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Coherence criterion for a mixed state of particle moving in solid film

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ABSTRACT

The time behavior of a packet width during the passage of particle through solid film is considered. The specific effect of memory, which follows from the wave nature of the micro-world is shown.

1. Introduction

An experimentalist and a theoretician often differ in the treatment of the interaction of a projectile with a surface of a solid. If the first, as a rule, considers the projectile as a point-like particle, the second considers a plane wave as a proper definition of the initial state of a projectile. One of the goal of this work consists in finding a solution to this contradiction using the quantum mechanics as a basic idea.

In a condition of constant interaction with environment, the state of a moving particle should not be described with the wave function rather with help of density matrix (DM). The DM, however, allowing the performance of calculations of all physical quantities, does not provide us with the qualitative understanding of the phenomenon under consideration. Its representation as the sum of pure state DM (in the sense by von Neumann) can help with reception of an evident representation about the physical content and logic of interaction. Moreover, sometimes this representation would be inevitable. As an example, consider the case when the projectile exits to vacuum after passage through solid film. Secondly, consider the nuclear reaction between a projectile and a specific nucleus intercalated in a lattice.

Study of the physics of phenomena occurring during the passage of a swift atomic projectile through solid has a long history [1–14]. A considerable amount of works has been performed and a wide class of phenomena revealed. Here we would like to very briefly pursue the main ideas in this scientific development. In particular, when particle passes through a crystal the so-called orientation phenomena (channeling, blocking, and so on) occur (see, e.g., [1–4]). The theory of such phenomena [5] is usually based on the assumption of a strong spatial localization of massive accelerated particles (nucleons, nuclei, atomic and molecular ions) which have a sufficiently great velocity in the solid.

The theory of conductivity in metals and semiconductors is a rather important branch of science. It was started by Drude and Lorenz approximately one century ago and has a lot of exciting and instructive achievements. This theory underwent an important development after the discovery of the quantum mechanical wave nature of the micro-world. It contains the unique combination of being able to deal with and provide answers on fundamental questions of physics while being relevant for applications in the nearest future. In fact, some of the experimental possibilities in this field have been developed with an eye on reducing sizes of electronic components.

The problem of the spatial localization of electrons in solids acquires the great attention during development of the modern transport theory in disordered conductors and semiconductors. Particularly, it was shown at a sufficient disorder that the electrons don't participate in charge transfer because of Anderson's localization (see, e.g., [7,8]). One of the confirmations of Anderson's theory was the model calculation performed in the work [9]. In this case one speaks about the static localization, when an electron is localized near a fixed atomic center in the lattice. On the other hand, some researchers (see, e.g., [10,11]) come to a conclusion that the charge carriers undergo a transition from the delocalized state

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to a localized one during their motion in a solid. In the work [10] the attention was paid to the possibility of a phase randomization of the wave function owing to interaction of the moving particle with its environment.

At the same time, the problem of spatial localization was considered within the scope of quantum theory of interaction of accelerated particles with solids. Instead of classical picture which was based on the assumption of a strong spatial localization of massive particles, the other point of view was proposed in [12], where it was stated that the particles moving in crystals should be described with the help of Bloch waves and obviously should be delocalized. It was shown that the channeling phenomena could be also well described by this theory. In our previous publications on this problem [13,14] it was revealed that a channeling quantum particle should nevertheless become spatially localized during the motion in a solid. In this works, the estimations of the wave packet width of a particle moving in a solid with a constant velocity were obtained.

The width of a particle's wave packet is important in some physical effects, e.g., in: interference & diffraction, channeling, conductivity, Hall effect, Bloch oscillations, nuclear reactions. We try to advance in the development of a mathematical formalism, based on some physical concepts, which follows in a natural way from the wave nature of the micro-world. As a rule, a non-relativistic projectile penetrating a thin solid film is considered. The film thickness is assumed to be small compared to the range of the particle in a solid.

Throughout the article we use the atomic units unless otherwise stated.

2. Decomposition of density matrix

Analyzing the expression for one-particle DM we shall take advantage of the famous theory by von Neumann [15], according to which it represents the weighted sum of the DM of pure states

$$\Gamma(\vec{x}_1,\vec{x}_2,t) = \sum_n W_n \tilde{\Gamma}_n = \sum_n W_n \psi_n^*(\vec{x}_1,t)\psi_n\left(\overleftarrow{x}_2,t\right), \qquad (1)$$

where the summation is made on some complete set of states of a particle being part of a quantum-mechanical system (here $\tilde{\Gamma}_n = \psi_n^*(\vec{x}_1,t)\psi_n(\overleftarrow{x}_2,t)$ is a DM of a "pure" state). The weights W_n represents the statistical probabilities to find a particle in one of the states described by the wave functions $\psi_n(\vec{x},t)$. The wave functions can be eigenfunctions of some linear operator. In (1) it is supposed, that the system of eigenfunctions represents an orthonormal basis in Hilbert space. Further generalization of the formula (1) is required if there are some speculations to use the normalized functions, but not explicitly orthogonal. They should belong to a continuous spectrum.

The following properties of the DM should be fulfilled:

1. The quantity $\Gamma(\vec{x},\vec{x},t) = \rho(\vec{x},t) \geqslant 0$ is equal to the probability density to find a particle in a point $\vec{x}$ at a time t.
2. The following normalization condition should be fulfilled:

$$Sp[\Gamma] \equiv \int \Gamma(\vec{x},\vec{x},t)d^3x = 1.$$

3. Generally speaking, DM should not be degenerate as it could not be represented as a finite sum of summands with separated variables ($m > 1$ – is a some integer), $\Gamma(\vec{x},\vec{x}',t) = \sum_{j=1}^m \Gamma_j^*(\vec{x},t)\Gamma_j(\vec{x}',t)$.
4. DM obeys the Hermitian self-conjugation $\Gamma(\vec{x},\vec{x}',t) = \Gamma^*(\vec{x}',\vec{x},t)$.
5. DM has a direct connection to the notion of coherence between the different parts of quantum field belonging to the projectile. This notion has been actively used by Glauber [16], Klauder and Sudarshan [17], Scully and Zubairy [18] and others in quantum optics.

Now it is necessary to carry out the critical analysis of the von Neumann's idea. As Landau and Lifshitz note in [19], the idea should not be understood literally. There is only a certain probability that during a measurement the particle can be found in one of those pure state, which enters into the appropriate decomposition (1), and this probability is determined by von Neumann's theory. At the actual application of (1) there is a question on unambiguity of this decomposition. As an example we shall consider a particle which moves with the large speed in a solid film and exits then in vacuum. Let's assume, that the DM of a particle is known. It is clear, that in vacuum in the neighborhood of an exit surface, the state of a particle has not enough time to change and is still described by a DM which relates to its previous movement in the solid. If a particle leaves the solid, does the DM now represent a superposition of DM of free particles? If it would be right, then the coherence length would be immediately increased in comparison with a motion inside the solid film. But from a physical point of view, it is impossible, because of large phase fluctuations which the particle obtains during the passage in the solid. These fluctuations don't disappear immediately after escape from the solid, so the disorder can not immediately be transformed into order.

This problem has a more general representation. Imagine that an elementary particle moves in a homogeneous medium being free, not interacting with any environment. Imagine that interaction is switched on at $t = 0$. The initial state of a particle described by a plane wave and a corresponding DM

$$\psi_0(\vec{x},t) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\vec{x}-iEt}\;; \quad \Gamma_0(\vec{x}_1,\vec{x}_2,t) = \frac{1}{\Omega} e^{-i\vec{k}(\vec{x}_1-\vec{x}_2)}$$

is to rearrange in a mixed state described by the density matrix $\Gamma_h(\vec{x}_1,\vec{x}_2,t)$. From the general consideration, using the homogeneity of a total system, we can conclude that this DM should depend only on a relative coordinate $\vec{x} = \vec{x}_1 - \vec{x}_2$, $\Gamma_h(\vec{x}_1,\vec{x}_2,t) = \Gamma_h(\vec{x},t)$. This DM has at least two different forms of decomposition, one – with plane waves,

$$\Gamma_h(\vec{x}_1,\vec{x}_2,t) = \Gamma_h(\vec{x},t) = \int \frac{d^3k}{(2\pi)^3} \tilde{\Gamma}_h\left(\vec{k},t\right) e^{i\vec{k}(\vec{x}_1-\vec{x}_2)} \qquad (2)$$

(here $\tilde{\Gamma}_h(\vec{k},t)$ – is a Fourier-image of DM) and other – with the help of continuously displaced equivalent states,

$$\Gamma_h(\vec{x}_1-\vec{x}_2,t) = \Gamma_h(0,t)\int \varphi^*(\vec{x}_1-\vec{a},t)\varphi(\vec{x}_2-\vec{a},t)d^3a. \qquad (3)$$

The Eq. (3) generalized (1) to a continuous spectrum. The deviation from a "simple" case (1) is found in that the functions $\varphi(\vec{x}-\vec{a},t)$ are equal and only displaced on various distances $\vec{a}$, belong to a continuous spectrum, are linearly independent and not orthogonal among themselves. In the first case (2) the plane waves describe the total delocalized states but in the other case (3) the functions $\varphi(\vec{x},t)$ allow us to consider the sufficiently localized states. Both representations obey von Neumann's approach but are very different in a physical sense.

Now we give the simple example of DM calculation in a case of an initial plane wave interacting with the homogeneous medium. The calculation was performed elsewhere [13,14] and gave

$$\Gamma_h(\vec{x}_1-\vec{x}_2,t) = \Gamma_0(0,t)e^{-P(\vec{x}_1-\vec{x}_2,t)}, \qquad (4)$$

where

$$P(\vec{x}_1-\vec{x}_2,t) = \sum_{\beta,\vec{q}} \left|Q_{\beta\vec{q}}(t)\right|^2 (1-\exp[i\vec{q}(\vec{x}_1-\vec{x}_2]). \qquad (5)$$

Here the quantities $\left|Q_{\beta\vec{q}}(t)\right|^2$ define the mean number of quasi-particles of type β obeying a momentum $\vec{q}$ which are generated by the moving projectile in a medium at the time t.