Spectrum of localized quasiparticle renormalized due to the interaction with three-mode phonons

Tkach M.V., Seti Ju.O., Hutiv V.V., Voitsekhivska O.M.

Department of Theoretical Physics and Computer Simulation, Yuriy Fedkovych Chernivtsi National University, 2, Kotsyubinsky Str., 58012, Chernivtsi, Ukraine,

E-mail: hutiv.vasyl@chnu.edu.ua

Introduction

Intensive development of nano scale physics during the last decades have been revealed the new physical properties of low-dimensional structures and stimulated the growth of different multi-layered nano heterostructures: quantum dots, wires, rings, etc. Also, it caused the experimental appearance of new unique nano devices which are widely used in medicine, ecology, communication and space, military, scientific investigation.

From the physical considerations, nano heterostructures are principally different with respect to 3D structures just due to the nano size of their composing elements. The effect of size quantization is always present in nano structures. It causes the multi-band spectra of quasiparticles (electrons, holes, excitons) and multi-mode spectra of polarization phonons.

It is well known that in order to optimize the operating parameters of modern nano devices functioning in infrared range, one should deeply understand the physical processes in multi-layered heterostructures, being their main elements. The quantum theory of photon- and phonon-assisted tunneling, being developed now, will provide this knowledge. The main problem of the theoretical investigation is to take into account the multi-phonon processes, which essentially renormalize the quasiparticles spectra. This cannot be done in the framework of perturbation method [1,2].

Consistently solving the complicated problem of renormalized spectrum of multi-level quasiparticle interacting with multi-mode polarization phonons, we have been modified the method of Feynman-Pines diagram technique and in the recent papers[3,4], using the Frohlich-like Hamiltonian, obtained the renormalized spectrum of multi-level quasiparticle interacting with one-mode phonons.

In the proposed paper, we solve the problem of renormalized energy spectrum of one-level quasiparticle interacting with three-mode phonons (for example, one mode of confined phonons and two modes of interface phonons).

Theory

The studied system consists of a localized quasiparticle (exciton, impurity, etc.), which strongly interacts with dispersionless three-mode polarization phonons at T = 0K. The Hamiltonian of this system in the representation of second quantization over all variables is written in Frohlich's form [1].

$$\hat{H}=\sum_{\vec{k}}E_{\vec{k}}\hat{A}^+_{\vec{k}}\hat{A}_{\vec{k}}+\sum_{\lambda=1}^{3}\sum_{\vec{q}}\Omega_\lambda\hat{B}^+_{\lambda\vec{q}}\hat{B}_{\lambda\vec{q}}+\sum_{\lambda=1}^{3}\sum_{\vec{k}\vec{q}}\varphi_\lambda(\vec{q})\hat{A}^+_{\vec{k}}\hat{A}_{\vec{k}}\left(\hat{B}_{\lambda\vec{q}}+\hat{B}^+_{\lambda-\vec{q}}\right) \quad (1)$$

Here $E_{\vec{k}}=E$ is the energy of non-interacting localized quasiparticle, Ω_λ is the energy of phonon mode (λ), $\varphi_\lambda(\vec{q})$ is a binding function. . Quasiparticle $\left(\hat{A}^+_{\vec{k}},\hat{A}_{\vec{k}}\right)$ and phonon $\left(\hat{B}^+_{\lambda\vec{q}},\hat{B}_{\lambda\vec{q}}\right)$ operators of second quantization satisfy Bose commutative relationships. Like in [1], we are studying the model of the system in which the condition is fulfilled

$$\hat{n}^2=\hat{n}=\sum_{\vec{k}}\hat{A}^+_{\vec{k}}\hat{A}_{\vec{k}} \quad (2)$$

It means that the eigenvalues of both of these operators($\hat{n}$ and $\hat{n}^2$) can be either 0 or 1, which is interpreted as a condition for the existence (1) or absence (0) of a "pure" quasiparticle state.

To calculate the spectrum of the system, at first the diagonalization of Hamiltonian (1) is performed by the transition from the operators $\hat{A}_{\vec{k}},\hat{B}_{\lambda\vec{q}}$ to new ones $\hat{a}_{\vec{k}},\hat{b}_{\lambda\vec{q}}$ using a unitary operator

$$S=\exp\left\{\hat{\sigma}\sum_{\vec{k}}\hat{a}_{\vec{k}}\hat{a}^+_{\vec{k}}\right\} \quad (3)$$

where

$$\hat{\sigma}=\sum_{\lambda\vec{q}}\Omega_\lambda^{-1}\left[\varphi^*_\lambda(\vec{q})\hat{b}^+_{\lambda\vec{q}}-\varphi_\lambda(\vec{q})\hat{b}_{\lambda\vec{q}}\right] \quad (4)$$

The Hamiltonian (1) in the new operators has a diagonal form

$$\hat{H}=\sum_{\vec{k}}\varepsilon_{\vec{k}}\hat{a}^+_{\vec{k}}\hat{a}_{\vec{k}}+\sum_{\lambda=1}^{3}\sum_{\vec{q}}\Omega_\lambda\hat{b}^+_{\lambda\vec{q}}\hat{b}_{\lambda\vec{q}} \quad (5)$$

where

$$\varepsilon_{\vec{k}}=E_{\vec{k}}-\sum_{\lambda\vec{q}}\Omega_\lambda^{-1}\left|\varphi_\lambda(\vec{q})\right|^2 \quad (6)$$

- energy of new elementary excitations generated by the operator $\hat{a}^+_{\vec{k}}$

Introducing at T = 0K a two-hour healed Green's function

$$G(\vec{k},t)=-i\theta(t)\left\langle 0\left|\left[\hat{A}_{\vec{k}}(t),\hat{A}_{\vec{k}}(0)\right]\right|0\right\rangle \quad (7)$$

taking into account (5) and the relationship between old and new operators

$$\hat{A}_{\vec{k}}=S\hat{a}_{\vec{k}}S^+=\hat{a}_{\vec{k}}\exp\{-\sigma\} \quad (8)$$

using the Weyl's operator identity, an exact expression is obtained

$$G(\vec{k},t)=-i\theta(t)\left\langle 0\left|e^{\hat{\sigma}(t)}e^{\hat{\sigma}(0)}\right|0\right\rangle\exp\left\{-\frac{i\varepsilon_{\vec{k}}t}{\hbar}\right\}=-i\theta(t)\exp\left\{-\frac{i\varepsilon_{\vec{k}}t}{\hbar}+g(t)\right\} \quad (9)$$

Here

$$g(t)=\sum_{\lambda=1}^{3}\alpha_\lambda\left\{\exp\left(-\frac{i\Omega_\lambda t}{\hbar}\right)-1\right\}, \quad (10)$$

where

$$\alpha_\lambda=\Omega_\lambda^{-2}\sum_{\vec{q}}\left|\varphi_\lambda(\vec{q})\right|^2 \quad (11)$$

is the dimensionless parameter which characterizes the binding energy of quasiparticle with λ -th mode of phonons.

The Fourier image of the Green's function (9) is written by the expression (12)

$$G(\vec{k},\omega+i\eta)=-\frac{i}{\hbar}\int_0^\infty\exp\left\{i(\omega-\hbar^{-1}\varepsilon_k+i\eta)t+\sum_{\lambda=1}^{3}\alpha_\lambda\left[\exp\left(-\frac{i\Omega_\lambda t}{\hbar}\right)-1\right]\right\}dt$$

The integration in (12) is performed exactly (laid ħ = 1, $\vec{k}=0$)

$$G(\omega+i\eta)=e^{-\sum_{\lambda=1}^{3}\alpha_\lambda}\left\{\frac{1}{\omega-E+\sum_{\lambda_1=1}^{3}\alpha_{\lambda_1}\Omega_{\lambda_1}}+\sum_{\lambda=1}^{3}\sum_{l_\lambda=1}^{\infty}\frac{\alpha_\lambda^{l_\lambda}}{l_\lambda!\left[\omega-E+\sum_{\lambda_1=1}^{3}\alpha_{\lambda_1}\Omega_{\lambda_1}-l_\lambda\Omega_\lambda+i\eta\right]}+\sum_{l_1,l_2,l_3=1}^{\infty}\frac{\alpha_1^{l_1}\alpha_2^{l_2}\alpha_3^{l_3}}{l_1!l_2!l_3!\left[\omega-E+\sum_{\lambda=1}^{3}\alpha_\lambda\Omega_\lambda-l_1\Omega_1-l_2\Omega_2-l_3\Omega_3+i\eta\right]}\right\} \quad (13)$$

According to the general theory [1,2], the poles of the Fourier image of the Green's function determine the energy spectrum of the system. Therefore, from formula (13) it is seen that the renormalized energy spectrum in this model is given by an exact analytical expression

$$E_{l_1,l_2,l_3}=E-\sum_{\lambda=1}^{3}\alpha_\lambda\Omega_\lambda+l_1\Omega_1+l_2\Omega_2+l_3\Omega_3 \qquad (l_1,l_2,l_3=0,1,2,...\infty) \quad (14)$$

It can be seen from (14) that since there is no a decay in the system, its spectrum is real. It contains the main renormalized level (at $l_1=l_2=l_3=0$)

$$E_{0,0,0}=E-\sum_{\lambda=1}^{3}\alpha_\lambda\Omega_\lambda \quad (15)$$

shifted to the low-energy region, with respect to the the basic (E) non-interacting quasiparticle, at magnitude $\sum_{\lambda=1}^{3}\alpha_\lambda\Omega_\lambda$. In addition, there arises an infinite number of discrete groups of satellite levels, which correspond to the bound states of a quasiparticle with all possible combinations of different numbers of phonons of these three modes.

The obtained renormalized spectrum (14) of the system has an interesting properties. Depending on the ratios between the energies of the phonon modes, the satellite part of the spectrum may be partially degenerated and partially non-degenerate.

If the energy ratios of any two or all three phonon modes are integers, then the discrete satellite spectrum of the system contains degenerated and non-degenerated levels. In the case when the ratios of all three phonon modes are integers, then the complete spectrum is equidistant with an energy step equal to the energy of the lowest phonon mode.

If the energy ratios of all three phonon modes are irrational numbers, then the whole renormalized spectrum of the system is non- degenerated.

The revealed analytical properties of the renormalized spectra of the system are well illustrated in Fig. 1a, b, where examples of the calculated spectra of degenerated and non-degenerate types, respectively, are given

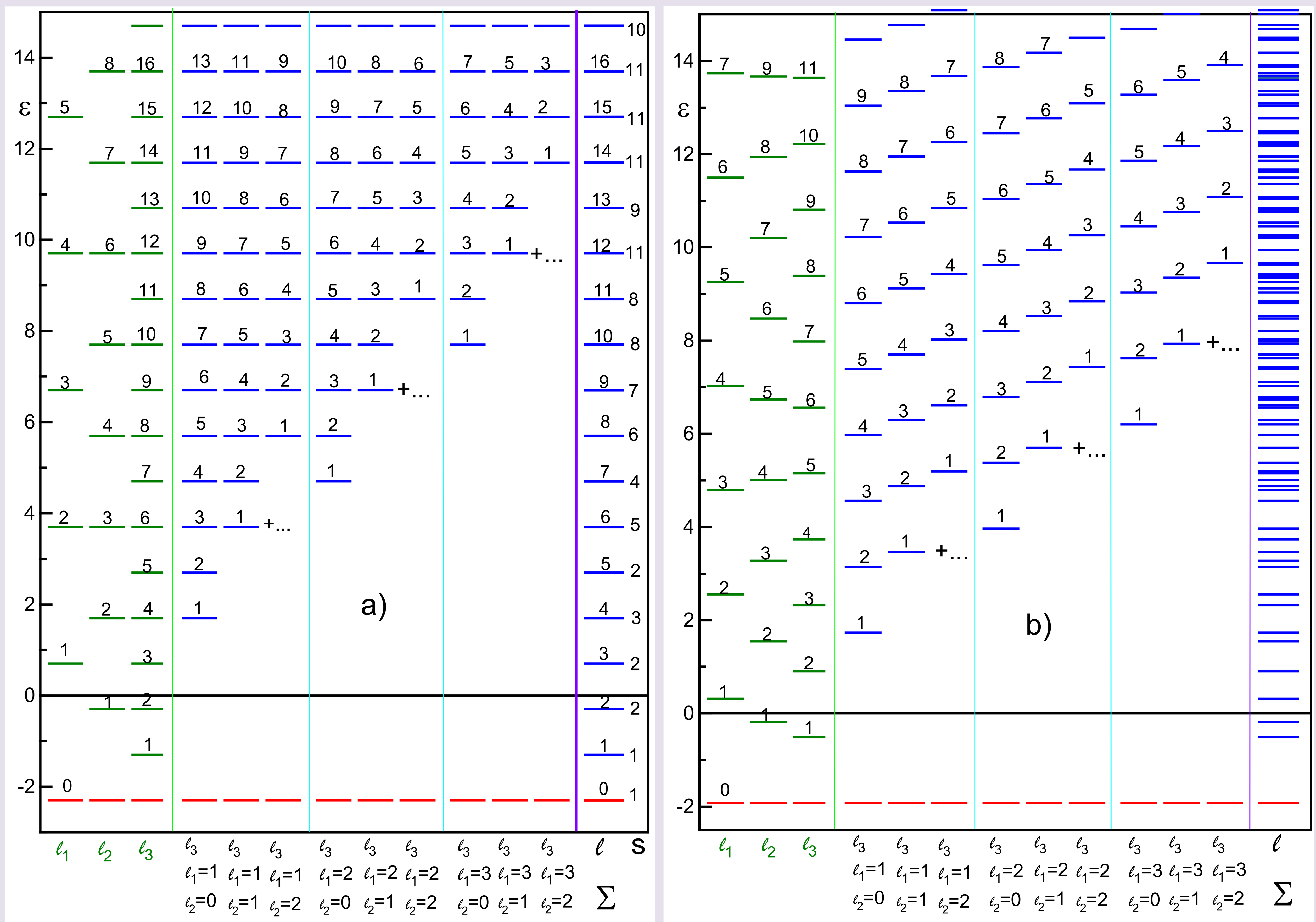

Fig.1. Scheme of the lower part of the degenerate renormalized spectrum of the main and degenerate a) and non-degenerate b) phonon satellite energy levels of the system. Basic level (red line), non-mixed satellite levels (green line), mixed satellite levels (blue line). Σ - total spectrum,ℓ- level number, S - the degree of degeneration. System parameters: $\alpha_1=0{,}5;\ \alpha_2=0{,}3;\ \alpha_3=0{,}2;$ a) $\Omega_1=3;\ \Omega_2=2;\ \Omega_3=1$; b) $\Omega_1=\sqrt{5};\ \Omega_2=\sqrt{3};\ \Omega_3=\sqrt{2}$.

Conclusion

In the proposed paper, for the first time, the problem of the renormalized energy spectrum of a one-level localized quasiparticle interacting with dispersionless three-mode phonons at T = 0K in a model of system with a limiting condition to quasiparticle states is solved exactly. It is shown that the renormalized spectrum of the system is stationary and discrete. In addition to the main level, it contains an infinite number of phonon satellite levels, which can be degenerated or non-degenerated depending on the ratio between the energy magnitudes of three phonon modes. Phonon satellite levels are formed by bound states of quasiparticle with all possible combinations of energies of all three phonon modes.

References

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