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Degeneracy effect of dynamical properties of quasi-particles of electronic origin in semiconductor materials

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The general dynamical properties of free quasi-particles are analyzed. Analyzed also the conditions under which the description of the dynamic properties of the quasi-particles is almost identical with those of real relativistic particles. The problem of the relation of quantum and classical methods of describing the quasi-particles in the case of the excited states of crystals is considered. Basic principles of construction of dynamic properties of classic type for quasi-particles at excitation of matter with the structure of solids (crystals) are analyzed. The results of analysis were demonstrated on the example of electronic excitations of crystals in the simplest case, when other effects are neglected (phonons, the response to excitation of the lattice, defects, high density of excitations, which requires the account of interactions between them, and so forth). It was shown that such excitations are described in three ways simultaneously. These descriptions make it possible to interpret the experimental data in terms of the usual relativistic dynamics, if the considered system allows the use of the considered approximations (plane wave in a phase, nearest neighbors and cubic grate).

В статье анализируются общие динамические свойства свободных квазичастиц а также условия, при которых описание динамических свойств квазичастиц практически совпадает с аналогичными свойствами реальных релятивистских частиц. Рассмотрена проблема соотношения квантового и классического способов описания квазичастиц в случае возбужденных состояний кристаллов. Проанализированы основные принципы построения динамических свойств классического типа для квазичастиц при возбуждении сред со структурой твердых тел (кристаллов). Результаты анализа продемонстрированы на примере электронных возбуждений кристаллов в самом простом случае, когда другими влияниями пренебрегают (фононы, реакция решетки на возбуждение, дефекты, высокая плотность возбуждений, которая требует учета взаимодействий между ними, и тому подобное). Показано, что такие возбуждения одновременно описываются тремя способами. Эти описания дают возможность интерпретировать экспериментальные данные в привычных терминах релятивистской динамики, если рассматриваемая система допускает использование указанных приближений (плоской волны в фазе, ближайших соседей и кубической решетки).

1. Introduction

At research of the excited states of semi-conductor materials often there are difficulties at interpretation of results in terms of quasi-particles. At the same time such interpretation is convenient, as quasi-particles represent analogues of particles of classical type. In small energy of quasi-particles (within a corresponding energy band) usually such difficulties does not arise. But in big energy (in the same limits) this question too little researched. In paper this question is analyzed in details for free quasi-particles. Comparison with properties of real particles is conducted. The relations which obtained,

allows comparing different ways of their description: quantum (initial) and two descriptions of classical type (exactly these two descriptions associate with a concept "quasi-particle") – wave and mechanical. In particular, it gives the chance to compare the dynamic properties of quasi-particles and real particles and may be useful from two points of view.

First of all it is useful for adequate application of classic method of description of the excited states of condensed matter in terms of quasi-particles for interpretation of experimental results. Such interpretation is especially important, if it applies in the wide range of such dynamic parameters, as wave vectors, quasi-impulse, dynamic effective masses, speeds and other. And also at the study of such physical properties, as transfer of energy [1–5], charge [6–8] or other physical characteristics [9–15], influences of the external fields on these processes, and others like that. Secondly, for more complete understanding of physical properties of the real particles.

Common dynamic properties of free quasi-particles are analyzed in paper. They are based on one of major characteristics of the excited states of condensed physical objects – on dispersion dependence of energy or frequency from a wave vector [1–27]. Terms at which description of dynamic properties of quasi-particles practically coincides with similar properties of the real relativistic particles are analyzed also. The problem of relation between quantum and classic methods of description of quasi-particles in the case of the excited states of crystals is considered.

2. Common remarks about dynamic properties

The main feature of the condensed matter is the presence of properties inherent only to this substance. One of such properties are, so-called, dispersion dependences of energy on a wave vector: $E(\mathbf{k})$.

It is known [28,29] that in the case when energy is a function from a parameter or family group of parameters, physical sense of such energy is interpreted depending on physical sense of this parameter or their group. A parameter $\mathbf{k}$ is always associated with an impulse: $\mathbf{P} = \hbar\mathbf{k}$, which in quantum mechanics name a wave impulse, and in the theory of solids – quasi-impulse. Therefore dependences $E(\mathbf{k})$ at once obtain the sense of Hamiltonian:

$$E(\mathbf{k}) \equiv H(\mathbf{P}). \tag{1}$$

Energies $E(\mathbf{k})$ in the solids are always the eigenvalues of the operators of Hamilton. Therefore it has the direct origin as Hamiltonian. After establishment (1) it is possible to find a speed of the proper classic object in accordance with the Hamilton equations:

$$V_i(\mathbf{k}) = \frac{\partial H(\mathbf{P})}{\partial P_i} \equiv \frac{1}{\hbar}\frac{\partial E(\mathbf{k})}{\partial k_i} \equiv \frac{\partial \omega(\mathbf{k})}{\partial k_i}. \tag{2}$$

It is visible from this determination, that the got speed coincides with group speed of processes, for example, in plasma: $\partial\omega(\mathbf{k})/\partial k_i$, and also with effective speed of quasi-particles in solids: $\partial E(\mathbf{k})/(\hbar\partial k_i)$. Thus, both group speed and effective speed are ordinary Hamilton speeds of some object of classic nature and depend on $\mathbf{P}$ or $\mathbf{k}$. Taking into account determinations (2) it is possible to notice that in general case speed $\mathbf{V}$ with components V_i is a function of an impulse $\mathbf{P} = \hbar\mathbf{k}$ with components $P_j = \hbar k_j$. Consequently mass has nature of tensor:

$$m_{ij}^{-1}(\mathbf{k}) = \frac{\partial V_i}{\partial P_j} \equiv \frac{1}{\hbar}\frac{\partial V_i(\mathbf{k})}{\partial k_i} \equiv \frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial k_i \partial k_j} \equiv \frac{\partial V_j}{\partial P_i}. \tag{3}$$

Equalities (3) show that this tensor is symmetric in relation to a main diagonal. This determination of reverse mass is the most general. It does not depend on the choice of point on a dispersion curve [16, 17], or from reality of the investigated substance. Tensor of reverse mass m_{ij}^{-1} is a dynamic parameter, as depends on an impulse $\mathbf{P} = \hbar\mathbf{k}$. It is now necessary to answer on an important question: is there some relation of such determination of mass with phenomenological inert mass, or not?

For an answer on this question we will take into account that dependences $E(\mathbf{k})$ and $\mathbf{V}(\mathbf{k})$ are the parametric type of dependence of energy from speed. Formal eliminating a parameter $\mathbf{k}$ gives a

possibility to get the energy as a function of speed. But, if energy is a function of speed, it has status of the Lagrangian, and in analogy with (1), it is possible to write down such equality:

$$E(\mathbf{k}) \equiv L_m(\mathbf{V}). \tag{4}$$

The origin of index "m" is related to the term "mechanical" and will become more clear after a formula (10).

Situation, when the same energy is simultaneously the Hamiltonian and the Lagrangian can cause the surprise. But determinations (1) and (2) show that it takes place always because these determinations always have the form of parametric dependence of energy from speed. Because the derivatives $\partial L_m(\mathbf{V})/\partial V_i$ determines an impulse, it is necessary to find out its physical sense and attitude to a wave impulse $\mathbf{P} = \hbar\mathbf{k}$. We will designate this impulse as $\mathbf{P}_m$. Then

$$P_m^{(i)} = \partial L_m(\mathbf{V})/\partial V_i. \tag{5}$$

Dependence $L_m(\mathbf{V})$ without specification of energy (in general case) is not known. Therefore we will take into account that this energy is also the Hamiltonian in relation to an impulse $\mathbf{P}$. In this case (5) it is possible to represent as: $P_m^{(i)} = \frac{\partial H(\mathbf{P})}{\partial P_j}\frac{\partial P_j}{\partial V_i}$. Taking into account determinations (2), at once it is possible to get:

$$P_m^{(i)} = V_j \cdot (\partial P_j/\partial V_i). \tag{6}$$

We will show now, that the derivative $\partial P_j/\partial V_i$ determine tensor of direct mass: m_{ij}. Indeed, if

$$m_{ij} = \partial P_i/\partial V_j, \tag{7}$$

equality must be executed:

$$m_{i\,k}^{-1} m_{kj} = \delta_{ij}. \tag{8}$$

Putting in (8) right parts of determinations (3) and (7), we will get

$$m_{i\,k}^{-1} m_{kj} \equiv (\partial V_i/\partial P_k)(\partial P_k/\partial V_j) = \partial V_i/\partial V_j = \delta_{ij}.$$

Thus, equality (8) is executed always, because the components V_i of vector of speed $\mathbf{V}$ are independent. It is possible to show that equality $m_{i\,k} m_{kj}^{-1} = \delta_{ij}$ is executed also, if the components P_i of vector $\mathbf{P}$ are independent.

Coming back now to equality (6), we use in it determination (7). As a result it is possible to get

$$P_m^{(i)}(\mathbf{k}) = m_{ij}(\mathbf{k})\, V_j(\mathbf{k}). \tag{9}$$

Symmetry of tensors m_{ij} and m_{ij}^{-1} was also taken into account in equality (9). As is obvious from equality (9), an impulse $\mathbf{P}_m$ differs from an impulse $\mathbf{P}$, at least, by two circumstances: by determinations and different attitude to mass. In accordance with determination: $\mathbf{P} = \hbar\mathbf{k}$, but

$$\mathbf{P}_m(\mathbf{k}) = \widehat{m}(\mathbf{k}) \cdot \mathbf{V}(\mathbf{k}). \tag{10}$$

With respect to attitude of these impulses toward mass, an impulse $\mathbf{P}_m(\mathbf{k})$, as is obvious from (9) and (10), is the generalized determination of ordinary mechanical impulse. In special case, when $m_{ij}(\mathbf{k}) = m(\mathbf{k})\,\delta_{ij}$, equalities (9) and (10) it is possible to lead, accordingly, to the kind: $P_m^{(i)}(\mathbf{k}) = m(\mathbf{k})\, V_i(\mathbf{k})$ and $\mathbf{P}_m(\mathbf{k}) = m(\mathbf{k})\,\mathbf{V}(\mathbf{k})$. Wave impulse $\mathbf{P} = \hbar\mathbf{k}$, on mass does not depend, but, in accordance with equality (3), determines it and does, at first, a dynamic parameter, and, secondly, a tensor.

For further it will be important, that energy $E(\mathbf{k})$ simultaneously is the Hamiltonian in relation to a wave impulse $\mathbf{P}$, and the Lagrangian in relation to a mechanical impulse $\mathbf{P}_m$.

Presence of two specifications of classic type for free quasi-particle, which are based on equalities

$$E(\mathbf{k}) \equiv H(\mathbf{P}) \equiv L_m(\mathbf{V}), \tag{11}$$

generates additional duality of classic-classic type. On today it is known only duality of quantum-classic type for the real particles and quasi-particle in solids. Between these two descriptions, except the equalities (11), exists another "intersection": both descriptions have identical speed determined by the common system of equalities $\mathbf{V} = \nabla_{\mathbf{P}}\{H(\mathbf{P})\} \equiv \frac{1}{\hbar}\nabla_{\mathbf{k}}\{E(\mathbf{k})\}$. These equalities can be continued as $\mathbf{V} = \nabla_{\mathbf{P}_m}\{H_m(\mathbf{P}_m)\}$. But for this purpose it is needed at first to define Hamiltonian $H_m(\mathbf{P}_m)$. It is possible to do this in a general case, having determinations for $L_m(\mathbf{V})$ and $\mathbf{P}_m$. But except of the Hamiltonian $H_m(\mathbf{P}_m)$, for complete symmetry in relation to both dynamic descriptions, it would be necessary to find also the Lagrangian $L(\mathbf{V})$, which, unlike $L_m(\mathbf{V})$, relates to wave description, instead of mechanical. But it is expedient to execute such work already when dispersion dependence $E(\mathbf{k})$ is specified. It will be done in the following to parts of the article.

3. Dynamics of quasi-particles in solids. Basic relations

In this part the questions listed above will be considered on the examples of the simplest excitations of single-particle type in solids. This is, first of all, electrons in the conductivity band of semiconductor or dielectric. In the application aspect such electrons provide the charge transfer (electric current). To the simplest excitations of single-particle type belongs also a Frenkel excitons in molecular crystals. It provides the transfer of energy. Such choice is explained by two circumstances. First of all, the concept of quasi-particle first arose up at research of solids. Secondly, primary description of the excited states of crystals, in a difference, for example, from plasma, is a quantum. This enables to establish connection not only between two classic descriptions considered higher, but each of them with primary quantum description also. Such analysis gives a possibility for transition from quantum description of the excited state of crystal to one of its classic analogues correctly. Correct implementation of such transition is important because classic description essentially easier in interpretation of results of researches. In addition, knowledge of basic features of intercommunications between different descriptions can matter in understanding and origin of properties of the real particles.

Typical Hamiltonian for single-particle electronic excitations in solids, without taking into account reaction of lattice of crystal on excitation, is determined by equality [30–33]. Crystals with a simple lattice are examined only (one atom or one molecule in an elementary cell). It enables to examine, so-called, normal dispersion dependences – with a minimum in a point $\mathbf{k} = \mathbf{0}$.

$$E_f(\{a\}) = \frac{1}{2}\left\{ {\sum_{\mathbf{n}\,\mathbf{l}}}' w_{\mathbf{n},\mathbf{n}+\mathbf{l}} + \sum_{\mathbf{n}} D^f_{\mathbf{n}} |a_{f\mathbf{n}}|^2 + {\sum_{\mathbf{n}\,\mathbf{l}}}' M^f_{\mathbf{n},\mathbf{n}+\mathbf{l}} \left(a^*_{f\mathbf{n}} a_{f,\mathbf{n}+\mathbf{l}} + a^*_{f,\mathbf{n}+\mathbf{l}} a_{f\mathbf{n}}\right) \right\}. \tag{12}$$

Primes over symbols of double sums mean here, that vectors $\mathbf{n}$ take on arbitrary values, but vectors $\mathbf{l}$ take on all values, except the value $\mathbf{l} = \mathbf{0}$. Determination (12) is a functional in relation to factors $a_{f\mathbf{n}}$. Vectors $\mathbf{n}$, $\mathbf{l}$ determines a spatial position of separate atom or molecule. In solids this is the vectors of crystalline lattice. They, as well as $a_{f\mathbf{n}}$, can be the variables of functional, if the reaction of lattice on excitation is taken into account [1,2,4,30–33]. A factor $a_{f\mathbf{n}}$, in accordance with its determination, is unknown part of wave function of electronic subsystem of crystal and is determined by the condition of dynamic minimization of functional (12) [2,30]. The eigenvalues $E_f(\mathbf{k})$ are determined simultaneously with $a_{f\mathbf{n}}$. The condition of dynamic minimization of functional (12) is equivalent to procedure of reduction to the diagonal type of the proper operator [3,4]. Procedure of reduction to the diagonal type of the proper operator enables to find energy $E_f(\mathbf{k})$ directly at the level of operator. A factor $a_{f\mathbf{n}}$ determines the spatio-temporal distributing of excitation within the limits of crystal and time of existence of excitation. The important feature of this factor is its dependence on an index f. This index determines the quantum state of crystal, excitation or injection of electron took place in which.

The set parts of wave function of crystal determine the matrix elements $w_{\mathbf{n},\mathbf{n}+\mathbf{l}}$, $D^f_{\mathbf{n}}$ and $M^f_{\mathbf{n},\mathbf{n}+\mathbf{l}}$ of functional (12). Energy $w_{\mathbf{n},\mathbf{n}+\mathbf{l}}$ is energy of interaction between separate atoms or molecules. Energy

$D^f_{\mathbf{n}}$ determines the change in an interaction between atoms or molecules at appearance of excitation. A matrix element $M^f_{\mathbf{n},\mathbf{n}+\mathbf{l}}$ also determines additional interaction between atoms or molecules at excitation of crystal. But this matrix element determines not so the change in an interaction, as processes of transfer of excitation on space of crystal, because describes the states with the simultaneous localization of excitation in two different space positions: $\mathbf{n}$ and $\mathbf{n}+\mathbf{l}$.

If three conditions of ideality are executed in a crystal (or is considered executed approximately): 1) a crystal has unlimited sizes; 2) does not have the defects of crystalline lattice; 3) the local reaction of crystalline lattice on electronic excitation is not taken into account, the potential energy $D^f_{\mathbf{n}}$ does not depend on a variable $\mathbf{n}$. In this case execute the equality $D^f_{\mathbf{n}} = D^f_{\mathbf{0}}$, and the functional (12) takes more simple form

$$E_f(\{a\}) = E_f^{(0)} + \frac{1}{2}{\sum_{\mathbf{n}\,\mathbf{l}}}' M^f_{\mathbf{n},\mathbf{n}+\mathbf{l}}\left(a^*_{f\mathbf{n}}a_{f,\mathbf{n}+\mathbf{l}} + a^*_{f,\mathbf{n}+\mathbf{l}}a_{f\mathbf{n}}\right). \tag{13}$$

Notations are entered here: $E_f^{(0)} \equiv U_0 + \frac{1}{2}D^f_{\mathbf{0}}N_f$ – it is the fixed part of energy in relation to the varied variables $\{a_{f\mathbf{n}}\}$ and $\left\{a^*_{f\mathbf{n}}\right\}$; in this energy $U_0 \equiv \frac{1}{2}{\sum_{\mathbf{n}\,\mathbf{l}}}' w_{\mathbf{n}\,\mathbf{l}}$ – is general potential energy of all crystal, and $N_f \equiv \sum\limits_{\mathbf{n}} |a_{f\mathbf{n}}|^2$ – is norm of function $a_{f\mathbf{n}}$ on a variable $\mathbf{n}$. Usually functions $a_{f\mathbf{n}}$ are built so that they were normalized on unit, i.e. that a condition $N_f = 1$ was performed. In general the inequality: $N_f < \infty$, is enough. More hard condition $N_f = 1$, is actual, when functions $a_{f\mathbf{n}}$ must form the base system. Using procedure of Hamilton dynamic minimization [2, 30]:

$$i\hbar\frac{\partial a_{f\mathbf{n}}}{\partial t} = \frac{\partial E_f(\{a\})}{\partial a^*_{f\mathbf{n}}},$$

it is possible to get equation

$$i\hbar\frac{\partial a_{f\mathbf{n}}}{\partial t} = -\frac{1}{2}{\sum_{\mathbf{l}}}' \left|M^f_{\mathbf{l}}\right| (a_{f,\mathbf{n}+\mathbf{l}} + a_{f,\mathbf{n}-\mathbf{l}}). \tag{14}$$

Here at once two circumstances were taken into account [30]. First of all, the matrix elements $M^f_{\mathbf{n},\mathbf{n}+\mathbf{l}}$ in the conditions of ideal crystal depend only on the difference of lower indexes. Secondly, in typical crystals they are negative. If to take into account these two circumstances in functional (13), it is possible to get

$$E_f(\{a\}) = E_f^{(0)} - \frac{1}{2}{\sum_{\mathbf{n}\,\mathbf{l}}}' \left|M^f_{\mathbf{l}}\right| \left(a^*_{f\mathbf{n}}a_{f,\mathbf{n}+\mathbf{l}} + a^*_{f,\mathbf{n}+\mathbf{l}}a_{f\mathbf{n}}\right). \tag{15}$$

It is impossible not to pay attention on one interesting fact. If in equation (14) to use the formal operator identity $a_{f,\mathbf{n}\pm\mathbf{l}} \equiv \exp\{\pm(\mathbf{l}\cdot\nabla)\}a_{f,\mathbf{n}}$, it takes form of the Schödinger equation

$$i\hbar\frac{\partial a_{f\mathbf{n}}}{\partial t} = \widehat{H}^{(f)}a_{f\mathbf{n}},$$

where

$$\widehat{H}^{(f)} \equiv -{\sum_{\mathbf{l}}}' \left|M^f_{\mathbf{l}}\right| \mathrm{ch}\,(\mathbf{l}\cdot\nabla_{\mathbf{n}}). \tag{16}$$

This remark will be important further, at the discussion of determination of operator of impulse for quasi-particles.

As the system is complex, at first we will represent a function $a_{f\mathbf{n}}$ in the most general form [34]

$$a_{f\mathbf{n}}(t) = \varphi_{f\mathbf{n}}(t)\ \exp\left[i\,\Gamma_{f\mathbf{n}}(t)\right]. \tag{17}$$

After putting (17) into (14) and separating a real and imaginary parts from one another, the system (14) disintegrates on two subsystems in relation to functions $\varphi_{f\mathbf{n}}$ and $\Gamma_{f\mathbf{n}}$:

$$\hbar\frac{\partial\varphi_{f\mathbf{n}}}{\partial t}+\frac{1}{2}\sum_{l}{}'\left|M_{\mathbf{l}}^{f}\right|\{\varphi_{f,\mathbf{n}+\mathbf{l}}\sin\left(\Gamma_{f,\mathbf{n}+\mathbf{l}}-\Gamma_{f\mathbf{n}}\right)-\varphi_{f,\mathbf{n}-\mathbf{l}}\sin\left(\Gamma_{f\mathbf{n}}-\Gamma_{f,\mathbf{n}-\mathbf{l}}\right)\}=0; \tag{18}$$

$$\hbar\varphi_{f\mathbf{n}}\frac{\partial\Gamma_{f\mathbf{n}}}{\partial t}=\frac{1}{2}\sum_{l}{}'\left|M_{\mathbf{l}}^{f}\right|\{\varphi_{f,\mathbf{n}+\mathbf{l}}\cos\left(\Gamma_{f,\mathbf{n}+\mathbf{l}}-\Gamma_{f\mathbf{n}}\right)+\varphi_{f,\mathbf{n}-\mathbf{l}}\cos\left(\Gamma_{f\mathbf{n}}-\Gamma_{f,\mathbf{n}-\mathbf{l}}\right)\}=0. \tag{19}$$

First approximation which results in the dynamics of quasi-particles, practically the identical to dynamics of free relativistic particle is ***approximation of plane wave in a phase***. Maybe, it is the main approximation which gives a possibility to compare dynamic properties of particles and quasi-particles. In this case phase function $\Gamma_{f\mathbf{n}}$ suppose equal: $\Gamma_{f\mathbf{n}}=\mathbf{k}\cdot\mathbf{n}-\omega_f t$. In this case for a wave function (17) and system of equations (18), (19) we will get: $a_{f\mathbf{n}}(t)=\varphi_{f\mathbf{n}}(t)\cdot\exp\left[i\left(\mathbf{k}\cdot\mathbf{n}-\omega_f t\right)\right]$,

$$\hbar\frac{\partial\varphi_{f\mathbf{n}}}{\partial t}+\frac{1}{2}\sum_{\mathbf{l}}{}'\left|M_{\mathbf{l}}^{f}\right|\sin\left(\mathbf{k}\cdot\mathbf{l}\right)\{\varphi_{f,\mathbf{n}+\mathbf{l}}-\varphi_{f,\mathbf{n}-\mathbf{l}}\}=0; \tag{20}$$

$$\frac{1}{2}\sum_{\mathbf{l}}{}'\left|M_{\mathbf{l}}^{f}\right|\cos\left(\mathbf{k}\cdot\mathbf{l}\right)\{\varphi_{f,\mathbf{n}+\mathbf{l}}+\varphi_{f,\mathbf{n}-\mathbf{l}}\}+\hbar\omega_f\varphi_{f\mathbf{n}}=0. \tag{21}$$

But since a phase was set, two subsystems for determination of one function $\varphi_{f\mathbf{n}}(t)$ appeared. It means that it is needed to search some compatibility conditions.

One of forms of such terms is a condition: $\varphi_{f\mathbf{n}}(t)\equiv\varphi_f=$ constant. In this case from determination (17) it is possible to get the solution which is known as plane wave:

$$a_{f\mathbf{n}}(t)=\varphi_f\cdot\exp\left[i\left(\mathbf{k}\cdot\mathbf{n}-\omega_f t\right)\right]. \tag{22}$$

Thus a subsystem (20) is satisfied identically, and a subsystem (21), after cancellation on φ_f, is reduce to equality: $\hbar\omega_f(\mathbf{k})=-\sum_{\mathbf{l}}{}'\left|M_{\mathbf{l}}^{f}\right|\cos\left(\mathbf{k}\cdot\mathbf{l}\right)$. The solution (22), as a wave function, is bad in the sense that in an infinite space has an endless norm: $N_f=\infty$. If to give up the first condition of ideality (endlessness of crystal) in the norm condition: $N_f\equiv\sum_{\mathbf{n}}\left|a_{f\mathbf{n}}\right|^2$, it takes a form: $N_f=N\varphi_f^2$, where N is number of atoms or molecules in the examined region of crystal. As in this case two parameters are indefinite: N_f and φ_f, suppose usually $N_f=1$. It does a wave function approximately normalized on unit. Thus: $\phi_f=1\Big/\sqrt{N}$, and (22) takes a form:

$$a_{f\mathbf{n}}(t)=\frac{1}{\sqrt{N}}\exp\left[i\left(\mathbf{k}\cdot\mathbf{n}-\omega_f t\right)\right]. \tag{23}$$

Substitution (23) in energy (15) gives a law of dispersion for the examined case (absences of reaction of lattice on excitation):

$$\varepsilon_f(\mathbf{k})=-\sum_{\mathbf{l}}{}'\left|M_{\mathbf{l}}^{f}\right|\cos\left(\mathbf{k}\cdot\mathbf{l}\right)\equiv\hbar\omega_f(\mathbf{k}), \tag{24}$$

where it is marked: $\varepsilon_f(\mathbf{k})\equiv E_f(\mathbf{k})-E_f^{(0)}$. As energy $\varepsilon_f(\mathbf{k})$ coincides with the eigenvalues $E_f(\mathbf{k})$ accurate within a constant $E_f^{(0)}$, in all dynamic determinations of previous section it is possible to use exactly $\varepsilon_f(\mathbf{k})$ instead of $E_f(\mathbf{k})$.

Comparison of expression (24) with determination of operator (16) shows that an operator $-i\nabla_{\mathbf{n}}$ may be put into accordance to a wave vector $\mathbf{k}$ (taking into account physical correctness of such accordance). As a wave vector $\mathbf{k}$ straightly determines a wave impulse $\mathbf{P}$ only, it is possible to come to the conclusion, that in transition from classic description to the quantum one, the operator of gradient is equivalent only to the wave impulse in sense of equality $\widehat{\mathbf{P}}=-i\hbar\nabla_{\mathbf{n}}$, but not to mechanical impulse, determined in (9), (10). As it will be shown, the accordance between a mechanical impulse and the operator of gradient is not such simple. At least, for quasi-particles it is so.

Formulas (24) enable already to specify common dynamic properties of quasi-particles for crystals with a simple lattice (one atom or one molecule in an elementary cell). Indeed, putting energy

(24) in determinations (2) and (3) for speed and mass we find enough concrete expressions: $V_f^{(i)}(\mathbf{k}) = \frac{1}{\hbar}\sum_{\mathbf{l}}{}' |\mathbf{l}|_i \left| M_{\mathbf{l}}^f \right| \sin(\mathbf{k}\cdot\mathbf{l})$ and $m_{ij}^{-1}(\mathbf{k}) = \frac{1}{\hbar^2}\sum_{\mathbf{l}}{}' |\mathbf{l}|_i |\mathbf{l}|_j \left| M_{\mathbf{l}}^f \right| \cos(\mathbf{k}\cdot\mathbf{l})$. Here $|\mathbf{l}|_i$, $|\mathbf{l}|_j$ are projections of vector of lattice $\mathbf{l}$ on co-ordinate directions: $\{i,j\} = \{x,y,z\}$. Solving the first equality in relation to a vector $\mathbf{k}$ and putting it in (24), energy indeed can be got as function from speed. It is possible also to obtain the mass as a function from speed. But to do this analytically is impossible. For this reason it is necessary to search other approximations in which it is possible. Such search is important for the getting of possibility to analyze the features of dynamics of classic type (wave and mechanical) exactly in an analytical form. In this sense a next, ***second approximation,*** there is an ***approximation of the nearest neighbours*** typical for crystals. This approximation is based on the fact, that in typical situations matrix elements $M_{\mathbf{l}}^f$ quickly (exponentially) decreasing with the increasing of $|\mathbf{l}|$. Energy (24) here is determined by expression: $\varepsilon_f(\mathbf{k}) = -\sum_{\alpha} \left| M_{\mathbf{b}_\alpha}^f \right| \cos(\mathbf{b}_\alpha \cdot \mathbf{k})$, where $\mathbf{b}_\alpha$ are base vectors of crystalline lattice. An index α, in the case of arbitrary lattice, has three values: $\alpha = \{1,2,3\}$ – in accordance with three crystalline directions. Not limiting generality, we will stop on the simplest case – an ***approximation of cubic lattice.*** In this case crystalline directions coincide with the axes of the Cartesian system of co-ordinates, i.e. $\alpha = i = \{x,y,z\}$, and the vector of lattice $\mathbf{b}_\alpha$ loses an index. This simplification can be considered as ***the third approximation***. It may be the most essential approximation, because the crystals with an ideal cubic lattice rarely meet.

In these approximations the energy (24) simplified to equality:

$$\varepsilon_f(\mathbf{k}) = -|M_f| \sum_i \cos(b k_i). \tag{25}$$

A new denotation is here entered: $M_b^f \equiv M_f$. Using determinations (2) and (3) it is possible to get:

$$V_f^{(i)} = \frac{1}{\hbar}\frac{\partial \varepsilon_f(\mathbf{k})}{\partial k_i} = C_f \sin(b k_i); \quad m_{ij}^{(f)} = \delta_{ij}\frac{m_f}{\cos(b k_i)} \equiv \delta_{ij}\frac{m_f}{\sqrt{1-\beta_i^2}}. \tag{26}$$

Standard denotation for a relativism dynamics is here used: $\beta_i \equiv V_f^{(i)} \big/ C_f$; a vector $\boldsymbol{\beta}$ has components β_i. Formulas (26) show also, that dimensionless speed does not depend on a quantum number f:

$$\beta_i = \sin(b k_i). \tag{27}$$

In the first of the determinations (26) a constant C_f has the dimension of speed, determines by the equality:

$$C_f \equiv b|M_f|/\hbar, \tag{28}$$

and have a sense of maximum possible speed of examined quasi-particle. The last property of it is similar to the constant C of relativistic dynamics (special theory of relativity): being a constant, it is invariant to any transformations. But, in same time, a constant C_f differs from C, it has different values for excitations in different states. As shown in [33] this problem have a solution in the proper setting of norms of wave vectors $\mathbf{k}$ for every state f.

In the second of determinations (26) a constant m_f has the dimension of mass and determines by the equality:

$$m_f \equiv \hbar^2 \big/ (|M_f| b^2). \tag{29}$$

It have a sense of not dynamic part of mass (i.e. not depends on a wave vector $\mathbf{k}$). By this property it is similar to the rest mass of relativistic dynamics and has an interesting feature: depends on the index of the state of crystal, determining the spectrum of the masses by this. For mass m_f it is possible to formulate another useful determination:

$$m_f \equiv \hbar / b\, C_f. \tag{30}$$

Farther, for prevention of bulky in formulas, an index f obviously will be used in the case of absolute necessity only, as it already has executed the main mission. I.e., instead of m_f, C_f, M_f, $\varepsilon_f(\mathbf{k})$, $V_f^{(i)}$, $a_{f\mathbf{n}}(t)$, $\omega_f(\mathbf{k})$ we will use, accordingly m, C, M, $\varepsilon(\mathbf{k})$, V_i, $a_{\mathbf{n}}(t)$, $\omega(\mathbf{k})$.

Due to the last two approximations, from listed above (nearest neighbors and, especially, cubic grate), tensor of mass becomes diagonal. And due to the third approximation (cubic grate) tensor nature of mass is determined by its dynamic properties only. A constant m is a scalar in these approximations. In this sense it is yet more similar to a mass of rest. From point of the relativistic approximation in the dynamics of quasi-particles there is important also an equality: $m\,C^2 = |M|$, which is possible to get with the help of determinations (28) and (29). I.e. in terminology of relativistic dynamics the rest energy of quasi-particle is proportional to the width of the proper energy band of crystal, excitation or injection happened in which. And energy (25) now can be represented as:

$$\varepsilon(\mathbf{k}) = -mC^2\sum_i \cos(b\,k_i). \tag{31}$$

The identity (1) in approximations of nearest neighbours and cubic lattice is determined by equality now:

$$\varepsilon(\mathbf{k}) \equiv H(\mathbf{P}) = -mC^2\sum_i \cos\left(\frac{b}{\hbar}P_i\right). \tag{32}$$

To obtain property (4) it is necessary, as mentioned above, to eliminate a wave vector $\mathbf{k}$ in (31) by the first of determinations (26). We will get as a result:

$$\varepsilon(\mathbf{k}) \equiv L_m(\boldsymbol{\beta}) = -mC^2\sum_i \sqrt{1-\beta_i^2}. \tag{33}$$

It is necessary to notice that the determination (33) of the Lagrangian differs a little from accepted in a relativistic dynamics [29,35]. There it is determined by an equality $L_m(\boldsymbol{\beta}) = -mC^2\sqrt{1-|\boldsymbol{\beta}|^2}$. But such difference tells, probably, that a question needs additional researches.

Using determinations (26) in relation (9) and taking into account that in examined three approximations the identity: $\cos(b\,k_i) \equiv \sqrt{1-\beta_i^2}$, is executed, it is possible to get:

$$P_m^{(i)} = \frac{m\,V_i}{\cos(b\,k_i)} \equiv m\,C\frac{\beta_i}{\sqrt{1-\beta_i^2}}. \tag{34}$$

Appearance of a factor $\sqrt{1-\beta_i^2}$ in dynamic relations at excitation of the condensed systems was mentioned in other articles also [1, 34].

The presence of determinations of the Lagrangian (33) and of impulse (34) enables to consider mechanical description of dynamics of quasi-particle completed and pass to wave description of its dynamics. Indeed, it remained only to find the mechanical Hamiltonian. For this purpose it is possible to use standard [28, 29] determination: $H_m(\mathbf{P}_m) = C\sum_i \beta_i P_m^{(i)} - L_m(\boldsymbol{\beta})$, in which it is necessary to eliminate speed β by equality (34). As a result it is possible to obtain: $H_m(\mathbf{P}_m) = m\,C^2\sum_i \sqrt{1+\left(p_m^{(i)}\right)^2}$, where is marked: $p_m^{(i)} \equiv P_m^{(i)}\Big/(m\,C) = \beta_i\Big/\sqrt{1-\beta_i^2}$. Here $p_m^{(i)}$ are the components of dimensionless mechanical impulse. As it was possible to expect, this determination also differs from generally accepted $H_m(\mathbf{P}_m) = m\,C^2\sqrt{1+\mathbf{P}_m^2}$.

Before consideration of a wave description we will stop on relation between impulses $\mathbf{P}$ and $\mathbf{P}_m$. Using in equality (34) determination (27) and replacing components k_i by the components P_i in accordance with determination: $k_i = P_i/\hbar$, we will get expression: $P_m^{(i)} = m\,C\,\mathrm{tg}\left(\dfrac{P_i}{m\,C}\right)$, which can be named the generalized relation of Louis de Broglie. While getting of dependence $P_m^{(i)}$ on P_i the determination of mass (30), written down in a form: $\hbar/b = m\,C$, was used. From this determination for mass follows also

the dimensionless determination of wave impulse $p_i \equiv \dfrac{P_i}{m\,C} \equiv b\,k_i$. As mentioned above at the discussion of operator (16) and energy (24) an operator $-\,i\,\hbar\,\nabla_{\mathbf{n}}$ is put into accordance to the wave impulse $\mathbf{P}$. It is now obvious, that to the mechanical impulse is put into accordance not so simple operator with components: $\widehat{P}_m^{(i)} = -i\,m\,C\,\mathrm{th}\left(\dfrac{\hbar}{m\,C}\nabla_{\mathbf{n}}\right)$. Or with an account of (30): $\widehat{P}_m^{(i)} = -i\dfrac{\hbar}{b}\,\mathrm{th}\,(b\nabla_{\mathbf{n}})$. Relation between impulses can be represented in a dimensionless form

$$p_m^{(i)} = \mathrm{tg}\,(p_i)\,. \tag{35}$$

Obviously, that equality (35) becomes an ordinary relation of Louis de Broglie: $\mathbf{p}_m = \mathbf{p}$, only in the case of very small impulses, and, accordingly, very small speeds. Relation $\mathbf{p}_m = \mathbf{p}$ looks here, as zero approximation. It is possible to select two approximations additionally. They are based on the inequality that is always executed: $p_m^{(i)} > p_i > \beta_i$. It appears from determinations of impulses $p_m^{(i)}$, p_i and also of speed β_i.

The description based on a wave impulse will be considered now. For final construction of this description we have determination of the Hamiltonian (32) and relation (26) between speed and wave impulse (in dimension form). In a dimensionless form the same relation has a form (27). For completion of this description it is enough to define the proper Lagrangian. Again we will use standard determination: $L\,(\boldsymbol{\beta}) = C\sum\limits_i \beta_i P_i - H\,(\mathbf{P})$. Further putting (32) in the last equality, eliminating an impulse $\mathbf{P}$ by means of relation (27) and forming a dimensionless form, we will get:

$$l\,(\boldsymbol{\beta}) = \sum_i \left(\beta_i\,\mathrm{arcsin}\,(\beta_i) + \sqrt{1-\beta_i^2}\right), \tag{36}$$

where it is marked $l\,(\boldsymbol{\beta}) \equiv L\,(\boldsymbol{\beta})/m\,C^2$. This Lagrangian at implementation of operations $\partial l\,(\boldsymbol{\beta})/\partial\beta_i$ indeed generates the components of wave impulse $p_i = \mathrm{arcsin}\,(\beta_i)$. The last equality is reverse in relation to determination (27) (at the account of relation $b\,k_i = p_i$). The necessity of implementation of reverse transformation means limitation on the components of impulse p_i by such inequalities $|p_i| \le \pi/2$. It differs from a similar limitation by the condition of Born-Karman: $|p_i| \le \pi$. Condition of Born-Karman is related to the terms of periodicity, but here we speak about the ordinary mathematical requirement: at implementation of reverse transformation it is necessary to be limited by the region of unambiguity. Condition of Born-Karman twice more of region, got here.

Thus, for consideration of quasi-particle, as classic object (material point), we have two descriptions, equal in rights. One description is mechanical one with the Lagrangian $l_m\,(\boldsymbol{\beta}) \equiv L_m\,(\boldsymbol{\beta})/\left(m\,C^2\right)$ and the Hamiltonian $h_m\,(\mathbf{p}_m) \equiv H_m\,(\mathbf{P}_m)/\left(m\,C^2\right)$. This is the description which can be named the relativistic approximation as it practically have the same form and was got in three approximations listed above (plane wave in a phase, nearest neighbors and cubic grate). Another description is wave description with the Hamiltonian function $h\,(\mathbf{p}) \equiv H\,(\mathbf{P})/\left(m\,C^2\right)$ and the Lagrangian $l\,(\boldsymbol{\beta}) \equiv L\,(\boldsymbol{\beta})/\left(m\,C^2\right)$. Both descriptions are equal in rights in the sense that identically adequately describe dynamic properties of quasi-particle, as classic object. In general case it is impossible to do the choice between them without additional researches. Except possibly the relativistic approximation considered here in which the mechanical Lagrangian $l_m\,(\boldsymbol{\beta})$ and the mechanical Hamiltonian $h_m\,(\mathbf{P}_m)$ have the acquainted relativistic form. Therefore, in conclusion, we will consider a question about attitude of both dynamic descriptions of classic type to quantum description, as one of methods, which gives a possibility to do such choice.

Quantum description in the accepted approximations (plane wave in a phase, nearest neighbors and cubic grate) relates to the wave function (23). In these approximations it takes such a form

$$a_{\mathbf{n}}\,(t) = \frac{1}{\sqrt{N}}\exp\left[i\,(p_j x_j - h\,(\mathbf{p})\;\tau)\right]. \tag{37}$$

A form $p_j x_j$ implies here, as usual, executing of adding up by an index j. Variables x_j are the components of vector of grate $\mathbf{n} = \{b x_1, b x_2, b x_3\} \equiv \{b x, b y, b z\}$ in approximation of cubic grate. In accordance with determination (32) the Hamiltonian $h\,(\mathbf{p})$ looks like $h\,(\mathbf{p}) = -\sum\limits_i \cos\,(p_i)$. It appears in

a phase due to a relations (24), from which, in particular, ensues $\omega(\mathbf{k}) = \varepsilon(\mathbf{k})/\hbar$, and due to relation (31), from which it is possible to get a Hamiltonian $h(\mathbf{p})$. Dimensionless time τ has such determination $\tau \equiv mC^2t/\hbar = |M|t/\hbar$. Because a function (37) is formulated in terms of wave impulse, it at once gives advantage to the wave "branch" of descriptions of classic type. In addition, quantum description is always formulated in the intrinsic frame of reference, what is important for the adequate location of classic description in a quantum description. For formulation of the solution (37) (its phases, if to be more exact) in the intrinsic frame of reference, we will find at first the point of conditional localization of excitation. As quasi-particle has a speed $\boldsymbol{\beta} = \{\beta_j\}$, its conditional location in the moment of time τ can be set by a vector $\mathbf{x}_0$ with the components $x_0^{(j)} \equiv \beta_j\tau$. In the case of irregular motion this relation is determined by more common equality: $d\mathbf{x}_0/d\tau = \boldsymbol{\beta}$. Executing in (37) identical transformation: $x_j \equiv x_j - x_0^{(j)} + x_0^{(j)}$, entering determination of relative variables: $x_j - x_0^{(j)} \equiv \xi_j$, and taking into account the dimensionless form of common determination of wave Lagrangian: $l(\boldsymbol{\beta}) = \sum\limits_i \beta_i p_i - h(\mathbf{p})$, it is possible, in final analysis, to get

$$a_{\mathbf{n}}(t) = \frac{1}{\sqrt{N}} \exp\left[i\left(p_j\xi_j + l(\boldsymbol{\beta})\,\tau\right)\right]. \tag{38}$$

Obviously, that phase part of solution actually disintegrated on two multipliers. First of it $\exp[i\ (\mathbf{p}\cdot\boldsymbol{\xi})]$, is the stationary quantum wave function of free particle in the frame of reference, related to the point $\mathbf{x}_0$, which moves in relation to a crystalline lattice with the speed $\boldsymbol{\beta}$. An argument of this multiplier can be brought to the form: $p_j\cdot(x_j - \beta_j\tau)$, and is visible that it meets condition of invariance of Galilei. However, taking into account the relation (35) written in a form: $p_i = \operatorname{arctg}\left(p_m^{(i)}\right)$, it is possible (in some set of exactness) to use approximation : $\mathbf{p}_m \approx \mathbf{p}$, $\mathbf{p} \approx \boldsymbol{\beta}$, but $\mathbf{p}_m \neq \boldsymbol{\beta}$, i.e. $p_m^{(i)} = \beta_i \Big/ \sqrt{1-\beta_i^2}$. It can be named the first approximation of Louis de Broglie. This approximation is possible due to inequalities that are always executed in examined case $p_m^{(i)} > p_i > \beta_i$, and it is always possible to find the range of values of these three variables in which such approximation is possible. In this case it is not difficult to show that an argument $p_j\cdot(x_j - \beta_j\tau)$ can be brought to Lorentz invariant form: $p_j\cdot(x_j - \beta_j\tau)\Big/\sqrt{1-\beta_i^2}$. Indeed, consistently using equalities: $\mathbf{p} \approx \mathbf{p}_m$, $p_m^{(i)} = \beta_i \Big/ \sqrt{1-\beta_i^2}$ and $\boldsymbol{\beta} \approx \mathbf{p}$, it is possible to get such sequence of transformations

$$p_j\cdot(x_j - \beta_j\tau) \to p_m^{(j)}\cdot(x_j - \beta_j\tau) \equiv \beta_j\cdot(x_j - \beta_j\tau)\Big/\sqrt{1-\beta_i^2} \to p_j\cdot(x_j - \beta_j\tau)\Big/\sqrt{1-\beta_i^2}.$$

But this transformation can be done only in such first approximation of Louis de Broglie.

Second multiplier $\exp(i\,l(\boldsymbol{\beta})\,\tau)$, depends on classic action $S(\tau) = l(\boldsymbol{\beta})\,\tau$, which determines the dynamics of point $\mathbf{x}_0 = \boldsymbol{\beta}\tau$ and the Lagrangian $l(\boldsymbol{\beta})$ is determined in (36). In general case classic action (in dimensionless formulation) is determined by expression: $S(\tau) = \int\limits_0^\tau l(\boldsymbol{\beta}')\,d\tau'$. Consequently, it is possible to assert that an indefinite phase element which a wave function (38) is determined within is a classic action of trajectory of motion of point of conditional localization of excitation (with the Lagrangian (36)). It will be shown in further our articles, that it is true also for the general case of dynamics of quasi-particle both in the external field and at interaction of quasi-particles.

In conclusion it is possible to mark that in the case of plasma the scalar and vector potentials execute the same role as a wave function in solids.

4. Conclusions

Basic principles of construction of dynamic properties of classic type for quasi-particles at excitation of environments with the structure of solids (crystals) are analyzed. Excitation is realized as dispersion dependences $E(\mathbf{k})$ or $\omega(\mathbf{k})$. The used methods of analysis have enough general character and can be

applied also in other physically or technologically actual regions, where energy is a function of some parameter. The results of analysis were shown on the example of electronic excitations of crystals in simplest case, when ignore other influencing. Phonons, reaction of grate on excitation, defects, high density of excitations, which requires the account of interaction between them, and others like that. It was shown that such excitations were simultaneously described by three methods. First is quantum, which gives description of the examined excitations in terms of wave functions and eigenvalues of energy. The second method is classic. It arises out from quantum method and is formulated in relation to a wave impulse. This method of description is based on the fact that eigenvalues of energy are an energy bands, i.e. dispersion dependences $E_f(\mathbf{k})$. Exactly dependence of energy on a parameter assumes its consideration in terms of classic mechanics as a Hamiltonian of some free point object. Description of quasi-particle in terms of the second method can be named a wave classic type description. The third method which originates from the second is also classic type description, but in relation to other impulse – mechanical. Interestingly, that in approximations used here (plane wave in a phase, nearest neighbors and cubic grate) the third method of description practically coincides with the known dynamic description of free relativistic particle. From point of more complete understanding of nature of the "real"particles, is impossible not to pay attention on this. At the same time this (third or second classic) description enables to interpret experimental information in the usual terms of relativistic dynamics, if the examined system assumes the use of the considered approximations. If this not so, the third, mechanical description, as well as the second, will differ from any of known descriptions. A question about the "relation" of both classic descriptions to the first – quantum – is found out. Also it is found out that the second, wave classic type description executes a certain transitional role from a basic quantum to the third, mechanical. This, second description exists in the phase of wave function as an element, sense of which is fully identical to classic action for the trajectory of point of conditional localization of excitation.

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Ефект виродження динамічних властивостей квазічастинок електронного походження у напівпровідникових матеріалах

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У статті аналізуються загальні динамічні властивості вільних квазічастинок, а також умови, при яких опис динамічних властивостей квазічастинок практично збігається з аналогічними властивостями реальних релятивістських частинок. Розглянуто проблему співвідношення квантового й класичного способів опису квазічастинок у випадку збуджених станів кристалів. Проаналізовано основні принципи побудови динамічних властивостей класичного типу для квазічастинок при збудженні середовищ із структурою твердих тіл (кристалів). Результати аналізу продемонстровано на прикладі електронних збуджень кристалів у найпростішому випадку, коли іншими впливами нехтують (фонони, реакція ґратки на збудження, дефекти, висока густина збуджень, що вимагає урахування взаємодій між ними, тощо). Показано, що такі збудження одночасно описуються трьома способами. Ці описи дають можливість інтерпретувати експериментальні дані у звичних термінах релятивістської динаміки, якщо розглянута система припускає використання розглянутих наближень (плоскої хвилі у фазі, найближчих сусідів і кубічної ґратки).