencies. It does not depend on any parameter of particle as far as we can suggest that the coupling constant and phonon frequency are independent of these parameters.

For small α we can see only one solution of (10), that is, the level shift without any phonon repetition (Fig.2 a)). Increasing absolute value of α allows more solutions of (10). Every solution differs from the previous by the same value (phonon frequency) and means phonon repetitions. As we can see, for $\xi < 5$ and $\alpha = 0.01$ we have only one solution of (10) – Fig.2 a); for $\alpha = 0.05$ we obtain two solutions – Fig.2b); three solutions for $\alpha = 0.08$ - Fig.2c); five solutions for $\alpha = 0.3$ – Fig.2d); six solutions for $\alpha = 0.5$ and $\alpha = 0.8$ – Fig. 2 c) and Fig – 2 d).

So we can conclude that increasing the absolute value of α means the decrease of energy level, because of electron-phonon interaction the increase of the number of phonon repetitions.

5. Conclusions

In this work we investigated the shift of constant energy level for a particle interacting with the polarization phonons and show the energy level shift and its dependence on the coupling constant and phonon energy.

We represented the virtual electron-phonon interactions with Feynman diagrams and with double permutations and found out the selection rules for phonon permutations corresponding to the Young schemes with one row, corresponding to mass operator.

We identified the double permutations corresponding to diagrams without crossing phonon lines, which contribute to Mass operator expressions.

We show that the increase of absolute value of electron-phonon coupling constant renormed to phonon energy leads to lowering the energy level and to increasing the number of phonon repetitions

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ЗМІСТ ПОСТІЙНОГО РІВНЯ ЕНЕРГІЇ ПІСЛЯ ВЗАЄМОДІЇ ЧАСТИНОК З ПОЛЯРИЗУЮЧИМИ ФОНОНАМИ

Корнелія Товстюк

У цій роботі досліджується зсув енергетичного рівня частинки, що взаємодіє з поляризаційними фононами. Енергія частинки і частота фонона постійні - вони не залежать від хвильового вектора (квазіімпульсу) частинок. Показано, як зменшується енергетичний рівень залежно від електрон-фононної константи зв'язку та енергії фонона. У цій роботі використано метод діаграм Фейнмана та метод подвійної перестановки, що дозволило ідентифікувати подвійні перестановки, що відповідають діаграмам Фейнмана, без перетину фононних ліній. Ми перестановок, що відповідають виразам, які утворюють масовий оператор, та виявили спільні риси для DPs, що утворюють ряди для одного, двох і трьох фононних наближень.

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Main scientific interests in the field of research of multiparticle interaction and its manifestation in strongly anisotropic materials.

Espetially the electron phonon interaction in layered crystals GaSe, InSe. She is author of serias of investigations of quantum dots: the energy of electron in quantum dots with different configurations; the energy shift of electron in quantum dot after electron – phonon interaction.

She developed the formalism of double permutations denoting the virtual interactions of electrons and electronwith phonons, where the pairwise averaging of phonon and electron operators are reflecting so that they contain selection rules derived from the conservation of energy and momentum.

Author of more than 130 scientific and scientific-methodical works.