# The energy shift of particles in the quantum dot caused by their interaction with polarizing phonons

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## 1. Motivation

The investigations carried out in this work correspond to the particles with the constant energy level, independent on its quasi-momentum. They are: electrons in quantum dots, impurities in semiconductors, intercalated atoms in the Van der Waals slit of layered crystals. Here we analyze the interaction of such particles with the polarization phonons.

This problem is very attractive because its simplicity for two reasons: a) we do not need to integrate on all possible quasi-impulses when calculating the Fourier image of the Green's function; b) for interaction of particles with constant energies the number of Feynman diagrams sharply reduces, because the diagrams with intersections of phonon lines are removed [1]. We compared the Feynman diagrams with double permutations (DP), which are also used to describe the electron-phonon interaction [2] and identified the DP corresponding to Feynman diagrams without intersecting phonon lines and DP corresponding to one-, two- and three phonon processes. Besides our results agree with the partial case of the considered problem, analyzed in [1] that proves the correctness of the used approximations and the carried-out calculations.

## 2. Analytical expressions

The electron – phonon interaction is described by the Froehlich Hamiltonian [3], where the energy of the particle ($E$) and the constant frequency of the phonon ($\Omega$) appear. The energy shift (due to electron-phonon interaction) is determined from the Fourier image of the Green's function, which can be reduced to dimensionless quantities by normalizing over the phonon frequency [1]. A definite mass operator, containing the average possible interactions between electrons and phonons, is added to the energy of a particle in denominator of the Fourier image of the Green's function. The energy of the particles is determined from the poles of this Green's function.

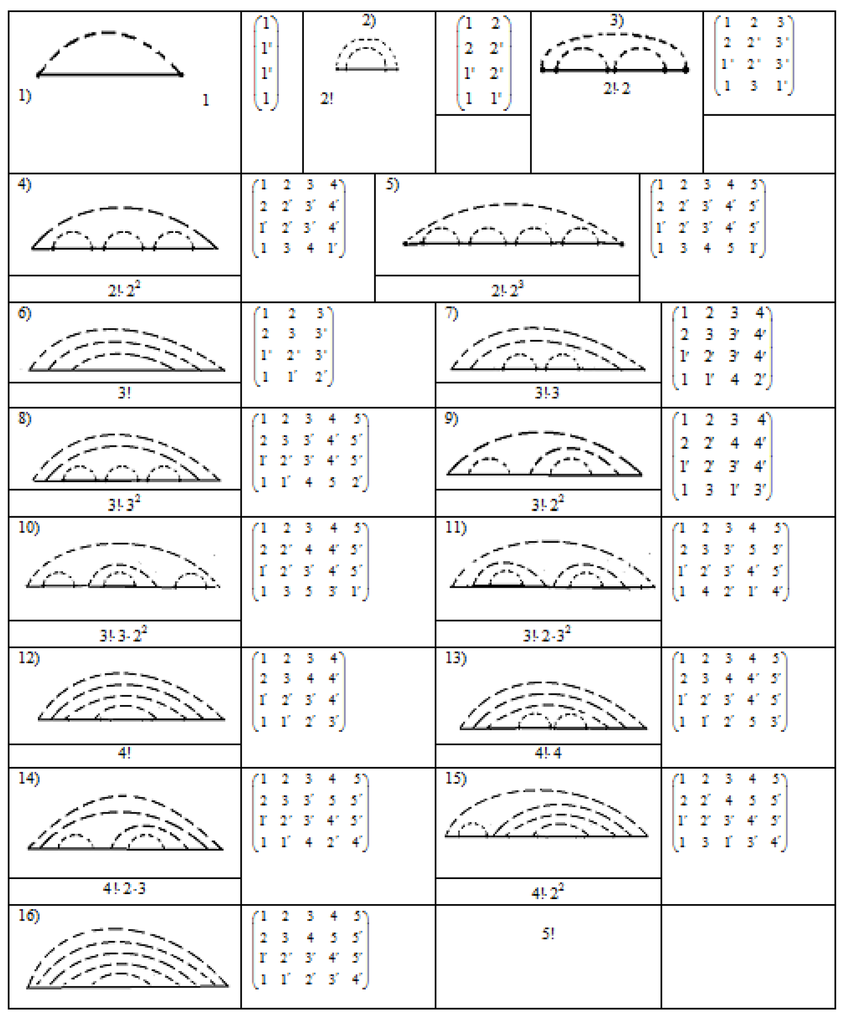
The mass operator is conveniently represented by Feynman diagrams [4], or by means of DP, proposed in [2] for electron - phonon interaction and in [5] for electron - electron interaction.

### 2.1. Mass operator in formalism of Feynman diagrams and double permutations

As it is shown in [1], for particles with the constant energy levels we have to coincident the analytical expressions for diagrams with nonintersecting phonon lines. Table 1 includes some diagrams, which form the mass operator together with the corresponding DPs and factors for each expression.

As we see from Table 1, all DPs that correspond to diagrams without intersections consist of degenerate columns (column that contain two identical digits) or quasi-degenerate columns (columns that contain a pair of digits that occurs in a degenerate column).

**Table 1**.
*Some expressions representing the virtual interaction of particles with the constant energy levels*



### 2.2 Partial summation in mass operator

When performing partial summation we consider the interaction of the particle with a certain number of virtual phonons. So to obtain a mass operator in the second approximation we consider an infinite number of diagrams which contain no more than two phonon lines above the base line. These are expressions 1, 2, 3, 4, 5 in Table 1. As we see, they are described by the DPs with all degenerate columns. Such infinite series gives:

$$m_2(\xi) = \frac{\alpha}{\xi - 1 - \dfrac{2\alpha}{\xi - 2}}. \qquad (1)$$

Here we used the dimensionless variables [1]:

$$\xi = \frac{\omega - E}{\Omega}; \quad \alpha = \sum_q \frac{|\varphi|^2}{\Omega^2}; \quad M = \frac{\mathrm{M}}{\Omega}. \qquad (2)$$

To describe the three phonon processes, we choose diagrams that do not contain more than 3 lines above the base. These are expressions 6, 7, 8 and expressions 9,10,11 from Table 1.

Diagrams 6,7,8,9,10 correspond to dP with one quasi-degenerate columns (column 2 in DPs 6,7,8 and column 3 in DPs 9 and 10) and PP 11 contain two quasi-degenerate columns (columns2 and 4). These infinite series allow us to determine

$$m_3(\xi) = \frac{\alpha}{\xi - 1 - \dfrac{2\alpha}{\xi - 2 - \dfrac{3\alpha}{\xi - 3}}}. \qquad (3)$$

Partial summation for two and three phonon processes in mass operator shows that it can be represented as chain fraction

$$MF(\xi,\alpha) = \frac{a1}{1 + \dfrac{a2}{1 + \dfrac{a3}{1 + \dfrac{a4}{1 + \dfrac{a5}{1 - ..}}}}}. \qquad (4)$$

where $a1 = \dfrac{\alpha}{(\xi - 1)}$, $an = \dfrac{-n\alpha}{(\xi - n + 1)\cdot(\xi - n)}$,

$E$ – electron energy level, $\Omega$ – photon energy, $\varphi(q)$ – the coupling function, which we also supposed to be independent on quasi-momentum, $MF$ – the dimensionless mass operator (the mass operator is divided by the phonon energy).

**Table 2**.
*Energy levels for different values of coupling function*

| $\alpha = 0{,}3$ | $\alpha = 0{,}5$ | $\alpha = 0{,}8$ |
|---|---|---|
| $\xi_1 = -0{,}3$ | $\xi_1 = -0{,}5$ | $\xi_1 = -0{,}8$ |
| $\xi_2 = 0{,}7$ | $\xi_2 = 1$ | $\xi_2 = 0{,}2$ |
| $\xi_3 = 1{,}7$ | $\xi_3 = 1{,}5$ | $\xi_3 = 1{,}2$ |
| $\xi_4 = 2{,}7$ | $\xi_4 = 2$ | $\xi_4 = 2{,}2$ |
| $\xi_5 = 3{,}7$ | $\xi_5 = 2{,}5$ | $\xi_5 = 3{,}2$ |

## 3. Calculation

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

$$\xi - M(\xi) = 0. \qquad (5)$$

The both functions from (5) are shown in Fig.1. The calculations were taken for α = 0.3; 0.5; 0.8. Fig.2 denotes the spline interpolation of the mass operator used by us in solving equation (5). The values of the energy level shift for some coupling functions are represented in Table 2. Fig. 3 shows the convergence of the solutions to their asymptotic values (-α) for different numbers of terms in the chain fraction (4). Numerical data are given above. Rows in matrices f correspond to a certain value of α (matrix α), the number of terms is in the name of the matrix (f2, f3, f5, f6 corresponds to the 2, 3, 5, 6 order in chain fractions (4) respectively).

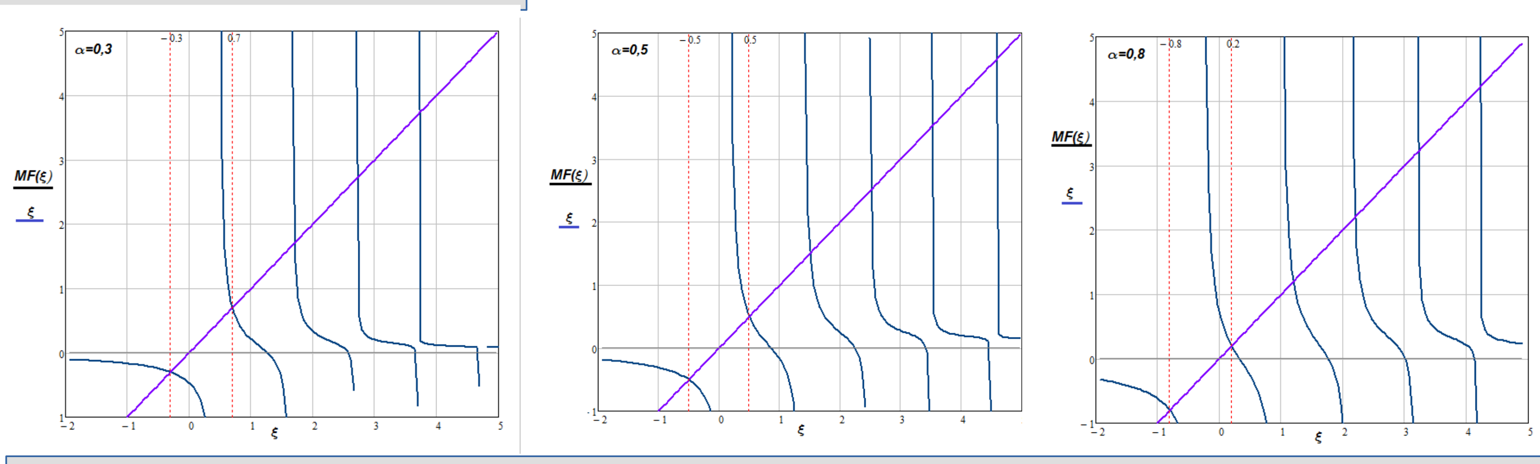



**Fig. 1**. *The crossing points define the energy of a particle for different values of the coupling constant at n = 100*

## 4. Results and discussion

The results of the calculations (Table 2) indicate a decrease of the energy level due to the electron-phonon interaction. Moreover, calculations at different values of the coupling constant indicate that the energy decreases to a value equal to α. The following solutions of the energy are associated with the interaction with one, two, … phonons: whole values of phonon energy are added to the ground state energy. For a bound particle (for example electron in a finite quantum dot), this may mean a transition to a free state. From Fig.3.a) we see the rapid convergence of the mass operator at small values of α. Thus, for $\alpha = 0.2$, we see the asymptotic value already on the third approximation in (4). The relative deviation for $n = 2$ is 1.5%. The increasing $\alpha$ leads to the need to consider a larger number of approximations in (4). Thus, at $\alpha = 0.4$ (or $\alpha = 0.6$) the asymptotic value is obtained in the fifth approximations (the relative deviation for the three approximations is 4.5% (7.7%) and 0.5% (1,7% ) for $n = 2$ and $n = 3$, respectively). At $\alpha = 0.8$ we achieve the asymptotic value in the 6-th approximation with the deviations of 10.8%, 2.9%, 0.13%, for $n = 2, 3, 5$, respectively. Although $\alpha = 1$ should become a bifurcation number (this value we cannot consider as a small parameter) the convergence of fractions (4) here does not go beyond the previous trend. For $\alpha = 1$ accounting of $n = 6$ leads to a relative deviation of 0.1% and we also see a good convergence even at $n = 5$ ($\delta = 0.2\%$). Therefore, we analysed the convergence of the chain fraction (4) and for some larger values of α (Fig. 3.b)). For $\alpha = 2$ the accounting of the sixth approximation leads to a relative deviations 0.8%; (5,6%), and for $n = 20$ it gives complete convergence. But for $\alpha = 6; 8$ for $n = 20$ we determined $\delta < 0.12\%; 0.1\%; 9.95\%$. As we see, for $\alpha > 1$ expression (4) coincides with the asymptotic value for small α (4) after considering 20 approximations in (4). For larger values of α, the analysis of the relative deviations of the series at $n = 20$ indicates its non-uniform convergence.

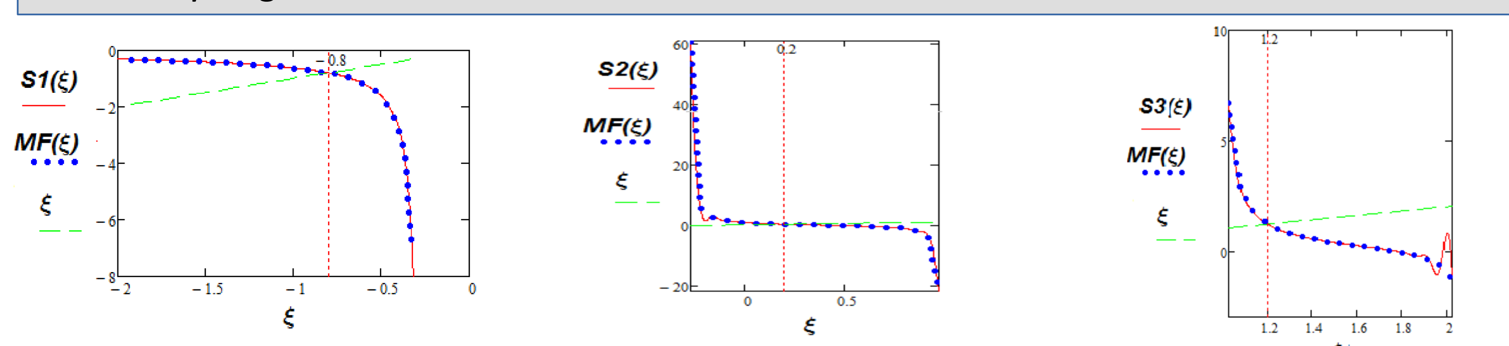



**Fig. 2**. *Spline interpolation of mass operator. S1 (ξ), S2 (ξ), S3 (ξ), - spline function for the first, second and the third solutions, respectively, MF (ξ) - mass operator obtained by chain fractions (4) for n = 100 (represented by the points ).*

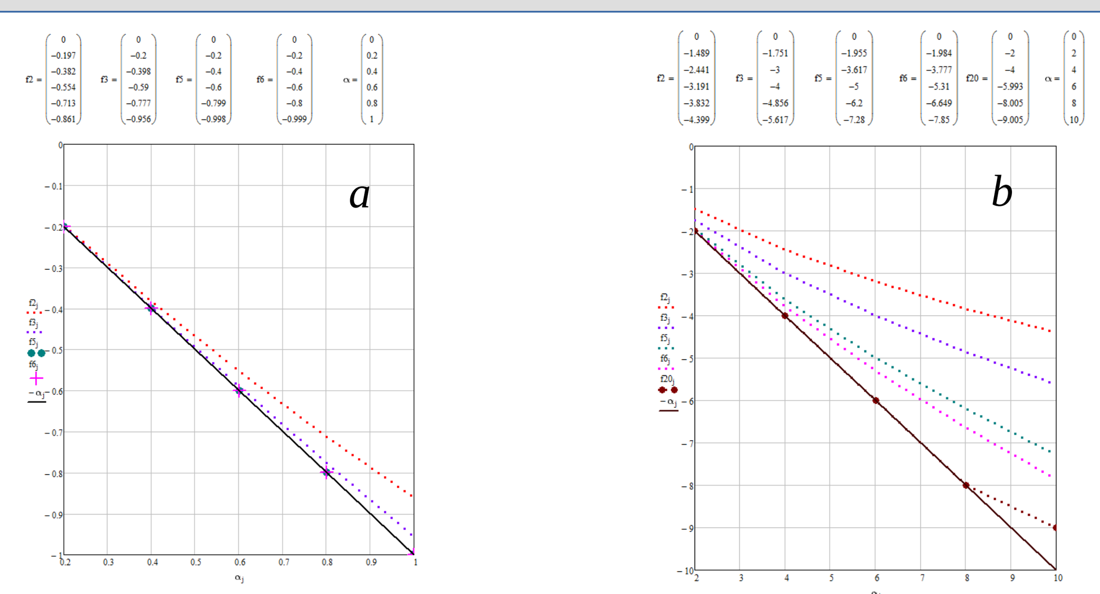



**Fig. 3**. *The convergence of solutions to their asymptotic value (-α) for different number of terms in the chain fraction (4) for small (a) and large (b) values of the coupling constant*

## 5. Conclusions

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

The comparison of double permutations and Feynman diagrams allowed to identify the DPs corresponding to diagrams without crossing phonon lines and to find common features in DPs corresponding to the interactions with one- two- and three virtual phonons.

The investigated convergence of the chain fraction for mass operator indicates its good convergence already in the sixth approximation for the small coupling constant, as well as in the 20th approximation for the average constant connection. Analysis of the relative deviations for large values of the constant relationship indicates uneven convergence of the series.

## References

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