ISSN 1027-5495. Functional Materials, 22, No.4 (2015), p. 524-534.
doi:http://dx.doi.org/10.15407/fm22.04.524

Features of generalized dynamics of quasiparticles in the presence of an external potential field. Part 1. General analysis of the problem

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Received 7 July, 2015

The influence of the external field (electrostatic) of an arbitrary spatial configuration on the common dynamic properties of the free quasiparticle of type of injecting in the semiconductor or dielectric electron is examined. In the quasi-linear approximation with respect to the external field and in the generalized approximation of flat wave in the phase of wave function the completely agreement of simultaneous quantum description (basic) and a description of the classical type (for the dynamics of quasiparticle) is possible. Correlations, which save determinations of basic dynamic characteristics of quasiparticle the same as they are in the absence of an external field established also.
Keywords: quasiparticle, quasi-linear approximation

Рассматривается влияние внешнего поля (электростатического) произвольной пространственной конфигурации на свойства свободной квазичастицы типа инжектированного в полупроводник или диэлектрик электрона. В квазилинейном приближении по внешнему полю и в обобщенном приближении плоской волны в фазе можно полностью согласовать одновременное квантовое описание (базовое) и описание классического типа (для неравномерной динамики квазичастицы). Установлены также соотношения, которые сохраняют определения основных динамических характеристик квазичастицы такими, какими они являются в отсутствие внешнего поля.

Про особливості узагальненої динаміки квазічастинки при наявності зовнішнього потенційного поля. Частина 1. Загальний аналіз проблеми. *Л.В.Шмельова, А.Д.Супрун*

Розглядається вплив зовнішнього поля (електростатичного) довільної просторової конфігурації на властивості вільної квазічастинки типу інжектованого в напівпровідник або діелектрик електрона. У квазілінійному наближенні по зовнішньому полю і в узагальненому наближенні плоскої хвилі у фазі можна повністю узгодити одночасний квантовий опис (базовий) та опис класичного типу (для нерівномірної динаміки квазічастинки). Встановлено також співвідношення, які зберігають визначення основних динамічних характеристик квазічастинки такими, якими вони є у відсутність зовнішнього поля.

1. Introduction

The features of dynamic properties of free quasiparticle of type of injected into semiconductor or dielectric electron were analyzed in the article [1]. There were shown, that these features based on one of the main characteristics of the excited states of condensed matter – on the dispersive dependence of energy or frequency on the wave vector [2 ÷ 5]. An electron is here considered, which is injected into the semiconductor (dielectric), in the external (electric) field of arbitrary, but weakly variable, spatial configuration. It is shown that under certain conditions the quantum description and the description of the classical type may be in full agreement. Thus, the description of the classic type is an element of the wave functions as a phase summand. This summand has a sense of physical action for the point of conditional localization of quasiparticle. The correlations that keep the determinations of the basic dynamic characteristics of the quasiparticles the same as they are in the absence of an external field were established.

2. Materials and methods (common remarks about dynamic properties of quasiparticles in external potential field)

2.1. Basic relations: functional of quasiparticle in the external potential field. For further analysis of influence of the external field on dynamic properties of a quasiparticle, we will use the standard functional [6, 7]:

$$E\left(\{a\}\right) = \sum_{\mathbf{n}} W_{\mathbf{n}}|a_{\mathbf{n}}|^2 + (1/2)\sum_{\mathbf{n}\,\mathbf{m}}{}^{/}\left(M_{\mathbf{n}\,\mathbf{m}} + W^M_{\mathbf{m}-\mathbf{n},\mathbf{n}}\right)\left(a^*_{\mathbf{n}}a_{\mathbf{m}} + a^*_{\mathbf{m}}a_{\mathbf{n}}\right).$$

Here $a_{\mathbf{n}}$ – has a meaning of the unknown part of a wave function of the excited state of crystal, which is to be determined by a conditions of the dynamical Hamiltonian minimization of the functional $E\left(\{a\}\right)$ [8], simultaneously with its eigen-values. This condition is equivalent to the procedure of diagonalization of the operator, which corresponds to the functional under investigation [9]. Other, known, parts of the wave function of crystal determines matrix elements$W_{\mathbf{n}}$, $W^M_{\mathbf{m}-\mathbf{n},\mathbf{n}}$ and $M_{\mathbf{n}\,\mathbf{m}}$. Particularly, $W_{\mathbf{n}}$ and $W^M_{\mathbf{m}-\mathbf{n},\mathbf{n}}$ – are energies, which determine interaction between excitation and the external field. For the electron, which was injected into the conduction band in the case of a monoatomic semiconductor, they are determined by the matrix elements:

$$W_{\mathbf{n}} \equiv \langle \phi^*_{\mathrm{c}}\left(\mathbf{r}-\mathbf{n}\right)\ \left|W\left(\mathbf{r}\right)\right|\phi_{\mathrm{c}}\left(\mathbf{r}-\mathbf{n}\right)\rangle \equiv \langle \phi^*_{\mathrm{c}}\left(\mathbf{r}\right)\ \left|W\left(\mathbf{r}+\mathbf{n}\right)\right|\phi_{\mathrm{c}}\left(\mathbf{r}\right)\rangle; \tag{1}$$

$$W^M_{\mathbf{m}-\mathbf{n},\mathbf{n}} \equiv \langle \phi^*_{\mathrm{c}}\left(\mathbf{r}-\mathbf{n}\right)\ \left|W\left(\mathbf{r}\right)\right|\phi_{\mathrm{c}}\left(\mathbf{r}-\mathbf{m}\right)\rangle \equiv \langle \phi^*_{\mathrm{c}}\left(\mathbf{r}\right)\ \left|W\left(\mathbf{r}+\mathbf{n}\right)\right|\phi_{\mathrm{c}}\left(\mathbf{r}-\left(\mathbf{m}-\mathbf{n}\right)\right)\rangle, \tag{2}$$

where $\phi_{\mathrm{c}}\left(\mathbf{r}-\mathbf{n}\right)$ – are the Wannier wave functions for the conduction band, which, in the case of a monatomic crystal, may be identified approximately as wave functions of the appropriate one-electron ion, which is centred by the spatial coordinate $\mathbf{n}$. Matrix elements $M_{\mathbf{n}\,\mathbf{m}}$ determine energy of the resonant exchange interaction, definition of which for various cases may be found in [6, 7]. Subscript "c" within definitions (1) and (2) symbolizes the quantum number, which corresponds to the conduction band, into which electron was injected.

Further, we will analyze the functional $E\left(\{a\}\right)$ in the approximation of the nearest neighbours, which is typical for crystals: $\mathbf{m} = \mathbf{n} + \mathbf{b}_\alpha$, where $b_\alpha$are vectors of the lattice constants ($\alpha = 1, 2, 3$). Then:

$$E\left(\{a\}\right) = \sum_{\mathbf{n}} W_{\mathbf{n}} \cdot |a_{\mathbf{n}}|^2 + (1/2)\sum_{\mathbf{n},\alpha}\left\{\left(M_{\mathbf{b}_\alpha} + W^M_{\mathbf{b}_\alpha,\mathbf{n}}\right)\left(a^*_{\mathbf{n}}a_{\mathbf{n}+\mathbf{b}_\alpha} + a^*_{\mathbf{n}+\mathbf{b}_\alpha}a_{\mathbf{n}}\right)\right\}. \tag{3}$$

2.2. Approximation of the homogeneous external potential field with respect to the variable n. Until now, functional (3) is an accurate one with respect to the field addends $W_{\mathbf{n}}$ and $W^M_{\mathbf{b}_\alpha,\mathbf{n}}$, because no assumptions were made with respect to these field addends. Energies $W_{\mathbf{n}}$ and $W^M_{\mathbf{b}_\alpha,\,\mathbf{n}}$ are regarded as weakly-varying within the approximation of the uniform external field with respect to the variable $\mathbf{n}$ and they may be expanded in Taylor's series near point $\mathbf{n}_*$. Summands, linear in relation to a difference $\mathbf{n}-\mathbf{n}_*$, are taken into account only. Vector $\mathbf{n}_*$ is constant with respect to the variable $\mathbf{n}$, but it may depend on time t because of a quasiparticle in the external field may have a non-uniform dynamics. It is possible to assert in this sense, that $\mathbf{n}_*$ has nature of variable of classic type (has the signs of material point).

Thus, there are the representations:

$$W_{\mathbf{n}} \approx W_{\mathbf{n}_*} + \{\mathbf{n}-\mathbf{n}_*\}\cdot\mathbf{J}_{\mathbf{n}_*};\quad W^M_{\mathbf{b}_\alpha,\mathbf{n}} \approx W^M_{\mathbf{b}_\alpha,\mathbf{n}_*} + \{\mathbf{n}-\mathbf{n}_*\}\cdot\mathbf{J}^M_{\mathbf{b}_\alpha,\mathbf{n}_*}, \tag{4}$$

where

$$\mathbf{J}_{\mathbf{n}_*} \equiv \nabla_{\mathbf{n}_*}(W_{\mathbf{n}_*})\,; \quad \mathbf{J}^M_{\mathbf{b}_\alpha,\mathbf{n}_*} \equiv \nabla_{\mathbf{n}_*}\left(W^M_{\mathbf{b}_\alpha,\mathbf{n}_*}\right). \tag{5}$$

From the point of view of the physical sense, variable $\mathbf{n}_*(t)$ may be interpreted as the point of conditional localization of the source of field. It is obvious that in order to ensure fulfilment of approximations (4) this point must have a certain dynamics, which is to be agreed with the dynamics of a quasiparticle. An issue of such consistency is one of the problems solved in this article.

Inequalities $\left|\mathbf{J}^M_{\mathbf{b}_\alpha,\mathbf{n}_*}\right| << |\mathbf{J}_{\mathbf{n}_*}|$, which follows from the definitions (1), (2), makes it possible to simplify functional (3) and reduce it to the approximate form:

$$E(\{a\}) = \sum_{\mathbf{n}}(W_{\mathbf{n}_*} + \{\mathbf{n}-\mathbf{n}_*\}\cdot\mathbf{J}_{\mathbf{n}_*})|a_{\mathbf{n}}|^2 + (1/2)\sum_{\mathbf{n},\alpha}\left\{\tilde{M}_{\mathbf{b}_\alpha,\mathbf{n}_*}\left(a^*_{\mathbf{n}}a_{\mathbf{n}+\mathbf{b}_\alpha} + a^*_{\mathbf{n}+\mathbf{b}_\alpha}a_{\mathbf{n}}\right)\right\}, \tag{6}$$

where the following designation is used: $\tilde{M}_{\mathbf{b}_\alpha,\mathbf{n}_*} \equiv M_{\mathbf{b}_\alpha} + W^M_{\mathbf{b}_\alpha,\mathbf{n}_*}$. Further on, it is possible to neglect by the field addend $W^M_{\mathbf{b}_\alpha,\mathbf{n}_*}$ in the weak fields, which are characterized by the inequality $|M_{\mathbf{b}_\alpha}| >> \left|W^M_{\mathbf{b}_\alpha,\mathbf{n}_*}\right|$. Then, only $M_{\mathbf{b}_\alpha}$will be present in functional (6) instead of $\tilde{M}_{\mathbf{b}_\alpha,\mathbf{n}_*}$. Taking this fact into consideration while minimizing functional (6) by means of the method of dynamic Hamiltonian minimization [1, 8], the Hamiltonian equation of classical mechanics may be written:

$$\frac{\partial a_{\mathbf{n}}}{\partial t} = \frac{1}{i\hbar}\cdot\frac{\partial E}{\partial a^*_{\mathbf{n}}}; \qquad i\hbar\,\frac{\partial a^*_{\mathbf{n}}}{\partial t} = -\frac{\partial E}{\partial a_{\mathbf{n}}}, \tag{7}$$

while analyzing purely quantum factors (functional $E(\{a\})$ and functions a_n) as classic ones. If we substitute functional (6) into (7), we will obtain:

$$i\,\hbar\,\frac{\partial a_n}{\partial t} - \{W_{\mathbf{n}_*} + \{\mathbf{n}-\mathbf{n}_*\}\cdot\mathbf{J}_{\mathbf{n}_*}\}a_{\mathbf{n}} - \frac{1}{2}\sum_\alpha M_{\mathbf{b}_\alpha}(a_{\mathbf{n}+\mathbf{b}_\alpha} + a_{\mathbf{n}-\mathbf{b}_\alpha}) = 0. \tag{8}$$

Equation (8) is a complex one, therefore most general representation of its solution determined by a record:

$$a_{\mathbf{n}}(t) = \phi_{\mathbf{n}}(t)\cdot\exp\left[i\cdot\Gamma_{\mathbf{n}}(t)\right]. \tag{9}$$

Taking representation of potential energies (4) into consideration, we will also construct solution (9) in linear approximation with respect to phase, while considering that this phase is equal to:

$$\Gamma_{\mathbf{n}}(t) = \mathbf{n}\cdot\mathbf{k}(t) - \gamma(t). \tag{10}$$

Substantially, representation of phase in the form of (10) is the generalized approximation of the plane wave in phase. Generality of this approximation is connected with the dependence of the wave vector $\mathbf{k}$ on time t and more general time dependence (if compared with $\omega\,t$ dependence) of the energy phase addend γ. Representation (10) also may be called Lagrange-Hamilton approximation in phase.

Substitution of (10) into (9), the further substitution of (9) into (8) and separation of real part from imaginary one, leads to the system of two equations. Further on, these two equations will be analyzed in the following approximations: cubic lattice approximation: $\mathbf{b}_\alpha = b_0\mathbf{e}_\alpha$, continuous approximation of the second order (taking into account the typical situation: $M_{b_0} = -|M_{b_0}|$, which immediately follows from the expression for matrix element $M_{\mathbf{n}\,\mathbf{m}}$), and accounting of the transformation to the dimensionless variables. As a result these two equations will take the following form:

$$\frac{\partial\phi}{\partial\tau} + \sin(p_\alpha)\,\frac{\partial\phi}{\partial x_\alpha} = 0; \tag{11}$$

$$\frac{1}{2}\cos(p_\alpha)\,\frac{\partial^2\phi}{\partial x_\alpha^2} + \left[\overset{\bullet}{\gamma} + \sum_\sigma\cos(p_\sigma) + v_{\mathbf{r}_*} - \mathbf{r}_*\cdot\mathbf{\Pi}_{\mathbf{r}_*} - \mathbf{r}\cdot\left\{\overset{\bullet}{\mathbf{p}} - \mathbf{\Pi}_{\mathbf{r}_*}\right\}\right]\phi = 0. \tag{12}$$

Here, the following designations are used: $\tau = \dfrac{|M_{b_0}|}{\hbar}t$; $\mathbf{\Pi}_{\mathbf{r}_*} \equiv -\dfrac{b_0 \mathbf{J}_{\mathbf{R}_*}}{|M_{b_0}|}$; $v_{\mathbf{r}_*} \equiv -\dfrac{W_{\mathbf{R}_*}}{|M_{b_0}|}$; $p_\alpha \equiv k_\alpha b_0$; $\overset{\bullet}{\mathbf{p}} \equiv \dfrac{d\mathbf{p}}{d\tau}$; $\overset{\bullet}{\gamma} \equiv \dfrac{d\gamma}{d\tau}$; obvious overdeterminations of variables $\mathbf{n}$ and $\mathbf{n}_*$ are made as well:

$$\mathbf{n} \equiv \mathbf{R_n} \Rightarrow \mathbf{R} = (X, Y, Z) \equiv b_0\,(x_1, x_2, x_3) \equiv b_0\mathbf{r}$$

$$\mathbf{n}_* \equiv \mathbf{R}_{\mathbf{n}_*} \Rightarrow \mathbf{R}_* = (X_*, Y_*, Z_*) \equiv b_0\left(x_*^1, x_*^2, x_*^3\right) \equiv b_0\mathbf{r}_*\ .$$

Here, x_1, x_2, x_3 are dimensionless forms of variables X, Y, Z, and x_*^1, x_*^2, x_*^3 are dimensionless forms of variables X_*, Y_*, Z_*.

It is necessary to note that there exists the relation $\mathbf{\Pi}_{\mathbf{r}_*} = \nabla_{\mathbf{r}_*}(v_{\mathbf{r}_*})$ between dimensionless energy $v_{\mathbf{r}_*}$ and dimensionless force (field intensity), which may be obtained by bringing of the first (left) relation in (5) to dimensionless form.

Further it is convenient to use the designations, which are well-founded in [1], as the main dynamic characteristics of a quasiparticle. Namely, to introduce such designations for the components of vector of dimensionless velocity and for the components of dimensionless tensor of efficient mass (here – the diagonal tensor), respectively:

$$\beta_\alpha \equiv \sin(p_\alpha)\,, \quad \mu_\alpha \equiv 1/\cos(p_\alpha). \tag{13}$$

It should be noted that relations (13) are only designations, which yet have no any "Hamiltonian-Lagrangian"sense, as in [1]. Therefore, purpose of the present research (at the least, one of the main purposes) – to find the answer on the question – whether it is possible to reproduce the same sense of these relations in the presence of an external field. Taking into consideration the designation (13) and introducing an additional designation: $\overset{\bullet}{\gamma} \equiv \Omega$, it is possible to write down equations (11) and (12), eventually, in the following form:

$$\frac{\partial\phi}{\partial\tau} + \boldsymbol{\beta}\cdot\nabla_{\mathbf{r}}\phi = 0; \tag{14}$$

$$\frac{1}{2\mu_\alpha}\cdot\frac{\partial^2\phi}{\partial x_\alpha^2} + \mathbf{r}\cdot\left\{\mathbf{\Pi}_{\mathbf{r}_*} - \overset{\bullet}{\mathbf{p}}\right\}\phi + \left(\Omega + \sum_\sigma \frac{1}{\mu_\sigma} + v_{\mathbf{r}_*} - \mathbf{r}_*\cdot\mathbf{\Pi}_{\mathbf{r}_*}\right)\phi = 0. \tag{15}$$

Here, $\boldsymbol{\beta}$ is the vector having componentsβ_α, which are determined in (13).

2.3. Solutions and their analysis. General solution of equation (14) is an arbitrary function of variable $\rho \equiv \mathbf{r} - \mathbf{r}_0$. In this case, vector $\mathbf{r}_0$ having components x_0^α $(\alpha = 1, 2, 3)$ will be determined by dynamic equations of a classic type:

$$\overset{\bullet}{\mathbf{r}}_0 = \boldsymbol{\beta}. \tag{16}$$

One of the purposes of the research consist in the consideration of the equation (16) as the equation, which follow from Hamiltonian equations.

Equation (15), which remained, is used to find the amplitude $\phi(\rho)$. If to formulate (15) relatively a new variable ρ, taking into account that $\mathbf{r}_0$ is constant with respect to $\mathbf{r}$, then this equation will take the following form:

$$\frac{1}{2\mu_\alpha}\cdot\frac{\partial^2\phi}{\partial\rho_\alpha^2} + \boldsymbol{\rho}\cdot\left\{\mathbf{\Pi}_{\mathbf{r}_*} - \overset{\bullet}{\mathbf{p}}\right\}\phi + \left(\Omega + \sum_\sigma \frac{1}{\mu_\sigma} + v_{\mathbf{r}_*} - \mathbf{r}_*\cdot\mathbf{\Pi}_{\mathbf{r}_*} + \mathbf{r}_0\cdot\left\{\mathbf{\Pi}_{\mathbf{r}_*} - \overset{\bullet}{\mathbf{p}}\right\}\right)\phi = 0. \tag{17}$$

Here, ρ_α – are components of vector $\boldsymbol{\rho} \equiv \mathbf{r} - \mathbf{r}_0$. Further it is necessary to take into attention the dependence on time of the momentum $\mathbf{p}$ with components p_α. Due to this fact, all addends to the equation (17) depend on time. In order to agree solutions of this equation with the solution of equation (14) in the form of arbitrary function $\phi(\rho)$, it is necessary to make sure of fulfilment of stationary conditions for this function provided that these conditions will ensure that no additional dependence on time τ will exist (except for $\mathbf{r}_0(\tau)$) in a certain approximation, at the very least. For this it is necessary, foremost, to define duly dimensionless energy Ω which, in accordance with equality $\overset{\bullet}{\gamma} \equiv \Omega$, has the physical sense of quantum eigenvalue of the examined system quasiparticle-field. This value here may, in general, depend on time. By introducing "eigenvalue" ε for equation (17) with the help of following relation:

$$\Omega = \varepsilon - \sum_{\sigma} \frac{1}{\mu_\sigma} - v_{\mathbf{r}_*} + \mathbf{r}_* \cdot \mathbf{\Pi}_{\mathbf{r}_*} - \mathbf{r}_0 \cdot \left\{ \mathbf{\Pi}_{\mathbf{r}_*} - \overset{\bullet}{\mathbf{p}} \right\}, \tag{18}$$

it is possible to reduce equation (17) to the form:

$$\frac{1}{2\mu_\alpha} \cdot \frac{\partial^2 \phi}{\partial \rho_\alpha^2} + \boldsymbol{\rho} \cdot \left\{ \mathbf{\Pi}_{\mathbf{r}_*} - \overset{\bullet}{\mathbf{p}} \right\} \phi + \varepsilon \phi = 0. \tag{19}$$

Taking into account the stationary conditions, it is necessary that new "eigenvalue"ε must be constant not only with respect to the variable ρ, but also with respect to the time. However, we do not make now any assumptions about the dependence of this energy from time.

Equation (19) allows the separation of variables, if the energy ε represented as a sum, and the amplitude of the wave function $\phi(\rho)$ – in the form of a product:

$$\varepsilon = \frac{1}{\mu_\alpha} \varepsilon_\alpha, \quad \phi(\rho) = \phi_1(\rho_1)\, \phi_2(\rho_2)\, \phi_3(\rho_3). \tag{20}$$

If to substitute (20) into equation (19) and divide the obtained result on , then for each component α, in accordance with the method of separation of variables, it is possible, ultimately, to obtain a separate equation:

$$\frac{1}{2\mu_\alpha} \cdot \frac{\partial^2 \phi_\alpha}{\partial \rho_\alpha^2} + \rho_\alpha \left(\Pi^\alpha_{\mathbf{r}_*} - \overset{\bullet}{p}_\alpha \right) \phi_\alpha + \frac{\varepsilon_\alpha}{\mu_\alpha} \phi_\alpha = 0. \quad \alpha = 1, 2, 3. \tag{21}$$

In this case (18) will take the form:

$$\Omega = -\frac{1}{\mu_\alpha} (1 - \varepsilon_\alpha) - v_{\mathbf{r}_*} + \mathbf{r}_* \cdot \mathbf{\Pi}_{\mathbf{r}_*} - \mathbf{r}_0 \cdot \left\{ \mathbf{\Pi}_{\mathbf{r}_*} - \overset{\bullet}{\mathbf{p}} \right\}. \tag{22}$$

Now, let us consider the choice of derivatives $\overset{\bullet}{p}_\alpha$. According to physical sense, values p_α are the components of the dimensionless wave momentum $\mathbf{p}$. Therefore, in the language of classical mechanics it comes to the formulation of the dynamic equations of motion, that will complement the equation (16), for spot quasiparticle localized in point $\mathbf{r}_0$. If one will introduce some force $\mathbf{G}$, which is unknown yet and which has components G_α, then such motion equation will formally take the form:

$$\overset{\bullet}{\mathbf{p}} = \mathbf{G}. \tag{23}$$

In this case, the system of equations (21) and equation (22) takes the form:

$$\frac{1}{2\mu_\alpha} \cdot \frac{\partial^2 \phi_\alpha}{\partial \rho_\alpha^2} + \rho_\alpha \left(\Pi^\alpha_{\mathbf{r}_*} - G_\alpha \right) \phi_\alpha + \frac{\varepsilon_\alpha}{\mu_\alpha} \phi_\alpha = 0, \quad \alpha = 1, 2, 3. \tag{24}$$

$$\Omega = -\frac{1}{\mu_\alpha} (1 - \varepsilon_\alpha) - v_{\mathbf{r}_*} + \mathbf{r}_* \cdot \mathbf{\Pi}_{\mathbf{r}_*} - \mathbf{r}_0 \cdot \{ \mathbf{\Pi}_{\mathbf{r}_*} - \mathbf{G} \}. \tag{25}$$

In equations (24) multipliers $\left(\Pi^\alpha_{\mathbf{r}_*} - G_\alpha \right)$ have sense of the components of force. At first it seems that is necessary to suppose the difference $\Pi^\alpha_{\mathbf{r}_*} - G_\alpha$ equal to G_α because it is the same forces. However, actually it is not so. That is, the force is really one and the same, but it is considered in different frames of reference. Namely, equation (23) is formulated in a global (laboratory) coordinate system, which is related to the crystal lattice. Consequently, the force (desired) has components G_α in this system. Equation (24), on the contrary, is formulated in the local frame of reference, which is connected with point $\mathbf{r}_0$. The dynamics of this point determined by motion equations (16) and (23). Consequently, in the equations (24), the components of this unknown force, which is denoted by F_α, would be possible to determine by the relation: $\Pi^{\alpha}_{\mathbf{r}_*} - G_\alpha = F_\alpha$. However, this is as well not the best choice, because, in addition, it is also necessary to take care on fulfilment of the stationary conditions (at least approximately). It may be seen at once that in the course of selection of components F_α with the help of the following relation:

$$\Pi^{\alpha}_{\mathbf{r}_*} - G_\alpha = \frac{F_\alpha}{\mu_\alpha}, \tag{26}$$

we may, firstly, cancel out multipliers $1/\mu_\alpha$ in all equations (24), because these multipliers essentially depend on time, and, secondly, we will get practically a transformation for the components of the desirable force, while we do not know its value yet. In the end, equation (24) will take the form:

$$\frac{1}{2} \cdot \frac{\partial^2 \phi_\alpha}{\partial \rho_\alpha^2} + \rho_\alpha F_\alpha \phi_\alpha + \varepsilon_\alpha \phi_\alpha = 0; \quad \alpha = 1, 2, 3. \tag{27}$$

These equations coincide with the dimensionless stationary equations of Schrödinger for the unit mass object in the external uniform field of arbitrary orientation (with respect to variables ρ_α) provided that components of forces F_α and energies ε_α are constants. It is obvious, that in the cases when F_α and ε_α are really constants, then stationary conditions will be complied with fully, and energies ε_α have an immediate status of eigenvalue in equations (27).

Consequently, it is possible to draw some conclusions. Firstly, taking into account (26), we have for energies (25):

$$\Omega = -\frac{1}{\mu_\alpha}(1 - \varepsilon_\alpha) - v_{\mathbf{r}_*} + \mathbf{r}_* \cdot \mathbf{\Pi}_{\mathbf{r}_*} - \mathbf{r}_0 \cdot \widehat{\mu}^{-1}\mathbf{F}. \tag{28}$$

Here, we have taken into account that μ_α are components of the diagonal tensor of the efficient mass, which may be designate as $\widehat{\mu}$. Then, it is possible to consider all components of factors $\frac{1}{\mu_\alpha} F_\alpha$ as components of the vector, formed as a product of matrix $\widehat{\mu}^{-1}$ on vector $\mathbf{F}$. Secondly, we have three of the Schrödinger equation (27) that are, at the time being, considered as stationary. It is worth to note that even if these equations are not stationary ones, i.e. when F_α and ε_α will depend on time, solutions will be the same, as in the stationary situation, because time is included to the equation (27) in parametric representation. Solutions of equations (27) are known and they are of the form of [10]:

$$\phi_\alpha(\rho_\alpha) = \sqrt[6]{\frac{4}{|F_\alpha|}} Ai\left(-\sqrt[3]{2|F_\alpha|}\left\{\rho_\alpha + \frac{\varepsilon_\alpha}{F_\alpha}\right\}\right), \tag{29}$$

where $Ai(x) \equiv \frac{1}{\pi}\int\limits_0^\infty \cos\left(xy + \frac{y^3}{3}\right) dy$. These solutions take such a form only in the case $F_\alpha \neq 0$. In other case, it is the plane wave: $\phi_\alpha(\rho_\alpha) \sim \exp\left(i\,\rho_\alpha\sqrt{2\varepsilon_\alpha}\right)$.

And, at last, we have a classical motion equations (16), (23):

$$\overset{\bullet}{\mathbf{r}}_0 = \boldsymbol{\beta}; \quad \overset{\bullet}{\mathbf{p}} = \mathbf{G}, \tag{30}$$

which describe classical dynamics of some object, which is localized in point $\mathbf{r}_0$, if value of force $\mathbf{G}$ as a function of $\mathbf{r}_0$ is already set, as well as, if the correlation between momentum $\mathbf{p}$ and velocity $\boldsymbol{\beta}$ is known. Here, such correlation determined with the help of the relations (13): $\beta_\alpha = \sin(p_\alpha)$, therefore we may raise a question about the Lagrangian-Hamiltonian nature of classical dynamics of this object.

As it was already mentioned above (after the expression (25)) forces $\mathbf{F}$ and $\mathbf{G}$ are one and the same force, but in different frames of reference. They remain unknown as yet, but are related by the conditions (26), vector form of which is as follows:

$$\mathbf{\Pi}_{\mathbf{r}_*} - \mathbf{G} = \widehat{\mu}^{-1}\mathbf{F}. \tag{31}$$

This equation is possible to interpret as the law of transformation of forces in the course of transition from one frame of reference to another one.

In the general case, components F_α of force $\mathbf{F}$ and energies ε_α will depend on time (particularly, through the dynamic variables $\mathbf{r}_0$ and $\mathbf{p}$ (or β)). This will leads, in its turn, to infringement of the stationary conditions (occurrence of additional (except for $\mathbf{r}_0(\tau)$) dependence of solution $\phi(\rho)$ on the dimensionless time τ). It is possible to make attempt to decrease an influence of such dependence by means of choice of "eigenvalues"ε_α, for example, in the form:

$$\varepsilon_\alpha = \xi_\alpha F_\alpha, \tag{32}$$

requiring that parameters ξ_α would be constants. In order to clarify physico-mathematical nature of parameters ξ_α we will substitute the value (32) into the energy ε, which is determined in (20). As the result of this, it is possible to provide this value to the form of scalar product: $\varepsilon = \boldsymbol{\xi} \cdot \widehat{\mu}^{-1}\mathbf{F}$, that is, product of a force vector $\widehat{\mu}^{-1}\mathbf{F}$ and vector of some coordinate $\boldsymbol{\xi}$. In the future, it will be important that vector $\boldsymbol{\xi}$, (more exactly, its components ξ_α) will undertake status of the eigenvalues (which are unknown yet) instead of the value ε_α and that they will be subject to further determination.

As it may be seen from the explicit form of the solutions $\phi_\alpha(\rho_\alpha)$, which are presented in (29), such replacement (32) does not provide us with possibility to avoid this additional dependence on τ completely, if even components ξ_α are constants. This is conditioned by the fact that dependence of the amplitude factor and growth rate from time may be irremovable if force $\mathbf{F}$ is not constant in time. In this case, there is no necessity for the time being to be anxious about constancy of vector $\boldsymbol{\xi}$, which has components ξ_α, also. But then it is necessary to investigate the conditions of quasi-stationarity, and for this is first necessary to consider the representation (32) in (27) - (29).

Taking into account the representation (32), energy (28) will take the form:

$$\Omega = -\sum_\alpha \frac{1}{\mu_\alpha} - v_{\mathbf{r}_*} + \mathbf{r}_* \cdot \mathbf{\Pi}_{\mathbf{r}_*} - \{\mathbf{r}_0 - \boldsymbol{\xi}\} \cdot \widehat{\mu}^{-1}\mathbf{F}, \tag{33}$$

equations of Schrödinger (27) and their solutions (29) will reduce to such expressions:

$$\frac{1}{2} \cdot \frac{\partial^2 \phi_\alpha}{\partial \rho_\alpha^2} + (\rho_\alpha + \xi_\alpha) F_\alpha \phi_\alpha = 0; \quad \alpha = 1,2,3, \tag{34}$$

$$\phi_\alpha(\rho_\alpha) \equiv A_\alpha Ai\left(-\lambda_\alpha\{\rho_\alpha + \xi_\alpha\}\right), \tag{35}$$

where the designations are obvious: $A_\alpha \equiv \sqrt[6]{\dfrac{4}{|F_\alpha|}}$, $\lambda_\alpha \equiv \sqrt[3]{2|F_\alpha|}$. It may be seen that the following correlations $A_\alpha = \sqrt{2/\lambda_\alpha}$ or $\lambda_\alpha = 2/A_\alpha^2$ are fulfilled between parameters A_α and λ_α.

Having now solutions of equations of Schrödinger (34) in the form of a (35), we will transform them (in accordance with definition $\boldsymbol{\rho} \equiv \mathbf{r} - \mathbf{r}_0$) into “global” frame of reference (which is connected with crystal):

$$\phi_\alpha(\tau, x_\alpha) = A_\alpha Ai\left(-\lambda_\alpha\{x_\alpha - x_0^\alpha + \xi_\alpha\}\right).$$

Now, in order to find conditions of quasi-stationarity of the entire solution:

$$\phi = \prod_{\alpha=1}^{3} A_\alpha Ai\left(-\lambda_\alpha\{x_\alpha - x_0^\alpha + \xi_\alpha\}\right), \tag{36}$$

it is necessary to return to the equation (14), taking into account that coefficients A_α and λ_α in the general case are functions of time τ. That is, conditions, under which signification of ϕ was obtained, satisfy the equation (14) accurately or approximately. That is, we seek conditions under which the signification obtained for ϕ exactly or approximately satisfies the equation (14).

If we will substitute solution (36) into equation (14) and take into account the first (left) equation from equations (30), then it is possible to obtain such condition:

$$\phi \sum_\alpha \left[\frac{\overset{\bullet}{A}_\alpha}{A_\alpha} - \left\{ \overset{\bullet}{\lambda}_\alpha (\rho_\alpha + \xi_\alpha) + \lambda_\alpha \overset{\bullet}{\xi}_\alpha \right\} \frac{Ai'(-\eta_\alpha)}{Ai(-\eta_\alpha)} \right] = 0. \tag{37}$$

In the condition (37), differentiation of function $Ai\,(...)$ is performed with respect to the variable η_α, which, in accordance with definition (35), determined by the identity: $\eta_\alpha \equiv \lambda_\alpha\,(\rho_\alpha + \xi_\alpha)$. Formally, condition (37) results to the fact that solution (35) satisfies the equation (14) accurately. However, it is clear that accurate fulfilment of such conditions is impossible, because imposes a correlation between four independent variables: between the time τ and components x_α of vector $\mathbf{r}$. This means that it is possible to speek about the condition of a quasistationarity only, for example, in the form:

$$\left|\phi \sum_\alpha \left[\frac{\dot{A}_\alpha}{A_\alpha} - \left\{\dot{\lambda}_\alpha\,(\rho_\alpha + \xi_\alpha) + \lambda_\alpha \dot{\xi}_\alpha\right\}\frac{Ai'\,(-\eta_\alpha)}{Ai\,(-\eta_\alpha)}\right]\right| < \delta; \quad \delta << 1.$$

Because of it is inessential now within which frame of reference it is necessary to analyze this condition, then it is convenient (for it simplification) to return to the local frame of reference (which is connected with the point of conditional localization of the excitation $\mathbf{r}_0$). Variables ρ_α do not depend on time τ in this frame of reference. Then it is easy to make sure that the last condition transforms into the simpler form:

$$\left|\phi \sum_\alpha \left[\frac{\dot{A}_\alpha}{A_\alpha} + \dot{\eta}_\alpha \frac{Ai'\,(\eta_\alpha)}{Ai\,(\eta_\alpha)}\right]\right| < \delta, \tag{38}$$

Value δ in this inequality determines degree of deviation from the stationary condition (37). In these circumstances, variables τ, $\boldsymbol{\rho}$ still remain independent, but range of their values is limited by the inequality (38). It is assumed that stationary conditions are fulfilled within this range of values.

2.4. Procedure of matching of quantum and classical descriptions. The last, what must be done in accordance with [1, 11] in order to go to the analysis of the consistency between quantum and classic descriptions – is the performance of the necessary transformation in the phase of the wave function $a_{\mathbf{n}}\,(t)$, which is determined in (9) and (10). If such transformations from "global-variable $\mathbf{r}$ to a "local-variable $\boldsymbol{\rho} \equiv \mathbf{r} - \mathbf{r}_0$ were performed in [1] without any explicit reasons, then such reasons were already obvious in [11]. There they were based on the fact that the amplitude of the wave function depends on such a variable. Therefore in order to separate the quantum description from the classical we had to go to the difference variable $\boldsymbol{\rho} \equiv \mathbf{r} - \mathbf{r}_0$ in the phase.

Thus, here we must reduce the phase part $\Gamma_{\mathbf{n}}\,(t)$ of the wave function $a_{\mathbf{n}}\,(t)$ to variables $\rho_\alpha + \xi_\alpha$. Within the continual approximation, which is used here, the phase (10) may be represented by means of the following relation:

$$\Gamma_{\mathbf{n}}\,(t) = p_\alpha x_\alpha - \int_0^\tau \Omega\, d\tau',$$

where the definition $\dot{\gamma} \equiv \Omega$ is taken in the account. Moving to the variables ρ_α from variables x_α in accordance with the definition $\rho_\alpha = x_\alpha - x_0^\alpha$, and further to variables $\rho_\alpha + \xi_\alpha$, we will transform this phase to the following form: $\Gamma_{\mathbf{n}}\,(t) = p_\alpha\,(\rho_\alpha + \xi_\alpha) + p_\alpha\,(x_0^\alpha - \xi_\alpha) - \int_0^\tau \Omega\, d\tau'$. As a result, the wave function $a_{\mathbf{n}}\,(t)$ will be transformed to the form:

$$a_{\mathbf{n}}\,(t) = \left[\prod_{\alpha=1}^{3} A_\alpha Ai\,(-\lambda_\alpha\{\rho_\alpha + \xi_\alpha\})\exp\{ip_\alpha\,(\rho_\alpha + \xi_\alpha)\}\right] \cdot \exp\left\{i\left[\mathbf{p}\cdot\{\mathbf{r}_0 - \boldsymbol{\xi}\} - \int_0^\tau \Omega\, d\tau'\right]\right\}.$$

As it visible now this function splits into two multipliers. One of it consists of three multipliers: $A_\alpha Ai\,(-\lambda_\alpha\{\rho_\alpha + \xi_\alpha\})\exp\{ip_\alpha\,(\xi_\alpha + \xi_0^\alpha)\}$, which have a form of the investigated wave function of a quasiparticle in the external field and in the local frame of reference, which is connected with point ... Conditions of quasistationarity (38) are considered as fulfilled. It means quasi-constancy of multipliers A_α within the limits of the accuracy, determined by parameter δ. In accordance with [1, 11], it is possible to consider the second multiplier $\exp\left\{i\left[\mathbf{p}\cdot\{\mathbf{r}_0-\boldsymbol{\xi}\}-\int\limits_0^{\tau}\Omega\,d\tau'\right]\right\}$ as a purely classic, and go to the analysis of classical part of the problem. Taking into account the results, which were obtained in [1, 11], the expression in the square brackets, must be a classic action, which determines dynamics of the point $\mathbf{r}_0$. That is: $S(\tau)=\mathbf{p}\cdot\{\mathbf{r}_0-\boldsymbol{\xi}\}-\int\limits_0^{\tau}\Omega\,d\tau'$. In order to find a Lagrangian we will perform the identity transformation: $S(\tau)=\int\limits_0^{\tau}\left\{\overset{\bullet}{\mathbf{p}}\cdot\{\mathbf{r}_0-\boldsymbol{\xi}\}+\mathbf{p}\cdot\left\{\overset{\bullet}{\mathbf{r}}_0-\overset{\bullet}{\boldsymbol{\xi}}\right\}-\Omega\right\}d\tau'$. It is obvious that with such definition of the action, the Lagrangian has the form:

$$l=\overset{\bullet}{\mathbf{r}}_0\cdot\mathbf{p}+\overset{\bullet}{\mathbf{p}}\cdot\{\mathbf{r}_0-\boldsymbol{\xi}\}-\overset{\bullet}{\boldsymbol{\xi}}\cdot\mathbf{p}-\Omega. \tag{39}$$

Derivatives $\overset{\bullet}{\mathbf{r}}_0$ and $\overset{\bullet}{\mathbf{p}}$ are already determined by the motion equations (30), therefore further they are considered as Hamiltonian variables. Because of velocity vector $\boldsymbol{\beta}$ and momentum vector $\mathbf{p}$ are interconnected by the relations (13), then it makes it possible to consider the pair of variables $\boldsymbol{\beta}$, $\mathbf{r}_0$ as the Lagrangian variables. Taking into consideration motion equation (30), we will reduce the wave Lagrangian (39) to the form:

$$l=\boldsymbol{\beta}\cdot\mathbf{p}+\{\mathbf{r}_0-\boldsymbol{\xi}\}\cdot\mathbf{G}-\mathbf{p}\cdot\overset{\bullet}{\boldsymbol{\xi}}-\Omega. \tag{40}$$

In order to definition (40) really got a significance of Lagrangian, it is necessary to take into consideration the following relation: $p_\alpha=\arcsin(\beta_\alpha)$, which is inverse to the first (left) of the relations (13). Then, taking into account the general relation between the Lagrangian l and relevant Hamiltonian h:

$$l=\boldsymbol{\beta}\cdot\mathbf{p}-h, \tag{41}$$

we will obtain, comparing (40) and (41), for the Hamiltonian of the system under consideration:

$$h=\Omega-\{\mathbf{r}_0-\boldsymbol{\xi}\}\cdot\mathbf{G}+\mathbf{p}\cdot\overset{\bullet}{\boldsymbol{\xi}}.$$

This expression includes components of three arbitrary vectors: $\mathbf{G}$, $\boldsymbol{\xi}$, and $\mathbf{r}_*$ (the last of which is found in Ω only). Availability of such arbitrary vectors makes it possible to raise a question, first of all, about coincidence of the Hamiltonian h and factor Ω. Such coincidence is very important from the physical point of view, because of the Hamiltonian of any closed system is kept in time. At the same time, factor Ω practically plays the role of quantum eigenvalue of the same system and it must be constant in time as well. In addition, availability of arbitrary vectors $\mathbf{G}$, $\boldsymbol{\xi}$, and $\mathbf{r}_*$ makes it possible to raise a question on the simultaneous compatibility of motion equations (30) both with the Hamiltonian h, and with the eigenvalue Ω. The simplest way to ensure fulfillments of the condition:

$$h=\Omega, \tag{42}$$

is to formulate the equation:

$$\mathbf{p}\cdot\overset{\bullet}{\boldsymbol{\xi}}=\{\mathbf{r}_0-\boldsymbol{\xi}\}\cdot\mathbf{G}, \tag{43}$$

which may be considered as one of equations for determination of vector $\boldsymbol{\xi}$. Equation (42) establishes that there is a possibility to study the question on providing to equations (30) the "Hamiltonian-Lagrangian"significance on the basis of Hamiltonian equations [12]:

$$\overset{\bullet}{\mathbf{r}}_0=\boldsymbol{\beta}=\nabla_{\mathbf{p}}(\Omega);\quad \overset{\bullet}{\mathbf{p}}=\mathbf{G}=-\nabla_{\mathbf{r}_0}(\Omega). \tag{44}$$

By substituting energies Ω in the explicit form from expression (33) into (44), taking into account the definition of components of the mass tensor $1/\mu_\alpha=\cos(p_\alpha)$ and velocity tensor $\beta_\alpha\equiv\sin(p_\alpha)$, as well as taking into consideration the relations $\boldsymbol{\Pi}_{\mathbf{r}_*}=\nabla_{\mathbf{r}_*}(v_{\mathbf{r}_*})$, we will obtain:

$$\overset{\bullet}{\mathbf{r}}_0=\boldsymbol{\beta}+\boldsymbol{\sigma}_{\mathbf{p}};\quad \overset{\bullet}{\mathbf{p}}=\mathbf{G}+\delta\mathbf{G}, \tag{45}$$

were for vectors $\boldsymbol{\sigma}_{\mathbf{p}}$ and $\delta\mathbf{G}$, after performance of the not so complicated, but sufficiently cumbersome transformations, we may obtain the following expressions in components:

$$\sigma_{\mathbf{p}}^{\alpha} \equiv \left[\left(\widehat{\mu}^{-1}\mathbf{F}\cdot\frac{\partial\boldsymbol{\xi}}{\partial p_{\alpha}}\right)+\left(\boldsymbol{\Phi}\cdot\frac{\partial\mathbf{r}_{*}}{\partial p_{\alpha}}\right)-\left((\mathbf{r}_{0}-\boldsymbol{\xi})\cdot\frac{\partial}{\partial p_{\alpha}}\left(\widehat{\mu}^{-1}\mathbf{F}\right)\right)\right]; \tag{46}$$

$$\delta G_{\alpha} \equiv \left\{\frac{F_{\alpha}}{\mu_{\alpha}}-G_{\alpha}-\left[\left(\widehat{\mu}^{-1}\mathbf{F}\cdot\frac{\partial\boldsymbol{\xi}}{\partial x_{0}^{\alpha}}\right)+\left(\boldsymbol{\Phi}\cdot\frac{\partial\mathbf{r}_{*}}{\partial x_{0}^{\alpha}}\right)-\left((\mathbf{r}_{0}-\boldsymbol{\xi})\cdot\frac{\partial}{\partial x_{0}^{\alpha}}\left(\widehat{\mu}^{-1}\mathbf{F}\right)\right)\right]\right\}.$$

In order to reduce cumbersome record, into these expressions were inserted the vector $\boldsymbol{\Phi}$, having components: $\Phi_{\alpha} \equiv \left(\mathbf{r}_{*}\cdot\dfrac{\partial\boldsymbol{\Pi}_{\mathbf{r}_{*}}}{\partial x_{*}^{\alpha}}\right)$.

It may be seen that dynamic equations (45) and equations (30) have different right-hand parts and the ***first condition*** arise immediately as follows (here we may consider this condition as a main):

$$\boldsymbol{\sigma}_{\mathbf{p}} = \mathbf{0}. \tag{47}$$

This condition is considered as basic, because its unconditional implementation provides automatic saving of all the definitions of the main dynamic characteristics of quasiparticles obtained in [1] (speed, mass, etc.).

The second condition, which was already discussed above, is connected with the equation (43). This condition will ensure fulfillment of the equation (42): $h = \Omega$.

The third condition, in analogy to ***first condition***, follows from the comparison of dynamic motion equations (45), (30) and reduced to the requirement: $\delta\mathbf{G} = \mathbf{0}$. It is possible to present this requirement in the explicit form as follows:

$$\widehat{\mu}^{-1}\mathbf{F}-\mathbf{G} = \boldsymbol{\sigma}_{\mathbf{r}_{0}}, \tag{48}$$

where $\sigma_{\mathbf{r}_0}$, similarly to the definition (46) for $\boldsymbol{\sigma}_{\mathbf{p}}$, denotes the vector, which has the following components:

$$\sigma_{\mathbf{r}_{0}}^{\alpha} \equiv \left[\left(\widehat{\mu}^{-1}\mathbf{F}\cdot\frac{\partial\boldsymbol{\xi}}{\partial x_{0}^{\alpha}}\right)+\left(\boldsymbol{\Phi}\cdot\frac{\partial\mathbf{r}_{*}}{\partial x_{0}^{\alpha}}\right)-\left((\mathbf{r}_{0}-\boldsymbol{\xi})\cdot\frac{\partial}{\partial x_{0}^{\alpha}}\left(\widehat{\mu}^{-1}\mathbf{F}\right)\right)\right]. \tag{49}$$

And, in the end, ***the fourth condition*** is the condition (31), which it would be better present here in the following form: $\widehat{\mu}^{-1}\mathbf{F}+\mathbf{G} = \boldsymbol{\Pi}_{\mathbf{r}_{*}}$, and which would add the condition (48) in order to transform it into the system of linear algebraic equations with respect to the forces $\mathbf{F}$ and $\mathbf{G}$:

$$\widehat{\mu}^{-1}\mathbf{F}+\mathbf{G} = \boldsymbol{\Pi}_{\mathbf{r}_{*}}; \tag{50}$$

$$\widehat{\mu}^{-1}\mathbf{F}-\mathbf{G} = \boldsymbol{\sigma}_{\mathbf{r}_{0}}, \tag{51}$$

if only subsystem (51) itself would not create the system of differential equations with respect to the vector $\mathbf{F}$, as it may be seen from the expression (49).

3. Conclusions

Was fulfilled the analysis of the dynamic properties of quasiparticles of type of injected into the semiconductor or insulator electrons in an external electrostatic field of general spatial configuration. To separate the properties under consideration from other factors, was used the most simplified model of the crystal (nearest neighbors, a cubic crystal lattice, the continuum approximation of the second order). Analysis of these dynamic properties of quasiparticles carried out in a uniform external field approximation (with respect to the quantum description) and in the generalized approximation of plane wave in the phase. The generality of approximation of plane wave in phase is expressed in that, the wave vector and energy phase summand are functions of time and they must be determined. It was shown that only in a generalized approximation of a plane wave in phase is implemented Lagrangian-Hamiltonian dynamics of quasiparticles in the usual forms (for example, in the relativistic form). In the presence of an external field, just as in the case of free quasiparticles, can be fully harmonize both the existing methods of describing the dynamics of quasiparticles (quantum and classical).

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