Nanostructure with periodic position dependent electron effective mass

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ABSTRACT

This communication has been dedicated to spectral properties of system composing of periodic arrays of layers which form superlattice with electron effective mass dependent on coordinate inside of each layer. We considered one dimensional model which admits to obtain the exact solution of wave equation. The position dependent mass inside the layer was represented by the linear function. We has found wave functions in their explicit and exact forms as well as the secular equation for the energy eiguen values. The energy spectrum of electrons as expected manifests properties typical for periodic nanostructures.

Keywords: superlattice; electron spectrum, position-dependent mass, Schrödinger equation

1. INTRODUCTION

For a long time yet semiconductors superlattices turned out [1] one of the most important functional elements of a lot of nanoelectronics devices such as pillar lasers structures or light emitting diodes et cet. In the last decades considerable progress based on molecular beam epitaxy methods or STM and AFM technologies allows to create numerous nanosystems, superlattices among them, with demanded spectral properties. As a rule, electron energetic spectrum consists of relatively narrow minibands which are formed due to the periodic modulation of the basic properties of supperlattice components such as the conduct band bottom and the valence band top in semiconductor heterojunctions or, for example, periodic doping semiconductor layers. Significant advances in nanoscience have opened the way for synthesis materials, for example, one-dimensional semiconductotr nanostructures [2], with exceptional properties which can allow to construct and produce electronic and optoelectronic devices based on completely new conceptions. Due to technology progress, we can't exclude possibility to create periodic structure like above mentioned examples by space modulation of electron effective mass. That is why a study of spectral properties of system with periodic position-dependent mass can be really interesting enough.

The quantum mechanics of a particle with an effective coordinate-dependent mass for a long time has been and continues to be the subject of a considerable number of studies. This fact is motivated by various circumstances. One of them involves the fun damental quantum dynamics principles related to the conception of mass. The quantum mechanics was created and built up for a particle whose mass as function of generalized coordinates is some constant. When the particle mass becomes position dependent the problem of operator ordering appears [3,4]. The fact is that the operator of linear moment can be positioned in different places in operator of the kinetic energy conducting to some ambiguity in explicit form of Hamiltonian. Considerable relevance of the problem can be confirmed by the fact that even founders of basics quantum conseptions have dedicated their attention and contributed a lot to its resolution. However the ordering ambiguity problem has no complete and final treatment yet. That is why researches of position dependent mass particle have serious reasons for quantum theory. On the other hand, the intensive development of nanotechnology, in the first place of energy bands engineering, fabrication of compositionally graded crystals, heterostructures transfer the above mentioned problem from a purely scientific plane to the practical one in order to create materials with predetermined and predictable properties, which are often determined by the effective mass. Among them we have to point out the density of states, coefficient of optical absorption, transport mobility and other mass sensitive parameters. Than in connection with the foregoing it will be interesting to study some special models of positon-dependent mass systems which admit the exact solution. One of the models is represented in this communication.

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2. DESCRIPTION OF MODEL. MODIFICATED WAVE EQUATION

We considered the layered periodic structure with the axis aliened along axis X. Inside of the layer the electron spectrum is parabolic with the isotropic effective mass in plane of layer and the mass dependent on coordinate X in the direction of superstructure axis. Position dependence of electron effective mass in its natural form appears in nonuniform solid state systems, when due to the coordinate dependent chemical composition some modification requires not only crystal field potential but also the kinetic energy operator. In order to study the effect of mass modification only we proceed from the assumption that the mass of charge carriers in their one-dimensional motion admits to be given by the expression:

$$m(x) = m_0 f(x) \tag{1}$$

where $f(x)$ is a function whose choice will be specified in the below following text.

Note that the explicit form of the kinetic energy operator, due to the above mentioned ambiguity, continues to be discussed intensively in the literature, for example, one can refer to works [3,4]. As it is quite well-known nearly the extreme points of non degenerated energetic bands accordingly to the Wannier theorem [5] the envelope factor of the wave function obeys a Schrödinger-like equation. However, the formal substitution of expression (1) instead the effective electron mass in this equation can not be accepted because this change conducts to the non-hermitian form of the Hamilton's operator. Then the above sub lined ambiguity of the operators ordering appears.

The nature of this ambiguity is quite obvious and lies in the fact the kinetic energy operator no longer commutes with the momentum linear operator $\hat{p}_x = -i\hbar\partial_x$ if the particle's mass $m(x)$ becomes position dependent. Consequently, the problem of momentum linear operator and particle mass ordering appears and demands its resolution. A natural correction of the kinetic energy operator can be reduced to representation [6,7,8] of the kinetic term by the symmetrized form, namely:

$$\hat{H}_c = \frac{1}{4}\left[\frac{1}{m(x)}\hat{p}_x^2 + \hat{p}_x^2\frac{1}{m(x)}\right] \tag{2}$$

but even this choice does not fix the ordering problem.

That is why the number of alternative forms have been proposed. One of the most commonly used approach to organize the momentum and mass operators has been suggested by von Roos [9,10] and can be given as follows:

$$\hat{H}_c = \frac{1}{4}\left[m^{\eta}(x)\hat{p}_x m^{\varepsilon}(x)\hat{p}_x m^{\rho}(x) + m^{\rho}(x)\hat{p}_x m^{\varepsilon}(x)\hat{p}_x m^{\eta}(x)\right] \tag{3}$$

where the parameters ε, ρ, η must satisfy the condition $\varepsilon + \rho + \eta = -1$. Beginning from this expression a lot of concrete models have been proposed and explored. Unfortunately, the early written symmetrical and very simple Hamiltonian does not fit into the scheme recommended by von Ross. This term was added to the von Ross's formula in order to include in consideration the symmetrized or Weyl ordered operator.

In this paper, we prefer to use frequently applied by a lot of authors, see for example works [11,12,14], values, namely $\varepsilon = -1$, $\rho = 0$ and $\eta = 0$, correspond to the Ben Daniel-Duke model [15]. Accordingly to the review [16] this choice allows to conserve the fundamental properties of Hamiltonian and considerable simplifies resolution of wave equation due to the more simple form of effective potential.

Because of the fact that in plane electron movement is free, in the wave equation the commonly used method of separation of variables can be applied. After this approach has been realized and assuming Ben Daniel-Duke's proposal we will have for the Schrödinger equation the following expression:

$$-\frac{\mathrm{h}^2}{2m_0}\partial_x\frac{1}{f(x)}\partial_x\Psi = E\Psi \tag{4}$$

where $\Psi \equiv \Psi(x)$ describes the motion along the superstructure axis and $E = \mathrm{E} - E(\vec{k})$ – energy counted from the energetic band corresponding to the free in plane motion.

Since we try to find an explicit and exact solution of equation (4) further consideration demands to specify the function $f(x)$ which describes coordinate dependence of particle's mass. There are a lot references [16] where some general forms of functions which provide the exact solutions of wave equation (4) have been established. In addition to these general forms in the extensive bibliography one can found some concrete examples where these exact solutions have been explicitly established and corresponding energy eigenvalues have been determined. Here we refer to the studies represented in the paper [5,14,17], where exact solutions of Schrödinger equation with mass given in terms of hyperbolic functions have been found and widely discussed. By the authors of works [12,13,14] the cases relative to description of mass in terms of polynomial functions were thoroughly investigated. Three coordinate distributions of masses combined with modified Morse's and Kratzer's potentials received complete treatment in the paper [17] where the authors applying the point canonical transformation method have found the wave equation exact solutions. A number of authors, see for references[17], develop the super symmetry theory in its operator methods. By using this approach they resolved the eigen functions and eigen values problems for a wide set of special mass distributions.

If exclude the ordering problem, to our knowledge, a majority of studies has been dedicated to resolution of wave equation with position-dependent mass given in terms of some smooth functions. However, for layered systems, such as superlattices, mass distribution is periodic and it can also manifest some sharp change into interfaces. That is why in this paper we try at least slightly to expand the list of exact solutions of position dependent mass problem considering the model which in our opinion could be relevant to nanostructures and other applications. Thus we treat the one-dimensional quantum dynamics of the particle with position dependent effective mass represented by the periodical function given as follows [23,24]:

$$f(x) = \frac{\kappa(x-nL)}{L} + 1 \; ; \; x \in [nL,(n+1)L] \; ; \; n \in Z \tag{5}$$

Accordingly to this choice parameter m_0 is the mass in the left point of period. We also assume that $k \geq 0$. The case corresponding to values $-1 < k \leq 0$ after changing $x \to -x$ admits to apply the below described approach.

Due to the coefficients of Schrödinger equation (4) are periodical functions with the period L its solutions have to satisfy to certain boundary conditions. Having recourse to Floquet theorem [19] we can write the first boundary condition as follows:

$$\Psi(x)\big|_{x=0} = e^{iqL}\,\Psi(x)\big|_{x=L} \tag{6}$$

Concerning the second one it comes up of probability's flux density continuity, that is:

$$\frac{1}{m_0 f(x)}\partial_x\Psi(x)\bigg|_{x=0} = e^{iqL}\,\frac{1}{m_0 f(x)}\partial_x\Psi(x)\bigg|_{x=L} \tag{7}$$

Here q is the wave vector which runs quasi continuous values into the first Brillouin zone $-\frac{\pi}{L} < q \leq \frac{\pi}{L}$

It is convenient to apply the method of coordinate transformation [4] in order to resolve the Couchy's problem (4),(6),(7). Hence we introduce a dimensionless variable y determining it by the expression [25,26]:

$$y = \frac{\kappa}{L} x + 1 \tag{8}$$

By substituting the formula (8) into the equation (4) we rewrite it as follows:

$$-\frac{\mathrm{h}^2}{2m_0}\left(\frac{\kappa}{L}\right)^2 \partial_y \frac{1}{y} \partial_y \Psi = E\Psi \tag{9}$$

In order to simplify the last and below written equations we assume a notice:

$$Q^2 = \frac{2m_0 E}{\mathrm{h}^2}\left(\frac{L}{\kappa}\right)^2 \tag{10}$$

Than we finally obtain

$$y\partial_y^2 \Psi - \partial_y \Psi + Q^2 y^2 \Psi = 0 \tag{11}$$

The equation (11) is the main result for further consideration.

3. WAVE FUNCTIONS AND EIGEN VALUES OF ENERGY

The system of fundamental solutions of equation (11) can be expressed in terms of the Bessel $J_\nu(\xi)$ and Neumann $N_\nu(\xi)$ functions. According to the reference book [19] we have such general solution:

$$\Psi(y) = AyJ_{2/3}\left(\frac{2}{3}Qy^{3/2}\right) + ByN_{2/3}\left(\frac{2}{3}Qy^{3/2}\right) \tag{12}$$

Substitution (12) in the boundary conditions (6) and (7) leads to the following system of equations for coefficients A and B:

$$\begin{cases} Ay_0 J_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right) + By_0 N_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right) = \\ \qquad = e^{iqL}\left[Ay_L J_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right) + By_L N_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)\right] \\ \frac{1}{y_0}\frac{\partial}{\partial y_0}\left[Ay_0 J_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right) + By_0 N_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)\right] = \\ \qquad = e^{iqL}\frac{1}{y_L}\frac{\partial}{\partial y_L}\left[Ay_L J_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right) + By_L N_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)\right] \end{cases} \tag{13}$$

where the notice

$$y_L = 1 + \kappa \tag{14}$$

was introduce.

The dispersion equation can be obtained in the standard way, namely, equaling to zero the system (13) determinant. To simplify the final result one can apply expressions corresponding to the Vronskian of equation (11), as well as the Vronskian relative to the Bessel equation independent solutions [20]. In this way we have found:

$$\frac{6}{\pi}CosqL = y_L\left[J_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)\partial_{y_0}N_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)-\partial_{y_0}J_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)N_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)\right]+$$
$$+y_0\left[J_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)\partial_{y_L}N_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)-\partial_{y_L}J_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)N_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)\right]+ \quad (15)$$
$$+\frac{(y_L^2-y_0^2)}{y_0y_L}\left[J_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)N_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)-J_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)N_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)\right]$$

After specifying all the derivates we have come to the master equation in its final form, namely:

$$\frac{6}{\pi}CosqL = \frac{2(y_L^2-y_0^2)}{y_0y_L}\left[J_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)N_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)-J_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)N_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)\right]-$$
$$-Q\sqrt{y_0}y_L\left[J_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)N_{5/3}\left(\frac{2}{3}Qy_0^{3/2}\right)-J_{5/3}\left(\frac{2}{3}Qy_0^{3/2}\right)N_{2/3}\left(\frac{2}{3}Qy_L^{3/2}\right)\right]- \quad (16)$$
$$-Qy_0\sqrt{y_L}\left[J_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)N_{5/3}\left(\frac{2}{3}Qy_L^{3/2}\right)-J_{5/3}\left(\frac{2}{3}Qy_L^{3/2}\right)N_{2/3}\left(\frac{2}{3}Qy_0^{3/2}\right)\right]$$

Approximate solutions of equation (16) can be obtained for two asymptotic cases, In the first case, taking into account the asymptotic expansions of the Bessel and Neumann functions [20], we come to the equation:

$$\frac{1}{2}\left[\left(y_L\right)^{1/4}+\left(y_L\right)^{-1/4}\right]Cos\left[\frac{2}{3}Q(y_L^{3/2}-1)\right]=CosqL \quad (17)$$

where the terms of order Q^{-1} and superior ones have been neglected. Let us point out that multiplicative factor in equation (16) satisfies to the condition $(y_L^{1/4}+y_L^{-1/4})/2\geq 1$ for all the actual values of parameter κ. Hence the equation (16) always has solutions. By resolving the equation (16), we have obtained:

$$E_n(q)=\frac{\mathrm{h}^2}{2m_0}\left(\frac{3\kappa}{2L(y_L^{3/2}-1)}\right)^2\left\{\pi n+arcCos\left[\frac{2CosqL}{y_L^{1/4}+y_L^{-1/4}}\right]\right\}^2 \quad (18)$$

Regarding the expression (16) and comparing it with the well known results of State Solid Theory [21] we make sure that periodic and linear modulation of particle mass produces the effect similar to the action of periodic potential of perfect crystal whose impact on the electron spectrum comes to the renormalization of the particle mass and formation of energetic bands. Accordingly to Eq. (18), that is for highly exited states , subbands reduce to non dispersed energetic levels and the electron moves in such a way as if its effective mass was constant and renormalized, as follows [27]:

$$m_{eff}=\frac{4}{9\kappa^2}m_0(y_L^{3/2}-1)^2 \quad (19)$$

It is quite obvious that the explicit form of mass renormalization depends on peculiarities of model and the last expression only can be valid for the mass modification determined by Eqs. (1), (5).

In order to verify validity of this result we considered the special case corresponding to limit $\kappa \to 0$.Due to the definitions (1) and (5) the particle mass becomes position independent if κ is equal to zero. Than we have to receive a free particle energy spectrum. Indeed in the case $\kappa = 0$ from equation (15) comes out

$$\lim_{\kappa \to 0} E_n(q) = \frac{\mathrm{h}^2}{2m_0}\left(q + \frac{\pi n}{L}\right)^2 \tag{20}$$

Passing to the extended Brillouin's scheme we naturally obtain the parabolic dispersion law inherent to the free particle.

Returning to the result (17) we note that the periodic modulation of the effective mass by some coordinate dependent function in relation to the energy eigen values plays the same role as the periodic potential, namely, the spectrum splits in allowed energy zones, in each of which the energy is a continuous function of the wave vector. Consequently, one can pass to conclusion that one of the way to expand technologic possibilities of zone spectrum engineering consists in the periodic modulation of the position dependent mass

The width W_n of allowed zone is determined by the expression:

$$W_n = \frac{\pi^2 \mathrm{h}^2 (2n+1)}{2m_0}\left(\frac{3\kappa}{2L(y_L^{3/2}-1)}\right)^2\left(1 - \frac{2}{\pi}\arccos\frac{2}{y_L^{1/4}+y_L^{-1/4}}\right) \tag{21}$$

while the forbidden zone gap E_{gn} has been found as follows:

$$E_{gn} = \frac{\pi^2 \mathrm{h}^2}{m_0}\left(\frac{3\kappa}{2L(y_L^{3/2}-1)}\right)^2\left(n + \frac{1}{2} + \frac{1}{\pi}\arccos\frac{2}{y_L^{1/4}+y_L^{-1/4}}\right) \tag{22}$$

It is interesting to note that neglecting by the dispersion one can obtain the results identical to ones corresponding to the well known problem of the particle in the rectangular potential well [22].

In the second case, that is, if $Qy_L^{1/2} = 1$, after applying the expansion of cylindrical functions in series and restricting us by the main terms only, we have

$$E(q) = \frac{10\mathrm{h}^2}{m_0}\left(\frac{\kappa}{L}\right)^2\left(\frac{1+CosqL}{1+(1+\kappa)^3}\right) \tag{23}$$

Consequently lowly laid branches of energy spectrum is analogous to the energy bands peculiar for the well-known in the Solid State Physics model of the nearest neighbours. It is easy also to see that for small values of wave number, the spectrum admits parabolic approximation with inverted scheme of quadratic energetic band and averaged electron mass which can be in obvious manner determined by correspondent expansion in series of equation (23)

4. CONCLUSION

In the context of the superlattice formed by periodic array of layers with effective mass dependent on coordinate into each of them, electron quantum dynamics has been studied. Assuming that the electron mass inside layer can be expressed as linear function of coordinate aligned along the superlattice axis, effective wave equation has been found in such special mathematic form that allows to obtain its exact solutions. These exact solutions were established not only for eigenfuntion but for secular equation too. The mentioned equation was found by joint applying of boundary conditions and the Floquet theorem and it shows the structure typical for well-known in Solids State Physics

Shrödinger's equations with periodic coefficients such as Kronig-Penney model for example [21,22]. However its solution in explicit form could only be found for two limits.

One of these cases corresponds to dimensionless wave number much more than one. In this case the dispersion law clearly shows the features of superlattice electron spectrum, namely, it consists of energetic subbands separated by forbidden zones. Characteristic properties such as subbands and forbidden zone widths depend on sublattice basic parameters that are period L and angular coefficient κ. Due to these peculiarities the creation of structures with predictable spectral properties becomes possible. The electron spectrum for highly situated energetic subbands turns out weakly depended on wave number and reveals behavior appropriated to one-dimensional rectangular well. The result points out that electron can be considered as the particle confined inside of the layer.

In the case correspondent to the wave number much less than one electron dispersion law is similar to the energetic spectrum in the nearest neighborhoods approximation with the renormalized effective mass and consists of one inverted energetic band.

The obtained results can be also applied to the frequency spectrum of layered photonic crystals with periodic and linear modulation of dielectric permeability.

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