Fluctuations of polarization fields of moving charged particles in solids

G. M. Filippov

Chuvash State University
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The fluctuations of polarization fields created by moving charged particles are calculated in the framework of the quantum-mechanical theory of interaction of charged particles with solids. The fluctuations depend strongly on quantum mechanical states of the particles: for narrow (in comparison with the screening radius of the field of a moving particle) wave packets the fluctuations are stationary and vanish with decreasing packet widths, while for wide wave packets the fluctuations increase with time.

1. INTRODUCTION

The polarization fields created by charged point particles moving in solids have been studied in detail in the framework of phenomenological classical electrodynamics (see Refs. 1 and 2). Such treatment is based on the use of the dielectric constant $\varepsilon(\mathbf{q},\omega)$, which gives the medium polarization properties and allows both for temporal and spatial dispersion. The problem of fluctuations of polarization fields does not arise, since in this "dielectric" approach they are simply equal to zero. Doubts that this result is valid outside the framework of phenomenological electrodynamics arise when one tries to find the dielectric constant by microscopic theory. It appears, in this case, that the dielectric constant gives only an averaged reaction of a medium to an external electromagnetic field, which does not exclude fluctuations. On the other hand, in the classical approach one also has to consider distributed charges, e.g., when calculating the deceleration of atoms.[3] In the latter case, the microscopic approach has shown[4] that there are situations when the results of classical and quantum-mechanical calculations coincide only for point charges.

In the present study we consider the problem of polarization-field fluctuations in the framework of the quantum-mechanical theory of interaction of moving atomic particles with a solid. We describe solid states in the form of a direct product of quasiparticle states.[5] It is shown in Ref. 5 that the surface affects only weakly the magnitude of the polarization field already at a relatively small penetration depth of order v/ω_0, where v is the mean particle velocity and ω_0 is the characteristic frequency of the electronic subsystem of the solid. As we are interested in large, in comparison with v/ω_0, values of depths, we consider the medium to be infinite and the moment when the particle enters the solid to be identical with the moment of a sudden switching on the interaction between the particle and quasiparticles.

We list briefly the basic considerations required for the construction of the version of the theory used below (these considerations are given at length in Ref. 5). The dependence of the quasiparticle energies $\omega_\beta(\mathbf{q})$ on their momenta $\mathbf{q}$ is determined by the zeros of the bulk dielectric constant $\varepsilon(\mathbf{q},\omega)$ (β denotes the branches of bulk elementary excitations; here and below we use atomic units $|e| = 1$, $\hbar = 1$ and $m_e = 1$). The electric field potential in a medium can be written as a sum of free oscillations of the form

$$\varphi_{\beta\mathbf{q}}(\mathbf{x},t)=g_{\beta\mathbf{q}}\exp(i\mathbf{q}\mathbf{x}-i\omega_\beta t) \quad (1)$$

Using the well-known expression for the energy of monochromatic field in a nonabsorbing medium

$$\mathscr{E}_{\beta\mathbf{q}}=\int\frac{dV\,dV'}{4\pi}\nabla\varphi_{\beta\mathbf{q}}(\mathbf{x},t)\nabla\varphi_{\beta\mathbf{q}}(\mathbf{x}',t)\frac{\partial}{\partial\omega}[\omega\varepsilon(\omega,\mathbf{x},\mathbf{x}')], \quad (2)$$

we can present the Hamiltonian function of the free oscillation field in a medium as a sum of the Hamiltonians of independent oscillators. Passing on then to the quantum theory, we obtain the operator of the electric field potential in a medium:

$$\hat\varphi(\mathbf{x},t)=\sum_{\beta,\mathbf{q}}g_{\beta\mathbf{q}}(\hat b_{\beta\mathbf{q}}\exp(i\mathbf{q}\mathbf{x}-i\omega_\beta t)+\hat b_{\beta\mathbf{q}}^{+}\exp(-i\mathbf{q}\mathbf{x}+i\omega_\beta t)), \quad (3)$$

where $\hat b^{+}_{\beta q}$ and $\hat b_{\beta q}$ are respectively, the quasiparticle creation and annihilation operators obeying the standard Bose Communication relations, and

$$g_{\beta\mathbf{q}}=\left[4\pi\Big/\left(\Omega q^2\frac{\partial\varepsilon(\mathbf{q},\omega)}{\partial\omega}\bigg|_{\omega=\omega_\beta(\mathbf{q})}\right)\right]^{1/2}. \quad (4)$$

Here Ω is the normalization volume.

2. QUANTUM THEORY EQUATIONS

The Hamiltonian of the system is the sum of the Hamiltonain H_p of the external particles, the Hamiltonain H_Q of the free quasiparticles, and the interaction Hamiltonian $H_{\rm int}$. The Hamiltonians can be conveniently presented in the second-quantization form

$$H_p=\sum_{\mathbf{k}}\frac{k^2}{2m}\hat a_{\mathbf{k}}^{+}\hat a_{\mathbf{k}},\quad H_Q=\sum_{\beta,\mathbf{q}}\omega_\beta(\mathbf{q})\hat b_{\beta\mathbf{q}}^{+}\hat b_{\beta\mathbf{q}}. \quad (5)$$

Here m is the external particle mass, $\hat a_{\mathbf{k}}^{+}$ and $\hat a_{\mathbf{k}}$ are the external quasiparticle creation and annihilation operators, respectively, in the states with a definite momentum $\mathbf{k}$ (for definiteness we consider the external particles fermions but neglect their spin). If the moving particle has a charge Z_1, then, in the interaction representation,

$$H_{\rm int}(t)=Z_1\int\hat\rho(\mathbf{x},t)\hat\varphi(\mathbf{x},t)\,d^3x, \quad (6)$$

where $\hat\rho(\mathbf{x},t)$ is the particle-density operator in the same representation. The standard perturbation theory constructed on the basis of the Hamiltonians (5) and (6) allows us to trace the evolution of the state vector only for a short (shorter than $1/\omega_0$) period of time after the particle enters

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the solid. We suggest below a modification of this theory applicable in a wider range (see below).

To construct a modified perturbation theory, the operator (6) should be presented as the sum of two operators: $H_{\rm int}^{(0)}(t)$ and $H_{\rm int}^{(1)}(t)$. The first one is obtained from $H_{\rm int}(t)$ by replacing the Fourier-components of the time-dependent density operator $\hat{\rho}_{\mathbf{q}}(t)$ by the expression $\hat{\rho}_{\mathbf{q}} f_{\mathbf{q}}(t)$, where $f_{\mathbf{q}}(t)$ is a function of time and momentum $\mathbf{q}$ chosen from additional considerations. It is expedient to demand that $f_{\mathbf{q}}(t)$ provide fulfillment of the Galilean invariance and conservation of the particle number in all orders of perturbation theory. The function

$$f_{\mathbf{q}}(t)=\exp[-i\mathbf{q}\mathbf{x}_0(t)],$$

where $\mathbf{x}_0(t)$ is the current mean value of the particle coordinate, satisfied the listed requirements. The second part of the Hamiltonian can be defined by the equation

$$H_{int}^{(1)}(t)=H_{int}(t)-H_{int}^{(0)}(t).$$

The expediency of singling out the Hamiltonian $H_{\rm int}^{(0)}(t)$ is justified by the fact that, since different operators $\hat{\rho}_{\mathbf{q}}$ obey the commutation relations (as was well-known long ago, see, e.g., Ref. 6), we can neglect the sequence in which the operators $\hat{\rho}_{\mathbf{q}}$ appear in all expressions and widely use the coherent-state theory technique.

Let us write down the "zeroth" evolution operator

$$U_0(t)=\exp\left\{\sum_{\beta,\mathbf{q}}[Q_{\beta\mathbf{q}}(t)\hat{\rho}_{\mathbf{q}}\hat{b}_{\beta\mathbf{q}}^{+}-Q_{\beta\mathbf{q}}^{*}(t)\hat{\rho}_{\mathbf{q}}^{+}\hat{b}_{\beta\mathbf{q}}-i\Phi_{\beta\mathbf{q}}(t)\hat{\rho}_{\mathbf{q}}^{+}\hat{\rho}_{\mathbf{q}}\right\}, \tag{7}$$

where

$$Q_{\beta\mathbf{q}}(t)=-iZ_1 g_{\beta\mathbf{q}}\int_{t_0}^{t}\exp[i\omega_\beta t'-i\mathbf{q}\mathbf{x}_0(t')]dt'.$$

$$\Phi_{\beta\mathbf{q}}(t)=\int_{t_0}^{t}\mathrm{Im}[Q_{\beta\mathbf{q}}^{*}(t')Q_{\beta\mathbf{q}}(t')]dt'+\mathrm{const}.$$

Here t_0 is a certain initial instant, when the interaction is switched on. Then we perform the canonical transformation of all operators:

$$\hat{A}(t)=U_0^{+}(t)A(t)U_0(t), \tag{8}$$

where $\hat{A}(t)$ is the operator in the interaction representation. In the new representation the state vector satisfies the equation

$$i\frac{d}{dt}|t)=\hat{H}_{int}^{(1)}(t)|t) \tag{9}$$

and is expressed through its initial value in the form $|t)=U_1(t)|t_0)$, where

$$U_1(t)=T\exp\left\{-i\int_{t_0}^{t}\hat{H}_{int}^{(1)}(t')dt'\right\}. \tag{10}$$

In the new representation the mean value of an arbitrary physical quantity is given by

$$\bar{A}(t)=(t|\hat{A}(t)|t).$$

Since we can choose the function $\mathbf{x}_0(t)$, this allows us to improve the convergence of the perturbation theory series in $H_{\rm int}^{(1)}(t)$. To this end, we demand that the equation

$$\bar{K}(t)=(t_0|\hat{K}(t)|t_0)$$

hold for a physical quantity $K(t)$. This quantity can be the energy of the moving particle, $E_p(t)$. Then the value of $E_p(t)$ is already obtained in the zeroth approximation in $H_{\rm int}^{(1)}(t)$. All other quantities will not, generally speaking, coincide with the zeroth approximation. Nevertheless, we can expect the corrections to be small. An example of calculations of corrections to the values of specific energy losses is given in Ref. 7. It has been found that the corrections do not exceed 20%.

The mean field

$$\varphi(\mathbf{x},t)=(t|\hat{\varphi}(\mathbf{x},t)|t)$$

to zeroth order in $H_{\rm int}^{(1)}(t)$ is

$$\varphi^{(0)}(\mathbf{x},t)=\sum_{\beta,\mathbf{q}}g_{\beta\mathbf{q}}\cdot 2\,\mathrm{Re}[\rho_{\mathbf{q}}^{(0)}Q_{\beta\mathbf{q}}(t)\exp(i\mathbf{q}\mathbf{x}-i\omega_\beta t)], \tag{11}$$

where $\rho_{\mathbf{q}}^{(0)}$ is the Fourier transform of the probability distribution in the initial state of the moving particle (we suppose that at $t=0$ the particle is, "on the average," at the origin; therefore $\rho_{\mathbf{q}}^{(0)}$ coincides with its value calculated in the particle coordinate frame). The expression (11) coincides with a similar one found in phenomenological electrodynamics. If the particle moves in a uniform medium with a constant velocity v, the set value of the field is found by making t_0 approach minus infinity and introducing a factor $e^{\delta t'}$ for $\delta\to+0$ into the integrand in the general formula for $Q_{\beta\mathbf{q}}(t)$. Taking into account the explicit values of the coupling constants (4), we find the standard expression (see, e.g., Ref. 1):

$$\varphi^{(0)}(\mathbf{x},t)=\int\frac{d^3q}{(2\pi)^3}\frac{4\pi Z_1}{q^2}[\varepsilon^{-1}(\mathbf{q},\mathbf{q}\mathbf{v})-1]\rho_{\mathbf{q}}^{(0)}\exp(i\mathbf{q}(\mathbf{x}-\mathbf{v}t)). \tag{12}$$

The corrections to Eq. (12) should cause the current value of the polarization field to be determined not only by the initial quantum-mechanical state of the particle, but also by the whole evolution of this state during the period of interaction of the particle with the medium.

3. CALCULATION OF THE POLARIZATION FIELD FLUCTUATIONS

The mean squared value of the polarization field fluctuations is given by the general formula

$$D^2(\mathbf{x},t)=(t|[\hat{\varphi}(\mathbf{x},t)-\varphi(\mathbf{x},t)]^2|t)$$
$$=(t|:\hat{\varphi}^2(\mathbf{x},t):|t)+D_0^2-\varphi^2(\mathbf{x},t), \tag{13}$$

where: $\tilde{\varphi}^2$: denote an N-ordered operator and D_0^2 is the contribution of zero-point fluctuations of the quasiparticle field vacuum. Calculating D_0^2, it is necessary to cut off the corresponding integral, allowing thus for the boundedness of the number of degrees of freedom in the solid. Since the quantity D_0^2 always exists, even in the absence of external particles, it cannot be related to the "self" polarization field of the particle. Therefore, in what follows, the expression $D_2(\mathbf{x},t)-D_0^2$ will mean the square value of the particle polarization field.

Let us calculate this expression in zeroth order, replacing the vector $|t)$ by the approximate value $|t_0)$. The obtained expression will have the same validity range as the approximation (11) for the polarization field. The calculations yield the following result:

$$D^2(\mathbf{x},t)-D_0^2$$

$$\approx \sum_{\beta,\mathbf{q}}\sum_{\beta',\mathbf{q}'} g_{\beta\mathbf{q}}g_{\beta'\mathbf{q}'}\rho^{(0)}_{\mathbf{q}-\mathbf{q}'}\cdot 2\,\mathrm{Re}\{[Q_{\beta\mathbf{q}}(t)Q_{\beta'\mathbf{q}'}(t)\exp(-i(\omega+\omega')t)$$

$$+Q_{\beta\mathbf{q}}(t)Q^{*}_{\beta'\mathbf{q}'}(t)\exp(-i(\omega-\omega')t)]\exp i(\mathbf{q}-\mathbf{q}')\mathbf{x})\}$$

$$-[\varphi^{(0)}(\mathbf{x},t)]^2, \qquad (14)$$

where $\omega=\omega_\beta(\mathbf{q})$ and $\omega'=\omega_{\beta'}(\mathbf{q}')$. The set value of this quantity, for motion with constant velocity, is

$$\bar{D}^2(\mathbf{x},t)-D_0^2\approx Z_1^2\sum_{\beta,\mathbf{q}}\sum_{\beta',\mathbf{q}'} g_{\beta\mathbf{q}}^2g_{\beta'\mathbf{q}'}^2\cdot 2\,\mathrm{Re}\Big\{(\rho^{(0)}_{\mathbf{q}-\mathbf{q}'}-\rho^{(0)}_{\mathbf{q}}\,\rho^{(0)}_{-\mathbf{q}'})$$

$$\times\exp(i(\mathbf{q}-\mathbf{q}')(\mathbf{x}-\mathbf{v}t))\Big[\frac{1}{(\omega-\mathbf{q}\mathbf{v}-i\delta)(\omega'-\mathbf{q}'\mathbf{v}+i\delta)}$$

$$+\frac{1}{(\omega-\mathbf{q}\mathbf{v}-i\delta)(\omega'-\mathbf{q}'\mathbf{v}-i\delta)}\Big]\Big\}. \qquad (15)$$

It follows from (15) that for point particles (usually considered in the classic case), owing to $\rho_\mathbf{q}^{(0)}=1$, the polarization-field fluctuations vanish. Such absolute localized states cannot be realized owing to the quantum mechanical uncertainty principle, therefore in reality polarization field fluctuations should always be present.

In further calculations we assume that the initial state of the particle is given by the Gaussian distribution:

$$\rho_\mathbf{q}^{(0)}=\exp(-q^2\delta_0^2/2), \qquad (16)$$

where δ_0 is the rms width of the wave packet. The expression (15) can be analyzed in this case by numerical calculation. However in this study we limit ourselves to qualitative analysis, considering the limiting cases of small, $\delta_0\ll v/\omega_0$, and large, $\delta_0\gg v/\omega_0$, widths. In the case of small widths, we find from (15) to first approximation in δ_0^2

$$\bar{D}^2(\mathbf{x},t)-D_0^2\approx 2\delta_0^2|\nabla\varphi(\mathbf{x},t)|^2. \qquad (17)$$

Thus, the self-fluctuations of the polarization field in the vicinty of the space-time point $(\mathbf{x},t)$ is equal numerically to the work done by the polarization forces on a unit charge to move it over the distance $2^{1/2}\delta_0$.

Consider now the case of large widths, approximating (16) by the δ-function

$$\rho_\mathbf{q}^{(0)}\approx(2\pi\delta_0^2)^{-3/2}\delta(\mathbf{q}), \qquad (18)$$

which is equivalent to (16), when we calculate the integrals in (14) and (15) in the range $|\mathbf{x}-\mathbf{v}t|<\delta_0$. In fact, if this inequality holds, the most quickly changing function in the integrands is the density $\rho^{(0)}_{\mathbf{q}-\mathbf{q}'}$. If we want to enlarge the validity range, the approximation (18) should be altered by introducing an extra factor $\exp[-(\mathbf{x}-\mathbf{v}t)^2/2\delta_0^2]$, which provides a rapid decrease in fluctuations at large distances exceeding δ_0 from the particle.

Substituting (18) into (15), we get a meaningless diverging expression, since the fluctuations are nonstationary. Substituting (18) into (14) we find for $t_0=0$, $t\gg 1/\omega_0$, and unity normalization volume

$$D^2(\mathbf{x},t)-D_0^2\approx 4\pi t(2\pi\delta_0^2)^{-3/2}Z_1^2\sum_{\gamma,\mathbf{q}}g_{\gamma\mathbf{q}}^4\delta(\omega_\gamma-\mathbf{q}\mathbf{v})$$

$$+8\pi^2(2\pi\delta_0^2)^{-3/2}Z_1^2\sum_{\sigma,\sigma',\mathbf{q}}g_{\sigma\mathbf{q}}^2g_{\sigma'\mathbf{q}}^2\delta(\omega_\sigma-\mathbf{q}\mathbf{v})\delta(\omega_{\sigma'}-\omega_\sigma), \qquad (19)$$

where the index γ lists collective modes corresponding to isolated branches of elementary excitations, and the indices σ and σ' denote individual modes within a certain band in the $(\mathbf{q},\omega)$-plane. As follows from (19), for wide packets the mean square value of the polarization field fluctuations grows linearly with time.

4. THE PROBLEM OF QUANTUM COHERENCE

The fact that the polarization-field fluctuations increase for wide packets means instability, in a medium, of that particle state in which the the quantum coherence length is much larger than v/ω_0. The same conclusion follows from analysis of the particle density matrix. First we find the measure of particle-state coherence, following the Glauber theory of optical coherence (see, e.g., Ref. 8). The constrast of the diffraction pattern formed by the particle states from the vicinities of space-time points $x\equiv(\mathbf{x},t)$ and $x'\equiv(\mathbf{x}',t)$ is given by the expression

$$R(x,x')=\frac{4|G(x,x')|}{(0|\hat{\rho}_H(x)|0)+(0|\hat{\rho}_H(x')|0)+2|G(x,x')|}, \qquad (20)$$

where $G(x,x')=(0|\hat{\psi}_H^+(x)\hat{\psi}_H(x')|0)$ is the correlation function of the particle states from the vicinities of the points x and x', $\hat{\psi}_H^+$ and $\hat{\psi}_H$ are the Heisenberg operators, and $\hat{\rho}_H(x)=\hat{\psi}_H^+(x)\hat{\psi}_H(x)$ is the Heisenberg density operator. As follows from (20), the contrast vanishes if the correlator $G(x,x')$ equals zero. In this case the wave fields at the points x and x' are incoherent and cannot belong to a pure state in the sense of von Neumann. The correlator $G(x,x')$ can be calculated in the framework of modified perturbation theory (see the Appendix). The quantum-coherence length of a particle state can be defined with the help of $R(x,x')$ as the distance $|\mathbf{x}-\mathbf{x}'|$ over which the quantity $R(x,x')$ decreases by a factor of e in comparison with its value at $\mathbf{x}'=\mathbf{x}$. If the initial state is a plane wave, this happens at $t'=t$ over distances (if the displacemnet is along the velocity, $i=1$, or in perpendicular directions, $i=2,3$)

$$\Delta_i=2[Ld\overline{\Delta k_i^2}/dx]^{-1/2}, \qquad (21)$$

where $d\,\overline{\Delta k_i^2}/dx$ is the increment of the mean square value of the fluctuation of the ith momentum component at a unit trajectory length, and L is the distance covered by the particle in the solid. When the initial state is given by a Gaussian packet with the rms width δ_0, the result depends both on δ_0 and the particle mass

$$\delta_i=\left\{\frac{\Delta_i^2}{1+\Delta_i^2/\delta_0^2}\left[1+\frac{t^2}{4m^2v^2\delta_0^2}(\delta_0^{-2}+\Delta_i^{-2})\right]\right\}^{1/2}. \qquad (22)$$

According to (22), the initial "fluctuation" compression of the packet is replaced by "dispersion" spreading. This happens at times obeying the condition

$$\frac{t^2}{4m^2v^2\delta_0^2}\left(\delta_0^{-2}+\frac{1}{4}vt\,\overline{d\Delta k_i^2/dx}\right)>1. \quad (23)$$

For heavy particles the dispersion spreading is important at such large distances, L, at which the assumption of smallness of particle velocity variations is already invalid. For small $|t-t'|\lesssim 1/\omega_0$ the widths (21) and (22) increase in proportion to $|t-t'|^2$.

The instability of the quantum state with a large coherence length of a particle moving in a sold, resulting in its localization, can serve, in particular, as an additional argument in favor of validity of the classical trajectory approximation in the analysis of charged particle beams in crystals (orientation effects) or in disordered solids (we mean, for example, calculations of mean projective paths). Serious deviations from "classical" results can be expected in the analysis of the diffraction of fast charged particles,[9] in the studies of energy-loss anomalies in the inner electron shells of target atoms (see, e.g., Ref. 10), and in the interpretation of spectra of convoy electrons.[11] The latter problem is of special interest, since for its solution one resorts to the idea of formation of quasibound localized electron states in the field of an ion moving in a medium. If such states really exist, they could be catalysts in nuclear fusion reactions. The experimentally observable phenomena of a so called preequilibrium particle deceleration in thin films can also be explained on the basis of particle localization upon entering the solid.[7]

Two conclusions can be drawn: (i) when a moving charged particle enters a solid, its polarization field reaches fairly quickly (in a time of order $1/\omega_0$) its classical value given by the wake potential, and (ii) along with this process, a rapid decrease in the polarization field fluctuations occurs.

APPENDIX

Allowing for

$$\hat{\psi}_H(x)=U_1^+(t)\hat{\psi}(x)U_1(t), \quad (A1)$$

where $U_1(t)$ is the evolution operator (10) (we assume that $t_0=0$), we write the correlator in the form

$$G(x,x')=(t|\hat{\psi}^+(x)U_1(t)U_1^+(t')\hat{\psi}(x')|t'), \quad (A2)$$

whence, to zeroth order in $H_{\rm int}^{(1)}$, we find

$$G(x,x')\approx(0|U_0^+(t)\hat{\psi}^+(x)U_0(t)U_0^+(t')\hat{\psi}(x')U_0(t')|0). \quad (A3)$$

Since the state $|0)$ is one-particle, after the action of the operator $\hat{\psi}(x')$ to the right there arises a vacuum particle state $|vac_p)$. The action of a pair of operators $U_0(t)U_0^+(t')$ on this state does not alter it. Furthermore, since the operator $\hat{\rho}_{\mathbf q}^+\hat{\rho}_{\mathbf q}$ does not alter the one-particle state either,

$$\hat{\psi}(x')U_0(t')|0)$$

$$=\exp\left\{-\frac{1}{2}\sum_{\beta,\mathbf q}(|Q_{\beta\mathbf q}(t')|^2+2i\Phi_{\beta\mathbf q}(t')]\right\}\hat{\psi}(x')$$

$$\times\exp\left\{\sum_{\beta',\mathbf q'}Q_{\beta'\mathbf q'}(t')\,\hat{\rho}_{\mathbf q'}\hat{b}^+_{\beta'\mathbf q'}\right\}|0). \quad (A4)$$

Let the initial state of the system be a direct product of a particle state with a definite momentum $\mathbf k_0$ and a vacuum state of the quasiparticle field $|0)=|\mathbf k_0;vac_Q)$. Expanding the expotential in a series, we find

$$\hat{\psi}(x')\exp\left\{\sum_{\beta,\mathbf q}Q_{\beta\mathbf q}(t')\hat{\rho}_{\mathbf q}\hat{b}_{\beta\mathbf q}^+\right\}|\mathbf k_0;vac_Q)$$

$$=\sum_{\mathbf k}\sum_{n=0}^{\infty}\frac{1}{n!}\exp(i\mathbf k_0\mathbf x'-i\varepsilon_{\mathbf k}t')\hat{a}_{\mathbf k}\left(\sum_{\beta,\mathbf q}Q_{\beta\mathbf q}(t')\hat{\rho}_{\mathbf q}\hat{b}^+_{\beta\mathbf q}e^{i\mathbf q\mathbf x'}\right)^n$$

$$\times|\mathbf k_0;vac_Q), \quad (A5)$$

where $\varepsilon_{\mathbf k}$ is the energy of a particle with momentum $\mathbf k$.

The expression $\varepsilon_{(\mathbf k_0-\mathbf q_1-\cdots-\mathbf q_n)}$ can be rewritten in the form

$$k_0^2/2m+\sum_{a=1}^{n}[q_a^2-2\mathbf q_a(\mathbf k_0-\delta\mathbf k/2)+\mathbf q_a(\varkappa_a-\delta\mathbf k)]/2m, \quad (A6)$$

where

$$\varkappa_a=\sum_{1\leqslant b\leqslant n}\mathbf q_b-\mathbf q_a$$

can be regarded as the momentum lost by the particle before the instant when the last quasiparticle with momentum $\mathbf q_a$ is emitted. The $\delta\mathbf k$ is defined as the mean with respect to different realizations of sets of emitted quasiparticles, $\delta\mathbf k=\overline{\varkappa_a}$, and can be regarded as mean momentum loss by the time t'. Then

$$\mathbf x_0(t')=(\mathbf k_0-\delta\mathbf k/2)t'/m$$

is the running coordinate of a particle moving with constant deceleration, since the mean deceleration force is approximately constant (we assume that the mean particle velocity changes very little when the particle moves through a sufficiently thin solid layer). Further, we consider an approximation based on neglect of the last term in the sum in (A6). The larger the particle mass, the better the approximation. A more rigorous estimate is obtained when an expansion of the exponential $\exp|it'(\mathbf q_a(\varkappa_a-\delta\mathbf k)+q_a^2)/2m|$ in a series is performed and the contribution of different terms is analyzed. As a result, we find the inequality $\overline{\Delta k_i^2}t'/4m<1$, where $\overline{\Delta k_i^2}$ is the mean square value of the fluctuation of the particle ith momentum component. Since the derivative $d\,\overline{\Delta k_i^2}/dt$ does not depend on time and can be directly calculated by standard techniques, the condition of validity of the approximation used, $t'<2\min[m/(\overline{dk_i^2}/dt)],^{1/2}$ is fairly convenient. For heavy particles, $m\gg 1$, and this inequality holds for layers of thickness of order 1000 Å passed by the particle.

Continuing our calculations under the given restrictions, we can reduce (A5) to the form

$$\sum_{\mathbf k,n}\frac{1}{n!}\exp(i\mathbf k_0\mathbf x'-i\varepsilon_{\mathbf k_0}t')$$

$$\times\left(\sum_{\beta,\mathbf q}Q_{\beta\mathbf q}(t')\exp\left(i\mathbf q\left(\mathbf x'-\mathbf x_0(t')+\frac{\mathbf q t'}{2m}\right)\right)\hat{b}^+_{\beta\mathbf q}\right)^n|vac)$$

$$=\exp\Big\{i\mathbf{k}_0\mathbf{x}'-i\varepsilon_{\mathbf{k}_0}t'$$

$$+\sum_{\beta,\mathbf{q}}Q_{\beta\mathbf{q}}(t')\exp\Big(i\mathbf{q}\Big(\mathbf{x}'-\mathbf{x}_0(t')+\frac{\mathbf{q}t'}{2m}\Big)\Big)\hat{b}_{\beta\mathbf{q}}^{+}\Big\}|vac). \tag{A7}$$

Taking (A7) into account and using the well-known Baker–Haussdorf formula,

$$e^Ae^B=e^{A+B}\exp\Big(\frac{1}{2}[A,B]_-\Big),$$

we can present (A3) in the form

$$G(x,x')\approx\exp\Big\{i\mathbf{k}_0(\mathbf{x}-\mathbf{x}')+i\varepsilon_{\mathbf{k}_0}(t-t')$$

$$+\sum_{\beta,\mathbf{q}}\Big[-\frac{1}{2}|Q_{\beta\mathbf{q}}(t)|^2-\frac{1}{2}|Q_{\beta\mathbf{q}}(t')|^2$$

$$+Q_{\beta\mathbf{q}}^*(t)Q_{\beta\mathbf{q}}(t')\exp\Big(i\mathbf{q}\Big(\mathbf{x}-\mathbf{x}_0(t)-\mathbf{x}'+\mathbf{x}_0(t')+\frac{\mathbf{q}(t-t')}{2m}\Big)\Big)$$

$$+i\Phi_{\beta\mathbf{q}}(t)-i\Phi_{\beta\mathbf{q}}(t')\Big]\Big\}. \tag{A8}$$

Owing to partial cancellation of temporal factors in (A3) for $G(x,x')$, the validity condition (A8) for small $|t-t'|\ll t$ differs from (A7) and has the form

$$|t-t'|<\min[m/(td\Delta\overline{k_i^2}/dt)].$$

Note that the reasoning, beginning with the formula (A6), can be omitted, if we limit ourselves to the calculation of the density matrix $\gamma(\mathbf{x},\mathbf{x}',t)$ found from (A3) at $t'=t$. Using (A5), we get

$$\gamma(\mathbf{x},\mathbf{x}',t)=\exp\Big\{-i\mathbf{k}_0(\mathbf{x}-\mathbf{x}')$$

$$-\sum_{\beta,\mathbf{q}}|Q_{\beta\mathbf{q}}(t)|^2(1-\exp i\mathbf{q}(\mathbf{x}-\mathbf{x}'))\Big\}, \tag{A9}$$

which coincides with the corresponding result of Ref. 12.

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