Inverse problem for multiple scattering fast charged particles in a mesoscopic medium

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We consider an inverse problem of multiple scattering for fast charged particles propagating in an inhomogeneous medium. The scattering processes are described by the diffusion-type equation in the small-angle approximation. It is shown that by using the scattering data given on some small interval it is possible to recover the spatial dependence of the density of the medium. This inverse problem is ill posed in the sense that small noise in the data may lead to large perturbations in $\epsilon(z)$ if no *a priori* assumptions are made about $\epsilon(z)$. This is clear from our presentation, since an analytic continuation of $\epsilon(z)$ is involved. One hopes that the proposed method can be applied to thin foils and to mesoscopic systems.

I. INTRODUCTION

The problem of multiple scattering of fast charged particles in different media has a long history.[1-5] In general, the problem is rather complicated, and can be considered only with the help of the integral-differential equation for the distribution function f of the scattering particles.[1,2] However, if the velocity of the particle is large enough (the modulus of the velocity does not change significantly in the process of scattering), one can use the small-scattering-angle approximation $\theta_{x,y} \ll 1$,[1-5] where $\theta_{x,y}$ are the projections of the scattering angle θ on the (x,y) plane. In this approximation it is possible to derive the diffusion-type equation for the distribution function $f(z,s,x,y,\theta_x,\theta_y)$, where s is the actual path length,[2,5] and x,y,z are the coordinates of the particle. We shall use the following equation for f:

$$\frac{\partial f}{\partial z} + \left(1 + \frac{\theta_x^2+\theta_y^2}{2}\right)\frac{\partial f}{\partial s} + \theta_x\frac{\partial f}{\partial x} + \theta_y\frac{\partial f}{\partial y} + \frac{kx}{p_0}\frac{\partial f}{\partial \theta_x} + \frac{ky}{p_0}\frac{\partial f}{\partial \theta_y} = \epsilon(z)\left(\frac{\partial^2}{\partial \theta_x^2} + \frac{\partial^2}{\partial \theta_y^2}\right) f, \quad (1)$$

where p_0 is the momentum of the particle, the constant $k = (eZ/c)q$ describes the interaction with the magnetic field $\vec{B} = (-qy, qx, 0)$, and eZ is the charge of the particle. The function $\epsilon(z)$ in (1) describes the multiple scattering of the particle in the medium. In what follows we shall assume that the radiation processes are negligible. In this case $\epsilon(z)$ in (1) is the normalized density of the medium. We assume that the density of the medium depends on the coordinate z only.

Assume that the data are the values

$$f|_{z=0}, \quad f|_{\zeta-h\le z\le\zeta}, \quad \epsilon|_{z=\zeta}, \quad (2)$$

where ζ is the coordinate of the boundary of the medium. The problem is, given data (2), to find $\epsilon(z)$ for z in the interval $(0, \zeta - h)$.

The unknown $\epsilon(z)$ may be an arbitrary continuous function. Any such function can be uniformly approximated on any fixed bounded interval by an analytic function of the form

$$\epsilon(z) = \frac{1}{2\pi}\int_{-a}^{a} b(t)e^{-izt}dt,$$

$$b(t) \in C(-a,a), \quad 0 < a < \infty, \quad (3)$$

(see Refs. 6 and 7, p. 211). Therefore we assume in this paper that $\epsilon(z)$ is of the form (3). Under this assumption we prove that $\epsilon(z)$ is uniquely determined by the data (2), and give a procedure for calculating $\epsilon(z)$. The problem is ill posed in the sense that small noise in the data may lead to large perturbations in $\epsilon(z)$ if no *a priori* assumptions are made about $\epsilon(z)$, and generally the method suggested can be used only for systems with sufficiently small spatial scale L in the z direction. We discuss the possibility of application of our results to thin foils and to mesoscopic systems.

II. ANALYSIS OF THE PROBLEM

A. Finding $\epsilon(z)$ for $\zeta - h < z < \zeta$

Assume, in what follows, that the magnetic field is absent ($q = 0$). The reasons we did not make this assumption at the start, in Eq. (1), are as follows: (1) it may be that another way will be found to solve the inverse prob-

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lem under study, and the other way will take advantage of the structure of Eq. (1); (2) Eq. (1) has been derived and discussed in the literature and we wish to use it as the starting point.

The analysis given in this paper is based on a simple idea: under *a priori* assumption (3) we can recover $\epsilon(z)$ from the data (2). There are two steps in the recovery procedure suggested in this paper. First, we recover $\epsilon(z)$ in the neighborhood of the boundary $\zeta - h < z < \zeta$. Second, we continue $\epsilon(z)$ analytically from this interval to the inteval $0 < z < \zeta - h$.

Both steps are linear with respect to $\epsilon(z)$. (1) In the first step, $\epsilon(z)$ is found on the interval $\zeta - h < z < \zeta$ from a linear equation (21). Of course, $\epsilon(z)$ is *not* a linear function of the data; the data γ and g are related to the data f_1 by formulas (13) and (19). (2) In the second step, $\epsilon(z)$ is found on the interval $0 < z < \zeta - h$ by analytic continuation [see formulas (25)–(31)]. The data $\varphi(z, \theta_x, \theta_y)$ are assumed to be known in the layer $\zeta - h < z < \zeta$; they generate the data $\psi(z, \lambda_1, \lambda_2)$ by formula (9), and the data $f_1(z, \lambda_1, \lambda_2)$ by formulas (8) and (11), in the same layer $\zeta - h < z < \zeta$. Therefore there is no need to solve Eqs. (4)–(6) for f or φ in this scheme in order to find φ in the layer $\zeta - h < z < \zeta$.

The first step is done by formula (23), the second is done analytically by formulas (25) and (28). In the first step, one could find $\epsilon(z)$ from Eq. (1) assuming that $f(z, s, x, y, \theta_x, \theta_y)$ is known for $\zeta - h < z < \zeta$ for all values of other parameters in a certain interval. However, such a procedure is considerably less stable than the one we use below. Indeed, Eq. (1) requires calculation of several derivatives of f up to the order 2. This is an unstable operation: small high frequency components of noise in the data are greatly amplified in the process of differentiation. Moreover, in the model equations (4)–(6) which we use, the δ functions in (4) are difficult to treat numerically if one calculates $\epsilon(z)$ directly from Eq. (4).

Let us derive a simple equation for a function φ defined below by formulas (4) and (5). Integrate Eq. (1) with respect to x, y over the plane $-\infty < x, y < \infty$, and with respect to s over the interval $(0, \infty)$, and take into account that $f \to 0$ as $|x| + |y| \to \infty$, to get

$$\frac{\partial \varphi}{\partial z} = \epsilon(z) \triangle \varphi - \delta(\theta_x)\delta(\theta_y), \quad z > 0, \tag{4}$$

$$\triangle \varphi := \frac{\partial^2 \varphi}{\partial \theta_x^2} + \frac{\partial^2 \varphi}{\partial \theta_y^2},$$

$$\varphi|_{z=0} = \varphi_0(\theta_x, \theta_y), \quad \varphi|_{\zeta - h \le z \le \zeta} = \varphi_1(z, \theta_x, \theta_y), \tag{5}$$

where

$$\varphi(z, \theta_x, \theta_y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dy \int_{-0}^{\infty} ds f(z, s, x, y, \theta_x, \theta_y).$$

Here we assumed that

$$f|_{z=0} = \delta(s)\delta(x)\delta(y)\varphi_0(\theta_x, \theta_y), \tag{6}$$

where δ is the delta function, and $\varphi_0(\theta_x, \theta_y)$ is fairly small outside a small neighborhood of the forward propagation direction.

Taking the Fourier transform in θ_x and θ_y in (4) and (5) one gets

$$\psi' - \lambda^2 \epsilon(z) \psi = -1, \quad z > 0, \quad \lambda^2 = \lambda_1^2 + \lambda_2^2, \tag{7}$$

$$\psi|_{z=0} = f_0(\lambda_1, \lambda_2), \quad \psi|_{\zeta - h \le z \le \zeta} = f_1(z, \lambda_1, \lambda_2). \tag{8}$$

Here $f_0(\lambda_1, \lambda_2)$, $f_1(z, \lambda_1, \lambda_2)$, and $\psi(z, \lambda_1, \lambda_2)$ are the Fourier transforms of $\varphi_0(\theta_x, \theta_y)$, $\varphi_1(z, \theta_x, \theta_y)$, and $\varphi(z, \theta_x, \theta_y)$ with respect to θ_x and θ_y, and λ_1 and λ_2 are the Fourier transform variables,

$$\psi(z, \lambda_1, \lambda_2) := \int_{R^2} \varphi(z, \theta_x, \theta_y) \exp\{i(\lambda_1 \theta_x + \lambda_2 \theta_y)\} d\theta_x d\theta_y. \tag{9}$$

Let L be the length of the sample in the z direction and $\bar{\epsilon}$ the average value of $\epsilon(z)$ over the length L: $\bar{\epsilon} \equiv L^{-1} \int_0^L \epsilon(z) dz$. The solution to (4), for constant $\epsilon = \bar{\epsilon}$, contains a factor $\varphi \sim \exp[-(\theta_x^2 + \theta_y^2)/4\bar{\epsilon}z] \le \exp[-(\theta_x^2 + \theta_y^2)/4\bar{\epsilon}L]$. This means that the function φ is bigger than the *arbitrary small* value δ only in the region of the angles $\theta_x^2 + \theta_y^2 < 4\bar{\epsilon}L \ln(1/\delta) \equiv \theta_{\max}^2$. If, for example, we choose $\delta = 10^{-6}$, then $\theta_{\max}^2 \approx 55\bar{\epsilon}L$. Let us assume that $55\bar{\epsilon}L \ll 1$. This assumption is sufficient for the validity of the small-angle approximation used in the paper (see also Refs. 3–5). We took the Fourier transform of the function φ in the variables θ_x and θ_y, and we used the standard argument that allows one to extend the integration limits for the Fourier transform from the physical region $-\pi \le \theta_x, \theta_y \le \pi$ to $-\infty < \theta_x, \theta_y < \infty$. Indeed, as we have shown above, the function φ is negligibly small ($\varphi < 10^{-6}$) outside the small neighborhood of the direction of forward propagation $\theta_x^2 + \theta_y^2 \lesssim \theta_{\max}^2 = 55\bar{\epsilon}L \ll 1$. Because of the uniqueness of the solution to the inverse problem under discussion, the coefficient $\epsilon(z)$, recovered by solving this inverse problem (with exact data), equals the coefficient in the original equation, which generates the data we use. This equation (with the imposed boundary conditions) is uniquely solvable. Therefore the solution to this equation with the $\epsilon(z)$ we found by solving the inverse problem is negligibly small outside a small neighborhood of the direction $\theta_x = \theta_y = 0$. We take $\varphi = 0$ outside this neighborhood and take the Fourier transform of the function φ so defined. From (7) and (8) one gets, using the notation $E(z) := \int_0^z \epsilon(t) dt$,

$$\psi(z, \lambda_1, \lambda_2) = e^{\lambda^2 E(z)} \left[f_0(\lambda_1, \lambda_2) - \int_0^z e^{-\lambda^2 E(t)} dt \right]. \tag{10}$$

Thus, with f_1 defined in (8), one has

$$f_1(z, \lambda_1, \lambda_2) = e^{\lambda^2 E(z)} \left[f_0(\lambda_1, \lambda_2) - \int_0^z e^{-\lambda^2 E(t)} dt \right]. \tag{11}$$

Let us expand (11) in the powers of λ,

$$f_1(z,0,0)+\lambda_1\frac{\partial f_1(z,0,0)}{\partial\lambda_1}+\lambda_2\frac{\partial f_1(z,0,0)}{\partial\lambda_2}+\frac{\lambda_1^2}{2}\frac{\partial^2 f_1}{\partial\lambda_1^2}+\lambda_1\lambda_2\frac{\partial^2 f_1}{\partial\lambda_1\partial\lambda_2}+\frac{\lambda_2^2}{2}\frac{\partial^2 f_1}{\partial\lambda_2^2}+\cdots$$

$$=\left[1+\lambda^2E(z)+\cdots\right]\left[f_0(0,0)+\lambda_1\frac{\partial f_0(0,0)}{\partial\lambda_1}+\lambda_2\frac{\partial f_0(0,0)}{\partial\lambda_2}+\cdots-\int_0^z[1-\lambda^2E(t)+\cdots]dt\right], \quad (12)$$

and equate the coefficients in front of the similar powers of λ_1 and λ_2 to get

$$f_1(z,0,0)=f_0(0,0)-z, \quad (13)$$

$$\frac{\partial f_1(z,0,0)}{\partial\lambda_j}=\frac{\partial f_0(0,0)}{\partial\lambda_j}, \quad j=1,2 \quad (14)$$

$$\frac{1}{2}\frac{\partial^2 f_1(z,0,0)}{\partial\lambda_1^2}=f_0(0,0)E(z)+\int_0^z E(t)dt+\frac{1}{2}\frac{\partial^2 f_0(0,0)}{\partial\lambda_1^2}, \quad (15)$$

$$\frac{\partial^2 f_1(z,0,0)}{\partial\lambda_1\partial\lambda_2}=\frac{\partial^2 f_0(0,0)}{\partial\lambda_1\partial\lambda_2}, \quad (16)$$

$$\frac{1}{2}\frac{\partial^2 f_1(z,0,0)}{\partial\lambda_2^2}=f_0(0,0)E(z)+\frac{1}{2}\frac{\partial^2 f_0(0,0)}{\partial\lambda_2^2}+\int_0^z E(t)dt. \quad (17)$$

From Eq. (15) one obtains an equation for $E(z)$ by differentiating (15) with respect to z:

$$E'+\frac{1}{f_0(0,0)}E=\frac{1}{2f_0(0,0)}\frac{\partial^3 f_1(z,0,0)}{\partial\lambda_1^2\partial z}. \quad (18)$$

Denote

$$\gamma:=\frac{1}{f_0(0,0)}, \quad g(z):=\frac{1}{2f_0(0,0)}\frac{\partial^3 f_1(z,0,0)}{\partial\lambda_1^2\partial z}. \quad (19)$$

Note that $g(z)$ is known for $\zeta-h<z<\zeta$.

Then (18) takes the form

$$E'+\gamma E=g(z). \quad (20)$$

Differentiate (20) to get

$$\epsilon'(z)+\gamma\epsilon(z)=g'(z). \quad (21)$$

The solution of (21) is

$$\epsilon(z)=\epsilon(\zeta)e^{-\gamma(z-\zeta)}+\int_\zeta^z g'(t)e^{-\gamma(z-t)}dt. \quad (22)$$

Thus, assuming that $\epsilon(\zeta)$ is known, one calculates $\epsilon(z)$ for $\zeta-h<z<\zeta$ by formula (22). Integrate by parts in (22) to get

$$\epsilon(z)=\epsilon(\zeta)e^{-\gamma(z-\zeta)}+g(z)-g(\zeta)e^{-\gamma(z-\zeta)}-\gamma\int_\zeta^z g(t)e^{-\gamma(z-t)}dt. \quad (23)$$

Since $g(z)$ for $\zeta-h<z<\zeta$ can be calculated from the data, formula (23) allows one to calculate $\epsilon(z)$ for $\zeta-h<z<\zeta$ from the data.

Let us assume now that $\epsilon(z)$ is calculated for $\zeta-h<z<\zeta$, and pass to the second step.

B. Calculation of $\epsilon(z)$ for $0<z<\zeta-h$ by analytic continuation

Since we assume (3), the function $\epsilon(z)$ is entire, and the problem of finding $\epsilon(z)$ for $0<z<\zeta-h$ from the knowledge of $\epsilon(z)$ for $\zeta-h<z<\zeta$ has a unique solution. A formula for finding analytic continuation (this formula solves the classical spectral extrapolation problem) is found in Refs. 6–9. The problem of numerical analytical continuation is considered in Refs. 10 and 11.

Let us describe the method given in Refs. 6–8 and applied to some inverse problems of geophysics in Ref. 9. The problem consists of recovery of $b(t)$ in (3) from the knowledge of $\epsilon(z)$ for $\zeta-h<z<\zeta$. Let

$$\xi:=z-\zeta+h/2, \quad (24)$$

and

$$\epsilon(z):=\nu(\xi). \quad (25)$$

We have

$$\frac{1}{2\pi}\int_{-a}^{a}e^{-it\xi}q(t)dt=\nu(\xi), \quad (26)$$

$$-\omega_0\le\xi\le\omega_0, \quad \omega_0:=h/2,$$

$$q(t):=b(t)e^{-it(\zeta-h/2)}. \quad (27)$$

The problem (26) consists of finding $q(t)$ from the knowledge of $\nu(\xi)$. This problem is solved in Ref. 9, p. 202, and we give the formula for solution. If $q(t)$ is found, then

$$b(t)=q(t)e^{it(\zeta-h/2)},$$

and $\epsilon(z)$ can be calculated by formula (3) if $b(t)$ is found.

Define

$$q_N(t):=\int_{-\omega_0}^{\omega_0}\nu(\xi)h_N(\xi)e^{i\xi t}d\xi, \quad (28)$$

where $\nu(\xi)$ is known, and

$$h_N(\xi):=\int_{-\infty}^{\infty}\delta_N(t)e^{-i\xi t}dt, \quad (29)$$

and where

$$\delta_N(t) := \left(\frac{N}{4\pi a^2}\right)^{1/2} \left(1 - \frac{t^2}{4a^2}\right)^N \left(\frac{\sin \frac{\omega_0 t}{2N+S}}{\frac{\omega_0 t}{2N+S}}\right)^{2N+S} . \quad (30)$$

Here $S \geq 1$ is an arbitrary number.

It is proved in Refs. 8 and 9 that

$$||q - q_N|| := \max_{-a \leq t \leq a} |q_N(t) - q(t)| \to 0 \quad \text{as } N \to \infty. \quad (31)$$

Moreover, if one assumes $q(t) \in L^2(-a, a)$, then (31) holds with $|| \cdots ||_{L^2(-a,a)}$ in place of $|| \cdots ||_{C(-a,a)}$. If one assumes *a priori* that

$$\max_{-a \leq t \leq a} \{|q(t)| + |q'(t)|\} \leq M, \quad (32)$$

then one proves[8,9] that

$$||q_N - q||_{C(-a,a)} \leq \frac{CM}{N^{1/2}} \quad \text{as} \quad N \to \infty. \quad (33)$$

Estimate (32) implies that $|\epsilon(z)| < (Ma/\pi) \exp(a|z|)$, as follows from (3), (27), and (32).

III. DISCUSSION

Equation (1) is derived under the small-angle approximation, which means that the scattering particle should have large velocity. Also, because the radiation processes (energy losses) were neglected, the function $\epsilon(z)$ in (1) can be considered as the renormalized density of the medium. As was mentioned above, the inverse problem of recovering the density of the medium $\epsilon(z)$ from scattering data given only on some small interval is ill posed. So the length L of the sample in the z direction should be rather small. It is convenient to present the length L of the sample in the dimensionless form, normalizing it by the characteristic value of the mean free path λ (see, for example, Ref. 2)

$$\frac{1}{\lambda} = \frac{4Z^2 Z'^2 e^4 \rho \pi}{\mu^2 c^4 (E_t - 1/E_t)^2 \eta_0^2}, \quad (34)$$

where

$$\eta_0 = \frac{\hbar}{a \mu c (E_t^2 - 1)^{1/2}}, \quad a = \frac{a_0}{Z'^{(1/3)}} = \frac{\hbar^2}{me^2 Z'^{(1/3)}}. \quad (35)$$

In (34) and (35) E_t is the total energy of the charged particle measured in units of its rest mass, μ is the rest mass, eZ' is the charge of the medium particles, and ρ is the dimensional density of the medium. When deriving (34) it was assumed in Ref. 2 that the scattering potential has the form $V = (e^2 Z'/r) \exp(-r/a)$, with the exponential factor representing the screening effect.

Consider the scattering of electrons of 2 Mev kinetic energy by small aluminum sample of $L \approx 300$ nm. Taking into account that in this case $\lambda \approx 3.8 \times 10^{-6}$ cm,[2] we have for the dimensionless length (the number of effective collisions) $\mathcal{L} = L/\lambda \approx 11$. The ratio $L/\lambda \approx 11$ can be considered as a small value in the following sense: this ratio defines the characteristic number of collisions. Therefore it should be, on one hand, big enough for the diffusion equation (1) to be applicable, and, on the other hand, it should be not too big, since the problem of recovery of $\epsilon(z)$ is ill posed. In this sense, the value $L/\lambda \sim 10$ is just what could be recommended for the experimental realization of the discussed approach. Also, in this case $E_t \approx 5$, and the electron is actually relativistic.

The authors propose a method for solving an inverse scattering problem for fast charged particles. They hope that numerical experiments with both simulated and real data will show the scope of the practical utility of this method.

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