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STRONG FIELD GENERALIZATION OF THE INTERBAND TRANSITIONS KINETICS

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A nonperturbative kinetic equation (KE) for description of two-band transitions under action of a strong time-dependent electric field is obtained for arbitrary dispersion laws of carriers in the c- and v-zones (the previously analogical KE was obtained in [1] for the case of quadratic mirror symmetric dispersion laws). The developed approach is based on the similarity to the dynamical Schwinger effect and considers the creation and annihilation processes as the coherent one.

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INTRODUCTION

In the present work the generalization of the KE of the work [1] is obtained for the case of arbitrary dispersion laws of electrons and holes in two-band solid state model. Both these works are based on the analogy with QED where the electron and positron evolution (in particular, their creation and annihilation) is considered as a coherent process. The KE received in this work is simple generalization of the KE [1] obtained for the quadratic mirror symmetric dispersion laws of the carriers. This KE is equivalent to the system of ordinary differential equations for the distribution and polarization functions (e.g., [3]) and has the same mathematical structure as the standard Bloch equations system based on the nonstationary perturbation theory in the framework of the dipole approximation.

We follow the work [1] and begin with the free carriers case (Sec. 1). The next generalization on the case of interaction with time-dependent space-homogeneous quasiclassical electric fields is considered in Sec. 2. The derivation of the KE is fulfilled here too. The last section contains the short summary of the work.

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1. THE FREE QUASIPARTICLE BASIS

In search of the relevant generalization we will rely on the work [1]. Let us consider a two-band system of the mirror asymmetric electron states in the v- and c-zones with dispersion laws

$$E_c = \frac{\triangle}{2} + \varepsilon_c(\mathbf{p}), \quad E_v = -\frac{\triangle}{2} - \varepsilon_v(\mathbf{p}). \tag{1}$$

The electron states in these zones will be considered coherent with the general dispersion law

$$(E - E_c)(E - E_v) = \left[E - \frac{\triangle}{2} - \varepsilon_c(\mathbf{p})\right]\left[E + \frac{\triangle}{2} + \varepsilon_v(-\mathbf{p})\right] = 0. \tag{2}$$

From here follows the equation of motion

$$\left[\hat{E} - \frac{\triangle}{2} - \varepsilon_c(\hat{\mathbf{p}})\right]\left[\hat{E} + \frac{\triangle}{2} + \varepsilon_v(-\hat{\mathbf{p}})\right]\Psi(\mathbf{x}, t) = 0 \tag{3}$$

with $\hat{E} = i\partial/\partial t$ and $\hat{\mathbf{p}} = -i\nabla(\mathbf{x})$. Going over to the momentum representation ($V = L^3$ is the volume of the system)

$$\Psi(\mathbf{x}, t) = \frac{(2\pi)^{3/2}}{V}\sum_{\mathbf{p}}\Psi(\mathbf{p}, t)\,\mathrm{e}^{i\mathbf{p}\mathbf{x}}, \tag{4}$$

we rewrite Eq. (4) in the form of an oscillator equation

$$\left[\hat{E} - \frac{\triangle}{2} - \varepsilon_c(\hat{\mathbf{p}})\right]\left[\hat{E} + \frac{\triangle}{2} + \varepsilon_v(-\hat{\mathbf{p}})\right]\Psi(\mathbf{p}, t) = 0, \tag{5}$$

which contains the term with the first time derivative, $[\varepsilon_v(\mathbf{p}) - \varepsilon_c(\mathbf{p})]\,\hat{E}$ describing the quantum beating of the electron states in the v- and c-zones.

For construction of the Lagrange and Hamilton formalism, it is convenient to transform Eq. (5) to the oscillator equation, which does not contain the first derivative. The phase transformation

$$\Psi(\mathbf{p}, t) = \exp\left\{\frac{i}{2}\left[\varepsilon_v(\mathbf{p}) - \varepsilon_c(\mathbf{p})\right]t\right\}\Phi(\mathbf{p}, t) \tag{6}$$

allows one to reach this purpose. The equation for the Φ function has the form

$$\ddot{\Phi}(\mathbf{p}, t) + \Omega^2(\mathbf{p})\Phi(\mathbf{p}, t) = 0, \tag{7}$$

where $\Omega(\mathbf{p},t)$ is the effective frequency

$$\Omega(\mathbf{p},t)=\frac{1}{2}\left[\varepsilon_v(\mathbf{p})+\varepsilon_c(\mathbf{p})+\triangle\right]. \tag{8}$$

The Lagrange function

$$L(\mathbf{p},t)=\frac{1}{\triangle}\left\{\left|\dot{\Phi}(\mathbf{p},t)\right|^2-\Omega^2(\mathbf{p})\left|\Phi(\mathbf{p},t)\right|^2\right\} \tag{9}$$

corresponds to Eq. (7). The factor $1/\triangle$ is fixed in accordance with the mirror symmetric dispersion laws $\varepsilon_v=\varepsilon_c=\varepsilon$ [1] (that correspond to the case of the independent bands, $\triangle\gg\varepsilon_{c,v}$). Fulfilling the inverse transformation (6), we obtain the Lagrange function in the Ψ representation

$$L(\mathbf{p},t)=\frac{1}{\triangle}\left\{\left|\dot{\Psi}^*+\frac{i}{2}\left(\varepsilon_v-\varepsilon_c\right)\Psi^*\right|^2-\Omega^2(\mathbf{p})\left|\Psi\right|^2\right\}. \tag{10}$$

The canonical momentum can be found

$$\pi(\mathbf{p},t)=\frac{\partial L}{\partial\dot{\Psi}}=\frac{1}{\triangle}\left[\dot{\Psi}^*+\frac{i}{2}\left(\varepsilon_v-\varepsilon_c\right)\Psi^*\right]. \tag{11}$$

The Legendre transformation brings now the Hamilton function in the momentum representation

$$H(\mathbf{p},t)=\pi\dot{\Psi}+\pi^*\dot{\Psi}^*-L, \tag{12}$$

where $L(\Psi,\Psi^*;\dot{\Psi},\dot{\Psi}^*)$ is defined by Eq. (10).

Let us take into account now, that the decomposition (4) is defined on the hypersurfaces $E_i(\mathbf{p})$ defined by the roots of Eq. (2). In order to take it into account, the additional Fourier transformation is fulfilled in Eq. (4)

$$\Psi(\mathbf{x},t)=\frac{(2\pi)^{3/2}}{V}\sum_{\mathbf{p}}\int dE\,\tilde{\Psi}(E,\mathbf{p})\,\mathrm{e}^{-iEt+i\mathbf{px}}, \tag{13}$$

and the Fourier transformation $\tilde{\Psi}(E,\mathbf{p})$ is fixed on the energy surface (2), i.e.,

$$\tilde{\Psi}(E,\mathbf{p})=\delta\left\{\left[E-\frac{\triangle}{2}-\varepsilon_c(\mathbf{p})\right]\left[E+\frac{\triangle}{2}+\varepsilon_v(-\mathbf{p})\right]\right\}\psi(E,\mathbf{p}). \tag{14}$$

Using the textbook relation

$$\delta[\phi(x)]=\sum_i\{|\phi'(x_i)|\}^{-1}\delta(x-x_i),\quad \phi(x_i)=0, \tag{15}$$

the decomposition (13) can be rewritten in the form typical of a two-band model (the electron state is a superposition of electron and hole contributions)

$$\Psi(\mathbf{x},t) = \frac{(2\pi)^{3/2}}{V} \sum_{\mathbf{p}} \sqrt{\frac{\Delta}{2\Omega}} \left\{ a_e(\mathbf{p})\, \mathrm{e}^{-i(\varepsilon_c+\Delta/2)t} + a_h(-\mathbf{p})\, \mathrm{e}^{i(\varepsilon_v+\Delta/2)t} \right\} \mathrm{e}^{i\mathbf{px}}. \tag{16}$$

The corresponding decomposition for the canonical momentum follows then from Eqs. (11) and (16):

$$\pi(\mathbf{x},t) = \frac{i(2\pi)^{3/2}}{V} \sum_{\mathbf{p}} \sqrt{\frac{\Omega(\mathbf{p})}{2\Delta}} \left\{ a_e^{\dagger}(\mathbf{p})\, \mathrm{e}^{i(\varepsilon_c+\Delta/2)t} - a_h^{\dagger}(-\mathbf{p})\, \mathrm{e}^{-i(\varepsilon_v+\Delta/2)t} \right\}. \tag{17}$$

Substitution of the decompositions (16) and (17) in Eq. (12) leads to the total Hamilton function

$$H = \frac{(2\pi)^3}{V} \sum_{\mathbf{p}} \left\{ \left[\varepsilon_c(\mathbf{p}) + \frac{\triangle}{2} \right] a_e^{\dagger}(\mathbf{p}) a_e(\mathbf{p}) + \left[\varepsilon_v(\mathbf{p}) + \frac{\triangle}{2} \right] a_h^{\dagger}(-\mathbf{p}) a_h(-\mathbf{p}) \right\}. \tag{18}$$

Quantization on the formal level brings to replacement of the amplitudes $a_{e,h}$ and $a_{e,h}^{\dagger}$ by the corresponding operators (we will not introduce new notations for them) defined on the stationary vacuum state. The operators of creation and annihilation obeyed the standard anticommutation relations $\{a_{e,h}(\mathbf{p}), a_{e,h}^{\dagger}(-\mathbf{q})\} = \delta_{\mathbf{p},\mathbf{q}}$, etc. The form of the corresponding Hamilton operator is identical to (18).

2. INTERACTION WITH A QUASICLASSICAL ELECTRIC FIELD

An interaction with a quasiclassical electromagnetic field in the original coordinate representation is introduced by the substitution $\partial_\mu \to D_\mu = \partial_\mu + ieA_\mu$ ($\mu = 0, 1, 2, 3$), where $A_\mu^{\mathrm{ex}} + A_\mu^{\mathrm{in}}$ is 4-potential of external and internal field and e is the electron charge with its sign. We will restrict ourselves below to the case of a nonstationary space-homogeneous electric field with 4-potential in the Hamilton gauge, $A_\mu = (0, A_1(t), A_2(t), A_3(t))$ and then $\hat{\mathbf{p}} \to \hat{\mathbf{P}} = \hat{\mathbf{p}} + e\mathbf{A}$. The corresponding procedure based on the decompositions (16) and (17) leads to the nondiagonal form of the Hamiltonian (12) in the momentum space, that makes the physical meaning of the $a_{e,h}$ operators difficult. The adequate interpretation is achieved by transition to the quasiparticle (QP) representation, where all observable operators have the diagonal form. Usually, the Bogoliubov method of time-dependent canonical transformations is used [2]. We will use below an economical method based on the holomorphic (oscillator) representation [3], that was developed for the problem of the relativistic kinetics of vacuum pair creation in strong electromagnetic field.

In accordance with the method of works [1, 3], it is necessary to make the substitution $\hat{\mathbf{p}} \to \hat{\mathbf{P}}$ in the dispersion law occurring in the decompositions (16) and (17) for the free field wave function and canonical momentum and also to introduce new time-dependent amplitudes (or operators) $a_{e,h}(\mathbf{p},t)$ by the replacement

$$a_e(\mathbf{p})\,\mathrm{e}^{-i(\varepsilon_c+\Delta/2)t} \to a_e(\mathbf{p},t), \quad a_h(-\mathbf{p})\,\mathrm{e}^{i(\varepsilon_v+\Delta/2)t} \to a_h(-\mathbf{p},t), \tag{19}$$

and so on. The result is the following:

$$\Psi(\mathbf{x},t) = \frac{(2\pi)^{3/2}}{\sqrt{V}} \sum_{\mathbf{p}} \sqrt{\frac{\Delta}{2\Omega(\mathbf{P})}} \left\{a_e(\mathbf{p},t) + a_h(-\mathbf{p},t)\right\} \mathrm{e}^{i\mathbf{p}\mathbf{x}}, \tag{20}$$

$$\pi(\mathbf{x},t) = \frac{i(2\pi)^{3/2}}{\sqrt{V}} \sum_{\mathbf{p}} \sqrt{\frac{\Omega(\mathbf{P})}{2\Delta}} \left\{a_e^\dagger(\mathbf{p},t) - a_h^\dagger(-\mathbf{p},t)\,\mathrm{e}^{-i\mathbf{p}\mathbf{x}}\right\}. \tag{21}$$

Here it is assumed, that the dispersion laws $\varepsilon_{e,h}(\mathbf{p})$ are not changed under action of the external field besides the trivial displacement $\hat{\mathbf{p}} \to \hat{\mathbf{P}}$, i.e., the dynamic Stark effect is not considered and magnitude of the gap and the band boundaries remain invariable. The total Hamiltonian $H_{\rm tot}$ can be obtained now from the free Hamiltonian (12) by the replacement $\partial \to D_k$ $(k = 1, 2, 3)$. The subsequent substitution of Eqs. (20), (21) brings at once to the diagonal form of the Hamiltonian in the QP representation

$$H_{\rm tot}(t) = \frac{(2\pi)^{3/2}}{\sqrt{V}} \sum_{\mathbf{p}} \left\{ \left[\varepsilon_c(\mathbf{P}) + \frac{\triangle}{2}\right] a_e^\dagger(\mathbf{p}) a_e(\mathbf{p}) + \right.$$
$$\left. + \left[\varepsilon_v(-\mathbf{P}) + \frac{\triangle}{2}\right] a_h^\dagger(-\mathbf{p}) a_h(-\mathbf{p}) \right\}. \tag{22}$$

The new time-dependent amplitudes $a_{e,h}(\mathbf{p},t)$ obey the exact equations of motion, which can be obtained from the minimal action principle

$$S = \int d\mathbf{x} \left\{ \pi(\mathbf{x},t)\dot{\Psi}(\mathbf{x},t) + \dot{\Psi}^*(\mathbf{x},t)\pi^*(\mathbf{x},t) - H_{\rm tot}(\mathbf{x},t) \right\} \tag{23}$$

in the QP representation with the decompositions (20), (21)

$$S = \int dt \frac{(2\pi)^3}{V} \sum_{\mathbf{p}} \left\{ \frac{i}{2} \Big([a_e(\mathbf{p},t) - a_h^\dagger(-\mathbf{p},t)][\dot{a}_c(\mathbf{p},t) + \dot{a}_h(-\mathbf{p},t)] - \right.$$
$$- [a_e(\mathbf{p},t) - a_h(-\mathbf{p},t)][\dot{a}_e^\dagger(\mathbf{p},t) + \dot{a}_h^\dagger(-\mathbf{p},t)] +$$
$$\left. + \lambda(\mathbf{p},t)[a_h^\dagger(-\mathbf{p},t) a_e(\mathbf{p},t) - a_e^\dagger(\mathbf{p},t) a_h(-\mathbf{p},t)] \Big) - H_{\rm tot}(\mathbf{p},t) \right\}, \tag{24}$$

where $H_{\rm tot}(\mathbf{x},t)$ and $H_{\rm tot}(\mathbf{p},t)$ are the Hamiltonian densities in the x- and p-representations. $\lambda(\mathbf{p},t)$ is the amplitude of interband transitions

$$\lambda(\mathbf{p},t)=\frac{1}{2}\sqrt{\Omega(\mathbf{p},t)}\frac{\partial}{\partial t}\frac{1}{\sqrt{\Omega(\mathbf{p},t)}}= \\ =-\frac{\dot{\varepsilon}_c(\mathbf{p},t)+\dot{\varepsilon}_v(-\mathbf{p},t)}{4\Omega(\mathbf{p},t)}=e\mathbf{E}(t)\frac{\mathbf{v}_c(\mathbf{p},t)+\mathbf{v}_v(-\mathbf{p},t)}{4\Omega(\mathbf{p},t)}, \quad (25)$$

where $E(t)=-\dot{A}(t)$ is the electric field strength and $\mathbf{v}_{e,h}(\mathbf{p},t)=\partial\varepsilon_{e,h}/\partial\mathbf{P}$ is the group velocities of the carriers. Then the operator equations of motion follow from Eq. (24) by variation on the amplitudes and subsequent transition to the occupation number representation with the anticommutation relations $\left\{a_{e,h}(\mathbf{p}),a^{\dagger}_{e,h}(\mathbf{q})\right\}=\delta_{\mathbf{p},\mathbf{q}}$ (the remaining elementary anticommutators equal zero). These Heisenberg-like equations of motion are the following:

$$\dot{a}_e(\mathbf{p},t)=\lambda(\mathbf{p},t)a_h^{\dagger}(-\mathbf{p},t)+i\left[H_{\rm tot}(t),a_e(\mathbf{p},t)\right], \\ \dot{a}_h(\mathbf{p},t)=\lambda(\mathbf{p},t)a_e^{\dagger}(-\mathbf{p},t)+i\left[H_{\rm tot}(t),a_h(\mathbf{p},t)\right]. \quad (26)$$

The first term in r.h.s. of these equations describes intermixing of the e- and h-states. Hence, the parameter (25) is the intermixing amplitude. It is very important, that the Hamiltonian and the total charge operator have the diagonal form in this representation. Thus, the oscillator representation is simultaneously a quasiparticle one.

It is assumed that the electric field is switched off in the in- and out-states and the quasiparticle excitations become «free» and available for direct observation. In addition, it is also supposed here, that the system is found in the ground state at the initial moment $t_0\to-\infty$ and, hence, the initial state is the vacuum state $|0>$ of electron and holes quasiparticles. This state is not equal to the out-state, where some quantity of electrons and holes can remain after switch off of the electric field.

The resulting closed form of the KE follows from the well-known procedure [1]:

$$\dot{f}(\mathbf{p},t)=2\lambda(\mathbf{p},t)\int\limits_{-\infty}^{t}dt'\,\lambda(\mathbf{p},t')[1-2f(\mathbf{p},t')]\cos 2\theta(\mathbf{p},t,t'), \quad (27)$$

where the dynamical phase

$$\theta(\mathbf{p},t,t')=\int\limits_{t'}^{t}d\tau\,\Omega(\mathbf{P},\tau) \quad (28)$$

corresponds to the quantum «beating» of the interband transition. This equation is equivalent to an integral equation of the Volterra type. The right-hand side of the KE (27) is responsible for creation and annihilation of electron–hole pairs and has the same form as in QED (with an essential difference in construction of the amplitude $\lambda(\mathbf{p}, t)$), where the corresponding KE describes the vacuum creation of electron–positron pairs. There is another essential difference from QED kinetics, where m is the unique mass parameter: the present model is the multiparameter one (the width of gap and zones) [1]. The KE (27) can be rewritten in the evident gauge invariant form by change of variables $\hat{\mathbf{p}} \to \hat{\mathbf{P}}$ in the distribution functions $f(\mathbf{p}, t) \to f(\mathbf{P}, t)$.

The KE (27) can be transformed to the system of ordinary differential equations, which is convenient for numerical analysis

$$\dot{f} = \lambda u, \qquad \dot{u} = 2\lambda(1 - 2f) - (2\varepsilon + \Delta)v, \qquad \dot{v} = (2\varepsilon + \Delta)u, \qquad (29)$$

where $u + iv = 2f^{(+)}$ and $f^{(+)}$ is

$$f^{(\pm)}_{e,h}(\mathbf{p}, t) = \int\limits_{-\infty}^{t} dt' \, \lambda(\mathbf{p}, t')[1 - f_e(\mathbf{p}, t') - f_h(-\mathbf{p}, t')] \, \mathrm{e}^{\pm 2i\theta(\mathbf{p}, t, t')}, \qquad (30)$$

$f_{e,h}$ — the quasiparticle distribution functions of electrons and holes. These equations have the first integral $(1 - 2f)^2 + u^2 + v^2 = 1$, according to which the phase trajectories are located on an ellipsoid with top coordinates $f = u = v = 0$ and $f = 1, u = v = 0$.

SUMMARY

The KE (27) is a nonperturbative result of the considered theory of the coherent excitations of interband transitions under action of a time altering electric field. Intensity of the electron–hole creation and annihilation processes is defined entirely by the effective dispersion law (8). The investigation of this KE is supposed to be continued in the next works.

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