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Passage of a charged particle through a thin solid film

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ABSTRACT

The inelastic collisions effect on the interaction of the projectile with a super thin solid film is considered. The wave nature of the particle and its transitions from delocalized to the strongly localized state defined many important properties of the interaction. As examples the effect of perforation the 1 nm carbon foil as well as the overwhelming passage through a thick porous layer are considered.

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BEAM INTERACTIONS WITH MATERIALS AND ATOMS

1. Introduction

There are some important physical phenomena revealed in experiments with the charged particle passage through a solid film (see, e.g., [1,2] from the past or [3–5] from present time). Until now not all the phenomena are found a proper physical explanation.

In condition of constant interaction with environment the state of a moving particle should not be described with the wave function rather with the help of density matrix (DM). The DM, however, allowing the performance of calculations of all physical quantities, don't 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 Newmann) can help with reception of evident representation about the physical content and logic of interaction. The physics of phenomena extended during the passage of a swift atomic projectile through solid has a long history. A considerable amount of works was performed and a wide class of phenomena was revealed. In particular, when particle passes through a crystal the so-called orientation phenomena (channeling, blocking, and so on) was occurred. The theory of such phenomena usually based on assumption of a strength spatial localization of massive accelerated particles (nucleons, nuclei, atomic and molecular ions) having a sufficiently great velocity in a solid.

We try to advance forward in development of a mathematical formalism, basing on some physical concepts, which by a natural

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http://dx.doi.org/10.1016/j.nimb.2015.01.004 0168-583X/© 2015 Elsevier B.V. All rights reserved. way follow from a wave nature of a micro-world. With the help of density matrix calculation we show a presence of a dynamic spatial localization for a projectile. The dynamical transformations of the packet width could be significant in some surface effects, in particular, at the formation of porous structures during the passage of high charged ions through a thin film [3,4] or at the penetration of the beam through a porous structure [5].

2. Coherence criterion

Let's put a task to determine wave functions, if a DM is known. But it is obvious the particle find in an environment could not find in a pure quantum-mechanical state due to the continuous interaction with the total system. In this case we consider the wave function as a not inevitable decomposition of a mixed state but mostly as a representation convenient for our understanding the phenomenon. In a decomposition we attach individuality to a particle in spite of it remains to be a part of a great system. There should be an additional criteria of choice of the individualization procedure which should be done with the help of some physical reasons. The most important criterion consists into quest the coherence of elements of a particle field concerning to various spatial - temporary points. The presence or absence of coherence determines the presence or absence of interference and diffraction phenomena, which play an important role in many physical and technological processes. Only that elements of a particle field which are found in relation of mutual coherence should be merged in the notion of an individual particle.

Please cite this article in press as: G.M. Filippov, Passage of a charged particle through a thin solid film, Nucl. Instr. Meth. B (2015), http://dx.doi.org/ 10.1016/j.nimb.2015.01.004 A density matrix $\Gamma(\vec{x}_1, \vec{x}_2, t)$ for the projectile directly relates to the definition of coherence of the projectile's wave field (see, e.g., in [6,7]). Namely, the relation

$$\tilde{\gamma}(\vec{x}_1, \vec{x}_2, t) = \frac{\Gamma(\vec{x}_1, \vec{x}_2, t)}{\sqrt{\Gamma(\vec{x}_1, \vec{x}_1, t) \Gamma(\vec{x}_2, \vec{x}_2, t)}}$$
(1)

determines degree of coherence of elements of a field found in vicinities of space–time points (\vec{r}_1, t) and (\vec{r}_2, t) . If we take the parts of a wave field of a projectile from the vicinities of points \vec{x}_1 , \vec{x}_2 (as example, with the help of Yung screen with two slits) then the interference picture at overlapping of two elected parts will be characterized by the function (1).

For this reason various terms in the von Newmann decomposition on statistically independent DM of states, should provide appropriate, equal to (1), shape of function of coherence. Let's denote this criterion as the criterion of coherence. Note, that for us is particularly important the behavior of (1) as a function of a distance between spatial points $\vec{x} = \vec{x}_1 - \vec{x}_2$ where observed parts of the particle wave field are taken from. In this approach the localized states don't the pure states in a sense of von Newmann's theory. They are mixed states due to the continuous binding of a particle with the all environment. Here we see a deviation from the von Newmann's procedure and a remarkable correspondence to the famous Landau and Lifchitz critics. The wave function which is defined by the coherence criterion procedure describe not a "pure" but an entangled state. In this case the particle is left to be a part of a total system but getting an "individuality" by gathering the parts of its wave field in which exists a notion of coherence or a partial coherence of its components. This circumstance is especially surprising when a projectile escapes from a solid but its coherence properties are tightly connected to the past interaction with a solid.

3. Application to a wave packet moving in a solid film

Consider more in detail the particular case when a particle (being not a plane wave) incident from vacuum in a thin foil target. An initial state of a particle is described with a wave function (Gauss wave packet)

$$|\chi_0) = \sum_{\vec{k}} C_{\vec{k}} |\vec{k}\rangle, C_{\vec{k}} = = \left(8\pi\delta_0^2\right)^{3/4} \frac{1}{\sqrt{\Omega}} \exp\left[-\delta_0^2 \left(\vec{k} - \vec{k}_0\right)^2 + i\phi\right].$$

The width of a free wave packet is $\delta(t) = (\delta_0^2 + t^2/(4m^2\delta_0^2))^{1/2}$ and spreads in time the slow the greater the particle mass *m* is (here and throughout of an article we put the width equal to the dispersion of Gauss distribution of probability density). In the consequence of a strong interaction with the medium the state of the particle doesn't be able to describe by the wave function but only by the DM. The briefly described way of calculation the DM presents in the Appendix B.

For further calculations we use the next formula

$$e^{-itk^2/2m} = \left(-i\frac{m}{2\pi t}\right)^{3/2} \int_{-\infty}^{\infty} e^{i(1+i0^+)ms^2/2t + i\vec{s}\vec{k}} d^3s,$$
(2)

where $0^+ = \lim_{\sigma \to +0} \sigma$ (in the following this symbol doesn't will be written explicitly). In this case one could get the more convenient accounting for the effect of the dispersion dependence of the energy on the momentum on the time evolution of DM. The result is (see Appendix B)

$$\Gamma(\vec{x}_{1},\vec{x}_{2},t) = \left(\frac{m}{2\pi t}\right)^{3} \iint d^{3}s_{1}d^{3}s_{2}e^{-im\left(s_{1}^{2}-s_{2}^{2}\right)/2t}\chi_{0}^{*}(\vec{x}_{1}+\vec{s}_{1},0)\chi_{0}(\vec{x}_{2}+\vec{s}_{2},0)$$
$$\times \exp\left\{-\sum_{\beta,\vec{q}}\left|Q_{\beta\vec{q}}(t)\right|^{2}\left(1-e^{i\vec{q}(\vec{x}_{1}+\vec{s}_{1}-\vec{x}_{2}-\vec{s}_{2})}\right)\right\}.$$
(3)

Here

$$Q_{\beta\vec{q}}(t) = -iZg_{\beta}(\vec{q}) \int_{0}^{t} \exp\left\{i\omega_{\beta}(\vec{q})t' - i\vec{q}\vec{x}_{0}(t')\right\}dt'$$
(4)

and $\vec{x}_0(t')$ – is a mean coordinate of the projectile to the instant t', Z – is the charge of the projectile, $\omega_\beta(\vec{q})$ – is the frequency of the elementary β – type excitation of the medium, $g_\beta(\vec{q})$ – is a bond coefficient between a particular elementary excitation and the projectile.

If the function $\chi_0(\vec{x})$ obeys the Gauss form then using the proper transformation of the last exponent in the expression (3), one obtain the integral of Gauss type which can be calculated explicitly. The widths of probability distribution relative (*r*) to coordinate $\vec{x} = \vec{x}_1 - \vec{x}_2$ as well as to the laboratory (*l*) coordinate $\vec{X} = (\vec{x}_1 + \vec{x}_2)/2$ are given by the formulae [8,9]

$$\begin{split} \delta_{j}^{(r)}(t) &= \delta_{0} \sqrt{\frac{1 + \left(1 + 4\Delta^{2}k_{jj}\delta_{0}^{2}\right)t^{2}/(4\delta_{0}^{4}m^{2})}{2\left(1 + 4\delta_{0}^{2}\Delta^{2}k_{jj}\right)}}, \quad \text{for } x; \\ \delta_{j}^{(l)}(t) &= \sqrt{2}\delta_{0} \sqrt{1 + \left(1 + 4\Delta^{2}k_{jj}\delta_{0}^{2}\right)t^{2}/(4\delta_{0}^{4}m^{2})}, \quad \text{for } X. \end{split}$$
(5)

We have introduced here the new quantities $\Delta^2 k_{ij}$, which equal to the squared mean momentum fluctuations for the projectile arisen in course of interaction with a solid. As we see, the fluctuations of momentum inside the solid influence on a projectile's states in opposite manner in comparison to the dispersion dependence of the projectile's energy on the momentum. If there is only dispersion broadening at free motion, in the solid the progressive momentum and energy fluctuations sufficiently changes all the picture. Especially it is important for the particle obeying a great mass. In this case during the comparatively long distance we can observe the rapid contracting in particle's coherence length. This behavior is mostly significant if an initial width of a packet is great. If a momentum fluctuation stops to increase, then, according to information received, in course of time the process resumes the dispersion broadening of the packet's width.

The values of parameters such as the initial width of the packet, the mass of the particle, the time of interaction with the environment, strongly influences the properties of the DM. If the particle has a large mass and the initial width of the packet is enough high, at the initial stage of evolution the determining factor is the growth of momentum fluctuations and the ensuing rapid decreases of the DM module when increases the distance between the points \vec{x}_1, \vec{x}_2 . In the opposite case, if both as the initial width as well as the mass of the particle are small, the broadening due to the dispersion prevails over all other factors after a comparatively short period of localization due to fluctuations, the width of the region in which the density matrix module is large, is growing rapidly. The result (2), naturally is applied only in cases of applicability of the first approximation in the modified perturbation theory. Among the other restrictions it is suggested the small variation of the particle's velocity during the passage through a solid.

It is important to emphasize that the packet width does not immediately follow a free particle behavior after exit from a solid. We obtain the particle's state which is strongly entangled with the state of the all environment. It means the wave packet conserves any information about its previous passage through the solid. We can consider it as a specific memory effect. In particular, at small times the width of the wave packet diminishes as a consequence of increasing the momentum fluctuations, following the law

$$\delta^{(r)}_j pprox rac{\delta_0}{\sqrt{2 \left(1+4\Delta^2 k_{jj} \delta_0^2
ight)}}, \quad t < m/\sqrt{\Delta^2 k_{jj}} + 1/(4\delta_0^2).$$

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