Nonperturbative kinetics of electron-hole excitations in strong electric field

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ABSTRACT
The nonperturbative kinetic description of the interband tunneling effect under action of the strong electric field (dynamical analog of the Zener effect) is proposed. The developed approach is based on the analogy with the Sauter-Schwinger effect and its dynamical analog in QED. The kinetic equation for quasiparticle excitations is derived on the dynamical basis in the framework of the oscillator representation. The numerical estimates are made for some simple cases of external field.

Keywords: electron-hole excitation, strong electric field, nonperturbative kinetics

1. INTRODUCTION
It is well known the fundamental analogy between Landau-Zener mechanism of interband tunneling and Schwinger’s mechanism os vacuum electron-positron creation in strong electric field (see e.g.\textsuperscript{1}). This similarity is used recently for the investigation of the transport properties of of strongly correlated quantum many-body systems.\textsuperscript{2,3}

In this work, we develop the nonperturbative kinetics of the electron-hole (e-h) excitations in dielectrics under the action of strong electric laser field using the direct analog of the QED formalism of vacuumpair creation. The proposed theory is oriented for description of an dynamic analog of the Zener effect. The proposed method allows taking into account all multiphoton processes accompanying excitation as against the standard one based on the perturbation theory with respect to an external field (e.g.,\textsuperscript{4,5} and the references therein).

The present work has the methodical character. The definition of the mixed e-h states is an essential distinctive element of our approach. We are employing the rich experience of relativistic QFT in describing the vacuum particle creation under the action of some external quasi-classical field (the Schwinger mechanism\textsuperscript{6–8}) and also using some naive analogy between the Dirac picture of electron-positron vacuum and some concepts of solid state band theory as a foundation of our approach. This leads to the second-order (with respect to time) equation of motion for the wave function describing both states with positive (electrons) and negative (holes) energies (Sect.2). For simplicity, electron and hole dispersions are assumed to be the same (mirror-like). For non-interacting electron-hole system we construct the Lagrange and Hamilton formalism and define corresponding decompositions of the field functions and canonical momentum with respect to the plane waves. This formalism represents a special form of electron-hole representation. The interaction with an external quasiclassical time-dependent homogeneous electric field is described in the Section 3. It is well known that the external electromagnetic field leads to non-diagonal form of the operators corresponding to physical observables, which makes the physical interpretation of the formalism difficult. The transition to quasiparticle (QP) representation is achieved by diagonalization of all operators relevant to the complete QP characteristics (e.g., energy, spin, charge).\textsuperscript{9} On practice, only the Hamiltonian diagonalization is often employed (incomplete QP representation). Usually, the transition to QP representation is done by time-dependent Bogoliubov transformation (e.g.,\textsuperscript{7}). Holomorphic (oscillator) representation developed at last years\textsuperscript{10} is more effective tool for this goal comparing to the Bogoliubov technique because it easily allows to obtain the diagonal Hamiltonian and to derive the Heisenberg-like equations of motion for creation and annihilation operators, where it also takes into account the mixing of the states with positive and negative energies. These equations provide the basis for derivation of the kinetic equation (KE) describing the electron-hole pair creation in the presence of an external electric field (Sect.4).
Some features of this process and dependence on different characteristics of the non-stationary electric field are investigated in Sect.5. The Sect.6 contains the summary.

Developed formalism reveals close similarity to the corresponding QED kinetics of vacuum electron-positron plasma created under the action of strong electromagnetic field. It can be used for simulation of such processes in the high-intensity fields of X-ray and optical lasers, where the electric field can reach the values close to the critical Schwinger strength \( E_c = m_e^2/e = 1.3 \times 10^{16} \text{V/cm} \). The experimental prove of this effect is however difficult. Therefore the study of similar effects in the solid state plasma could be useful for simulation and prediction of the corresponding effects in the strong laser fields. We are limited below the collisionless approximation and neglect the interaction between different charge carriers.

The natural units \( \hbar = c = 1 \) will be used throughout the paper.

2. DESCRIPTION OF ELECTRON-HOLE MIXED STATES

Let us consider two energy bands with the completely filled lower band and the mirrored electron and hole dispersions, \( \varepsilon_e = \varepsilon(p) \), \( \varepsilon_h = -\Delta - \varepsilon(p) \). It is assumed that the energy gap \( \Delta \) is space homogeneous and stationary. Two Schrödinger equations can be associated with these dispersions:

\[
(\hat{E} - \hat{H})\psi = 0,
\]

where \( \hat{E} = i\partial/\partial t \) and

\[
\Psi = \begin{pmatrix} \psi_l \\ \psi_h \end{pmatrix}, \quad \hat{H} = \begin{pmatrix} 0 & -\Delta - \varepsilon(\hat{p}) \\ -\varepsilon(\hat{p}) & 0 \end{pmatrix}
\]

with \( \hat{p} = -i\nabla \). For arbitrary dispersions, this leads to independent description of electron and holes. In this section it is assumed that the external electromagnetic fields and interparticle interaction are absent. On the other hand, we can consider a hole as an antiparticle to the electron. Their states are correlated and allow joint description in analogy with QED. It results to the second order dispersion

\[
(E - \varepsilon_e)(E - \varepsilon_h) = \left[ E - \varepsilon(p) \right]\left[ E + \Delta + \varepsilon(p) \right] = 0
\]

(3)

(the analogous determinant equation is used in the theory of the stationary Zener effect) and leads to the corresponding equation of motion for the total wave function also of the second order with respect to time,

\[
\{\hat{E}^2 + \Delta \hat{E} - \varepsilon(\hat{p})[\Delta + \varepsilon(\hat{p})]\}\Psi = 0
\]

(4)

where \( \Psi(x,t) \) is now the one-component wave function.

Our next target now is to develop the Lagrange and Hamilton formalisms for this equation. To this end, it is convenient to transform this equation to the uniform differential form of the second order with respect to time without the first-order time derivative stipulated by the asymmetry of electron and hole energy states in reference energy frame. The such equation can be obtained by the transformation to the auxiliary wave function \( \Phi \):

\[
\Psi = \Phi \exp \left( \frac{i}{2} \Delta t \right),
\]

(5)

which obeys the equation of the Klein-Gordon type \( (\ddot{\Phi} = \partial^2 \Phi/\partial t^2) \)

\[
\ddot{\Phi} + \left[ \varepsilon(\hat{p}) + \frac{1}{2} \Delta \right]^2 \Phi = 0.
\]

(6)

The Lagrange density for this equation is \( (\Phi, k = \partial \Phi/\partial x_k) \)

\[
L[\Phi] = \alpha \left\{ \Phi^* \dot{\Phi} - \frac{\Delta}{2m} \Phi^* \Phi_{,k} \Phi_{,k} - \frac{1}{4m^2} \Phi^* \Phi_{,kl} \Phi_{,kl} - \frac{1}{4} \Delta^2 \Phi^* \Phi \right\},
\]

(7)
where the dimensional constant $\alpha$ will be determined below. For the simplicity, we use the quadratic isotropic dispersion law, $\varepsilon(p) = \hbar^2 p^2 / 2m$. Using the inverse transformation (5), we obtain

$$L[\Psi] = \alpha \left\{ \dot{\Psi}^* \Psi - \frac{i}{2} \Delta |\Psi^* \Psi - \Psi^* \Psi| - \frac{\Delta}{2m} \Psi^*_k \Psi, k - \frac{1}{4m^2} \Psi^*_k \Psi, kl \Psi, kl \right\}. \tag{8}$$

Let us take advantage of the standard definitions of the canonical momentum

$$\pi = \frac{\partial L[\Psi]}{\partial \dot{\Psi}}, \quad \pi^* = \frac{\partial L[\Psi]}{\partial \dot{\Psi}^*} \tag{9}$$

and the Hamilton density

$$H = \pi \dot{\Psi} + \pi^* \dot{\Psi}^* - L[\Psi]. \tag{10}$$

Using the Eq.(8), we obtain

$$\pi = \alpha [\dot{\Psi}^* + \frac{i}{2} \Delta \Psi^*], \tag{11}$$

$$H = \alpha \left\{ \dot{\Psi}^* \dot{\Psi} + \frac{\Delta}{2m} (\nabla \Psi^*)(\nabla \Psi) + \frac{1}{4m^2} (\nabla^2 \Psi^*) (\nabla^2 \Psi) \right\}, \tag{12}$$

so that the Hamilton density contains also the higher-order space derivatives.

As in the QFT, the wave function $\Psi$ now loses the meaning of the state amplitude. The corresponding charge and current densities are ($k=1,2,3$)

$$\rho = \alpha e \left[ |\Psi|^2 + i(\Psi^* \dot{\Psi} - \dot{\Psi}^* \Psi) \right], \tag{13}$$

$$j_k = ie \alpha \left\{ \frac{\Delta}{2m} \left[ (\Psi^*_k \Psi^* - \Psi^* \Psi^*_k) - \frac{1}{4m^2} \left[ (\Psi^*_k \Psi^* - \Psi^* \Psi^*_k) + (\Psi^*_k \Psi^* + \Psi^* \Psi^*_k) - \Psi^* \Psi^*_k \right] \right\}. \tag{14}$$

The transition to the momentum representation can be done in analogy with QFT. Let us carry out the decomposition of wave function $\Psi(x,t)$ over the plane wave system,

$$\Psi(x,t) = (2\pi)^{-3/2} \int dE dp \, \tilde{\Psi}(E, p) e^{-iEt + ipx} \tag{15}$$

and take into account the dispersion equation (3),

$$\tilde{\Psi}(E, p) = \delta\{|E - \varepsilon(p)|[E + \varepsilon(p)] + \Delta\}\psi(E, p). \tag{16}$$

Using the textbook relation

$$\delta[\phi(x)] = \sum_i \{[\phi'(x_i)]^{-1}\delta(x - x_i), \tag{17}$$

the decomposition (15) can be written in the form

$$\Psi(x,t) = (2\pi)^{-3/2} \int dp \, \sqrt{\frac{\Delta}{\Delta + 2|\varepsilon(p)|}} \left\{ a_e(p)e^{-i\varepsilon(p)t} + a_h^+(p)e^{i|\varepsilon(p)|t} \right\} e^{ipx}, \tag{18}$$

where $a_e(p)$ and $a_h(p)$ are the positive (electron) and negative (hole) amplitudes in momentum representation. In the Eq.(18) we redefine the amplitudes $[\Delta/(\Delta + \varepsilon)]^{-1} a_{e,h} \rightarrow a_{e,h}$ and the multiplier $\alpha$ emerging in the Eqs.(7),(8) and (12) was changed to $\alpha = \Delta^{-1}$ in order for the observables (12)-(14) to make sense (see below). The canonical momentum (11) in the same representation (18) has the form

$$\pi(x,t) = \frac{i}{2}(2\pi)^{-3/2} \int dp \, \sqrt{\frac{\Delta + 2|\varepsilon(p)|}{\Delta}} \left\{ a_h^+(p)e^{i|\varepsilon(p)|t} - a_h(p)e^{-i|\varepsilon(p)|t} \right\} e^{-ipx}. \tag{19}$$
Substituting Eqs. (18) and (19) in the Eqs. (12)-(14), we obtain the total Hamiltonian and charge in the diagonal form (the quasiparticle representation 7, 9)

\[ H_{\text{tot}} = \int dp \left\{ \varepsilon(p) a_e^+(p) a_e(p) + [\Delta + \varepsilon(p)] a_h^+(-p) a_h(-p) \right\}, \]

\[ Q = e \int dp \left\{ a_e^+(p) a_e(p) - a_h^+(-p) a_h(-p) \right\}. \]

The specific correspondence principle is: the electron and hole states become independent at \( \Delta \to \infty \) and the derived relations turn into the ordinary quantum mechanical analogs (after elimination of the high frequency components of the wave function with help of Eq. (5)).

3. QUASIPARTICLE REPRESENTATION IN AN EXTERNAL ELECTRIC FIELD

Interaction with an external quasiclassical electromagnetic field in the original coordinate representation is introduced by the substitution \( \partial \to D_\mu = \partial_\mu + ieA_\mu \) (\( \mu = 0, 1, 2, 3 \)), where \( A_\mu \) is 4-potential and \( e \) is the electron charge with its sign. We will restrict ourself below to the case of a nonstationary space-homogeneous electric field with a 4-potential in the Hamilton gauge, \( A_\mu = (0, A_1(t), A_2(t), A_3(t)) \) and then \( \hat{p} \to \hat{P} = \hat{p} + e\hat{A} \). The substitution into the Hamiltonian (12) leads to its non-diagonal form in the momentum representation. The conventional interpretation of the formalism is achieved by transition to quasiparticle representation, in which all observable operators have the diagonal form.

We will use an economical method based on the holomorphic (oscillator) representation, 16 that was developed in work 10 for the problem of the relativistic kinetics of vacuum pair creation in strong electromagnetic field. We will use that approach below.

In accordance with the method of work 10 it is necessary to make substitution \( p \to P \) in the dispersion law occurring in the decomposition (18) and (19) for the free field function and canonical momentum and also to introduce new amplitudes \( a_{e,h}(p, t) \) by the replacement

\[ a_{e,h}(p) \exp \left[ -ie(p)t \right] \to a_{e,h}(p, t) \]

and so on. The result is the following:

\[ \Psi(x, t) = (2\pi)^{-3/2} \int dp \sqrt{\frac{\Delta}{\Delta + 2\varepsilon(p)}} \left\{ a_e(p, t) + a_h^+(-p, t) \right\} e^{ipx}, \]

\[ \pi(x, t) = \frac{i}{2} (2\pi)^{-3/2} \int dp \sqrt{\frac{\Delta + 2\varepsilon(p)}{\Delta}} \left\{ a_e^+(p, t) - a_h(-p, t) \right\} e^{-ipx}. \]

The new time-dependent amplitudes \( a_{e,h}(p, t) \) obey the exact equations of motion, which can be obtained either from the minimal action principle 10 or using the Hamilton equations

\[ \dot{\Psi} = \frac{\delta H_{\text{tot}}}{\delta \pi(x, t)}, \quad \dot{\pi} = -\frac{\delta H_{\text{tot}}}{\delta \Psi^*(x, t)}. \]

Here the total Hamiltonian in the presence of an external electric field according to the Eq. (12) is:

\[ H_{\text{tot}}(t) = \int dx \left\{ \pi^* \pi + \frac{\Delta}{2m} (D_k^* \Psi^*) (D_k \Psi) + \frac{1}{4m^2} (D_k^* D_k^* \Psi^*) (D_k D_k \Psi) \right\}. \]

The equations system (25) takes then the form:

\[ \dot{\Psi} = \pi^*, \quad \dot{\pi} = \frac{\Delta}{2m} D_k^* D_k \Psi - \frac{1}{4m^2} D_k^* D_k D_k^* D_k \Psi. \]
These equations are compatible with the Eq.(4). Substituting the decompositions (23) and (24) brings the equations of motion for the electron and hole amplitudes in external electric field,

\[ \dot{a}_e(p, t) = \lambda(p, t) a_h^+(p, t) + i [H_{tot}(t), a_e(p, t)], \]
\[ \dot{a}_h(p, t) = \lambda(p, t) a_e^+(p, t) + i [H_{tot}(t), a_h(p, t)], \]  

(28)

where \( \lambda(p, t) \) is amplitude of the interband transition,

\[ \lambda(p, t) = -\frac{\dot{\varepsilon}(P)}{\Delta + 2\varepsilon(P)} = -\frac{ePE(t)}{m[\Delta + 2\varepsilon(P)]}, \]  

(29)

where \( E(t) = -\dot{A}(t) \) is the strength of the electric field. Specific for this Heisenberg-like equations of motion (28) is the presence of the terms describing the states with opposite signs of energy (the first terms in r.h.s.).

The form of the Eqs.(28) implies that transition to the occupation number representation can be done using the Fermi-Dirac statistic, i.e.,

\[ \{a_{e,h}(p, t), a_{e,h}^+(q, t)\} = \delta(p - q) \]  

(30)

(the remaining elementary anti-commutators equal zero). It is very important, that the Hamiltonian (26) and the total charge operator (27) have the diagonal form in this representation. Thus, the oscillator representation is simultaneously quasiparticle one (we are not investigated here the possibility of diagonalization of the spin operator, therefore the question about the completeness\(^3\) of that representation remains opened).

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 with the initial moment \( t_0 \rightarrow -\infty \) and, hence, the initial state is the vacuum state \( |0\rangle \). This state is not out-state, where some quantity of electrons and holes can remain after switch off of the electric field.

4. KINETIC EQUATION AND OBSERVABLES

The basic object of the kinetic theory in the presence of an external strong field is the quasiparticle distribution function, which is defined on the in-vacuum state \( |0\rangle \). In the case of space-homogeneous system, considered here, the quasiparticle distribution functions of electrons and holes are:

\[ f_{e, h}(p, t) = <0| a_{e,h}^+(p, t) a_{e,h}(p, t)|0\rangle. \]  

(31)

Differentiating the functions (31) with respect to time, and using the equations of motion (28) we obtain:

\[ \dot{f}_{e, h}(p, t) = \lambda(p, t) \{ f_{e, h}^{(+)}(p, t) + f_{e, h}^{(-)}(p, t)\}, \]  

(32)

where the auxiliary correlation functions of electrons are introduced

\[ f_{e}^{(+)}(p, t) = <0| a_e^+(p, t) a_e(p, t)|0\rangle, \]
\[ f_{e}^{(-)}(p, t) = <0| a_e(p, t) a_e(p, t)|0\rangle. \]  

(33)

The corresponding hole correlation functions are defined in similar way. The equation of motion for the functions (33) can be obtained by analogy with the equation (32). We can write it down in the integral form

\[ f_{e}^{(\pm)}(p, t) = \int_{-\infty}^{t} dt' \lambda(p, t') [1 + 2 f_{e}^{(\pm)}(p, t')] e^{\pm 2i\varepsilon(p, t', t')}, \]  

(34)

where the asymptotic conditions have been introduced,

\[ \lim_{t \rightarrow -\infty} f_{e}^{(\pm)}(p, t) = 0. \]  

(35)
The analogous relations take place for the distribution functions (31) (absence of electrons and holes in the initial state). In Eq.(34), the dynamical phase

$$\theta(p,t,t') = \int_t^{t'} d\tau \varepsilon(P(\tau))$$

(36)

corresponds to the quantum 'beating' of the mixed states. In the Eq.(34) it was taken into consideration also, that the system is neutral at each moment, i.e.,

$$f_e(p,t) = f_h(p,t) = f(p,t)$$

(37)

According to that, we skip the indexes of the distribution functions in the Eqs.(34) and (35) below.

The resulting closed form of KE follows now from the Eqs.(32) and (34)

$$\dot{f}(p,t) = 2\lambda(p,t) \int_{-\infty}^{t} dt' \lambda(p,t')[1 + 2f(p,t')]\cos 2\theta(p,t,t').$$

(38)

The right-hand side of the KE (38) represents the source of "vacuum" creation and annihilation of electron-hole pairs and has the same form as in QED\textsuperscript{11–13} (with essential difference in construction of the amplitude $\lambda(p,t)$).

There is another essential difference from QED kinetics, where $m$ is the unique mass parameter: in the present model there are such parameters $m$ and $\Delta$. That leads to some specific in the eh-system behavior (see Sect.5). Thus, this non-Markovian KE is a non-perturbative result in the mean-field approximation. KE (38) can be rewritten in the evident gauge invariant form if we make the change of variables $p \to P$ in the distribution functions

$$\dot{f}(p,t) \to \dot{f}(P,t).$$

The KE (38) can be transformed to a system of ordinary differential equations, which is convenient for numerical analysis,$^{11–13}$

$$\dot{f} = \lambda u, \quad \dot{u} = \lambda(1 + 2f) - 2\varepsilon v, \quad \dot{v} = 2\varepsilon u.$$  

(39)

The general study of this system was carried out in the works\textsuperscript{11–13} (existence of one first integral, its geometrical interpretation, non-Hamiltonian structure and so on). After the distribution functions of electron and hole quasiparticles have been obtained, we can write the densities of observables by averaging over vacuum state of the operator energy (20), electron charge (21), total electron-hole current etc. As a result, we have the densities of energy $\omega(t)$, electron number and total current in the form:

$$\omega(t) = 2\int d\mathbf{p} \varepsilon(p,t)f(p,t),$$  

(40)

$$n(t) = \int d\mathbf{p} f(p,t),$$  

(41)

$$j(t) = \frac{2e}{m} \int d\mathbf{p} \mathbf{p}\{f(p,t) + u(p,t)\}.$$  

(42)

The last term in r.h.s. of Eq.(42) describes the vacuum polarization current.$^{11–13}$

If the electric field is rather large ($|E(t)| \sim \Delta^2/|\varepsilon|$), it is necessary to take into account the secondary electric field $E_{in}(t)$ produced by the electron-hole plasma in the primary external field $E_{ex}(t)$ (back reaction of the system). Thus, the total field is

$$E_{tot}(t) = E_{in}(t) + E_{ex}(t).$$  

(43)

The internal field $E_{in}(t)$ obeys the Maxwell equation with the current (42)

$$\dot{E}_{in}(t) = \frac{2e}{m} \int d\mathbf{p} \mathbf{p}\{f(p,t) + u(p,t)\}.$$  

(44)
5. ELECTRON-HOLE EXCITATIONS IN STRONG ELECTRIC FIELD

For numerical estimation, we will consider below the linear polarized electric field of two kinds: the pulse field\(^7\) with the Narozhny-Nikishov potential \( A_{ex} = (0, 0, A_{ex}(t)) \),

\[
A_{ex}(t) = E_0 b [\tanh (t/b) + 1], \quad E_{ex}(t) = E_0 \cosh^{-2} (t/b),
\]

(45)

where \( b \) is the pulse width, and periodic field with the frequency \( \nu \),

\[
A_{ex}(t) = -(E_m/\nu) \cos \nu t, \quad E_{ex}(t) = E_m \sin \nu t.
\]

(46)

The parameters of this field must be satisfied to the quasiclassical field condition,\(^17\) which is necessary for application of used formalism,

\[
E_m \gg \nu^2.
\]

(47)

The parameters of semiconductor are chosen close to ones for silicon: the mass gap \( \Delta = 1 \text{ eV} \) and the effective mass \( m = m_e \). The carrier densities time evolution calculated on the basis of KE (38) and Eq. (41) are presented on the Fig.1,2 for the pulse field (45) with \( b = 1.5 \times 10^{-12} \text{ c} \) and the monochromatic field (46) with \( \lambda = 1 \text{ mm} \).
for different amplitudes $E_0 = E_m = 10^2, 10^3$ and $10^4$ V/cm. The initial strong growth and the next saturation regime is observed for pulse field whereas the periodical field action is accompanied with "accumulation" of density similarly to results of works\textsuperscript{14} for vacuum pair creation.

6. SUMMARY

The new variant of the kinetic equation for description of the e-h excitations (interband tunneling transition) under action of the nonstationary electric field (Zener’s dynamical effect) was obtained on nonperturbative dynamical basis. We used the direct analogy with QED formalism of vacuum pair creation in strong field. The obtained kinetic equation was used for some simple numerical estimation of carriers density dynamics in the monochromatic and pulse fields.

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