CORRECTION TO MOLIÈRE'S FORMULA
FOR MULTIPLE SCATTERING

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The semiclassical correction to Molière's formula for multiple scattering is derived. The consideration is based on the scattering amplitude obtained with the first semiclassical correction taken into account for an arbitrary localized but not spherically symmetric potential. Unlike the leading term, the correction to Molière's formula contains the target density n and thickness L not only in the combination nL (areal density). Therefore, this correction can be referred to as the bulk density correction. It turns out that the bulk density correction is small even for high density. This result explains the wide range of applicability of Molière's formula.

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1. INTRODUCTION

Multiple scattering of high-energy particles in matter is a process that plays an important role in experimental physics. The basis of the theoretical description of this process goes back to Refs. [1–4]. The theory of multiple scattering was further developed in numerous publications (see, e.g., Refs. [5, 6] and the references therein). Detailed experimental investigation of multiple scattering has also been performed (see Refs. [7, 8]).

The celebrated Molière's formula describes the angular distribution $dW/d\Omega$ for small-angle scattering. It was shown by Bethe in Ref. [4] that the simplest way to derive this formula is to use the transport equation. As a consequence of this equation, the angular distribution $dW/d\Omega$ depends on the thickness L and the density n only in the combination nL, which is the areal density of a target. It can be expected that the applicability of Molière's formula is restricted to low densities. But experimental results obtained for small scattering angles show that the deviations from Molière's formula are small for all data available. In the present paper,

we explain such surprising behavior by calculating the leading bulk-density correction to Molière's formula.

We start with the expression for the small-angle scattering amplitude. This expression was obtained in Ref. [9] in the semiclassical approximation with the first correction taken into account. The applicability of this approximation is provided by small scattering angles and high energy ε of the particle, $\varepsilon \gg m$ (m is the particle mass; the system of units with $\hbar = c = 1$ is used). This amplitude has been obtained for an arbitrary localized potential without the requirement of its spherical symmetry. As is known, the semiclassical wave function has a much wider range of applicability than the eikonal wave function. However, as was shown in Ref. [9], the scattering amplitude obtained with the use of the semiclassical wave function coincides with that obtained in the eikonal approximation (see also Ref. [10]). Using the semiclassical scattering amplitude with the first correction taken into account, we calculate the corresponding cross section and average it over the positions of atoms in the target. Dividing this cross section by the area of the target, we arrive at the angular distribution $dW/d\Omega$. The leading term of this distribution coincides with Molière's formula. The correction depends not only on the areal density nL of

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the target but also on the bulk density n alone. We discuss the magnitude of the correction for different target parameters and scattering angles.

2. DIFFERENTIAL PROBABILITY

We direct the z axis along the initial momentum $\mathbf{p}$ of the particle such that

$$\mathbf{r} = z\,\mathbf{p}/p + \boldsymbol{\xi}.$$

The small-angle high-energy scattering amplitude in a localized potential $V(z, \boldsymbol{\xi})$ has the form [9]

$$f = -\frac{i\varepsilon}{2\pi} \int d^2\xi\, e^{-i\mathbf{q}\cdot\boldsymbol{\xi}} \Bigg\{ e^{-i\mathcal{K}(\boldsymbol{\xi})} - 1 + e^{-i\mathcal{K}(\boldsymbol{\xi})} \times$$
$$\times \Bigg[\frac{1}{2\varepsilon} \int\limits_{-\infty}^{\infty} dx\, x \Delta_{\boldsymbol{\xi}} V(x, \boldsymbol{\xi}) - \frac{i}{\varepsilon} \int\limits_{-\infty}^{\infty} dx \times$$
$$\times \int\limits_{-\infty}^{x} dy\, y\, (\nabla_{\boldsymbol{\xi}} V(x, \boldsymbol{\xi})) \cdot (\nabla_{\boldsymbol{\xi}} V(y, \boldsymbol{\xi})) \Bigg] \Bigg\}, \quad (1)$$

$$\mathcal{K}(\boldsymbol{\xi}) = \int\limits_{-\infty}^{\infty} dx\, V(x, \boldsymbol{\xi}),$$

where $\mathbf{q} = \mathbf{p}' - \mathbf{p}$, $\mathbf{p}'$ is the final momentum, $\nabla_{\boldsymbol{\xi}} = \partial/\partial\boldsymbol{\xi}$, and $\Delta_{\boldsymbol{\xi}} = \nabla_{\boldsymbol{\xi}}^2$. The second term in braces in Eq. (1) corresponds to the correction. For $\mathbf{q} \neq 0$, the unity in the leading term can be omitted. The differential cross section corresponding to the amplitude f and having the same accuracy as Eq. (1) is given by

$$\frac{d\sigma}{d\Omega} = \frac{\varepsilon^2}{2\pi^2} \operatorname{Re} \int d\boldsymbol{\xi}_1\, d\boldsymbol{\xi}_2 \exp\left[-i\mathbf{q}\cdot(\boldsymbol{\xi}_1 - \boldsymbol{\xi}_2)\right] \times$$
$$\times \exp\left\{-i\left[\mathcal{K}(\boldsymbol{\xi}_1) - \mathcal{K}(\boldsymbol{\xi}_2)\right]\right\} \times$$
$$\times \Bigg\{ 1 + \frac{1}{2\varepsilon} \int\limits_{-\infty}^{\infty} dx\, x \Delta_{\boldsymbol{\xi}_1} V(x, \boldsymbol{\xi}_1) - \frac{i}{\varepsilon} \int\limits_{-\infty}^{\infty} dx \times$$
$$\times \int\limits_{-\infty}^{x} dy\, y\, (\nabla_{\boldsymbol{\xi}_1} V(x, \boldsymbol{\xi}_1)) \cdot (\nabla_{\boldsymbol{\xi}_1} V(y, \boldsymbol{\xi}_1)) \Bigg\}. \quad (2)$$

The total potential of atoms in the target has the form

$$V(\mathbf{r}) = \sum_i u(\mathbf{r} - \mathbf{r}_i), \quad (3)$$

where $u(\mathbf{r})$ is the potential of an individual atom, which we assume to be spherically symmetric. We average over the atom positions using the prescription

$$\langle f \rangle = \int \prod_i \frac{dx_i\, d\boldsymbol{\rho}_i}{LS} f, \quad (4)$$

corresponding to the dilute gas approximation. As a result, we obtain

$$\frac{dW}{d\Omega} = \left\langle \frac{d\sigma}{S d\Omega} \right\rangle = \frac{\varepsilon^2}{2\pi^2} \operatorname{Re} \int d\boldsymbol{\rho}\, e^{-i\mathbf{q}\cdot\boldsymbol{\rho}} \times$$
$$\times \left\{ F_1^N - \frac{iN}{\varepsilon} F_1^{N-1} F_2 - \frac{iN(N-1)}{\varepsilon} F_1^{N-2} F_3 \right\}, \quad (5)$$

where

$$F_1 = \int \frac{d\boldsymbol{\rho}_1}{S} \exp\left\{-i\left[\chi(\boldsymbol{\rho}_1) - \chi(\boldsymbol{\rho}_1 - \boldsymbol{\rho})\right]\right\},$$

$$F_2 = \frac{L}{4} \int \frac{d\boldsymbol{\rho}_1}{S} \exp\left\{-i\left[\chi(\boldsymbol{\rho}_1) - \chi(\boldsymbol{\rho}_1 - \boldsymbol{\rho})\right]\right\} \times$$
$$\times \left[(\nabla_{\boldsymbol{\rho}_1}\chi(\boldsymbol{\rho}_1)) \cdot (\nabla_{\boldsymbol{\rho}_1}\chi(\boldsymbol{\rho}_1)) + i\Delta_{\boldsymbol{\rho}_1}\chi(\boldsymbol{\rho}_1)\right] +$$
$$+ \int\limits_{-\infty}^{\infty} dx \int\limits_{-\infty}^{x} dy\, y \int \frac{d\boldsymbol{\rho}_1}{S} \times$$
$$\times \exp\left\{-i\left[\chi(\boldsymbol{\rho}_1) - \chi(\boldsymbol{\rho}_1 - \boldsymbol{\rho})\right]\right\} \times$$
$$\times (\nabla_{\boldsymbol{\rho}_1} u(x, \boldsymbol{\rho}_1)) \cdot (\nabla_{\boldsymbol{\rho}_1} u(y, \boldsymbol{\rho}_1)), \quad (6)$$

$$F_3 = \int\limits_{-\infty}^{\infty} dx \int\limits_{-\infty}^{\infty} dy \iint \frac{d\boldsymbol{\rho}_1}{S} \frac{d\boldsymbol{\rho}_2}{S} \times$$
$$\times \exp\left\{-i\left[\chi(\boldsymbol{\rho}_1) -\right.\right.$$
$$\left.\left.- \chi(\boldsymbol{\rho}_1 - \boldsymbol{\rho}) + \chi(\boldsymbol{\rho}_2) - \chi(\boldsymbol{\rho}_2 - \boldsymbol{\rho})\right]\right\} \times$$
$$\times \left[\frac{L}{6} - \frac{(x-y)^2}{4L}\right] \times$$
$$\times (\nabla_{\boldsymbol{\rho}_1} u(x, \boldsymbol{\rho}_1)) \cdot (\nabla_{\boldsymbol{\rho}_2} u(y, \boldsymbol{\rho}_2)).$$

Here,

$$\chi(\boldsymbol{\rho}) = \int\limits_{-\infty}^{\infty} dx\, u(x, \boldsymbol{\rho}),$$

and hence

$$\mathcal{K}(\boldsymbol{\rho}) = \sum_i \chi(\boldsymbol{\rho} - \boldsymbol{\rho}_i).$$

We next pass to the limit $N, S \to \infty$ and $N/S = nL = {}$ $= \text{const}$. In this limit,

$$F_1^N = \left(1 + \int \frac{d\boldsymbol{\rho}_1}{S} \left[\exp\left\{-i\left[\chi(\boldsymbol{\rho}_1)\right. - \right.\right.\right.$$
$$\left.\left.\left. - \chi(\boldsymbol{\rho}_1 - \boldsymbol{\rho})\right]\right\} - 1\right]\right)^N \to \exp\left[-nL \int d\boldsymbol{\rho}_1 \times\right.$$
$$\left. \times \left(1 - \exp\left\{-i\left[\chi(\boldsymbol{\rho}_1) - \chi(\boldsymbol{\rho}_1 - \boldsymbol{\rho})\right]\right\}\right)\right]. \quad (7)$$

Substituting Eqs. (6) and (7) in Eq. (5), we finally obtain

$$\frac{dW}{d\Omega} = \frac{\varepsilon^2}{(2\pi)^2} \int d\boldsymbol{\rho}\, e^{-i\mathbf{q}\cdot\boldsymbol{\rho}} \times$$

$$\times \exp\left\{ -nL \int d\boldsymbol{\rho}_1 \left[1 - \cos\left(\chi\left(\boldsymbol{\rho}_1\right) - \chi\left(\boldsymbol{\rho}_1 - \boldsymbol{\rho}\right)\right) \right] \right\} \times$$

$$\times \left\{ 1 - \frac{nL}{\varepsilon} \int\limits_{-\infty}^{\infty} dx \int d\boldsymbol{\rho}_1 \times \right.$$

$$\times \sin\left(\chi\left(\boldsymbol{\rho}_1\right) - \chi\left(\boldsymbol{\rho}_1 - \boldsymbol{\rho}\right)\right) \boldsymbol{\rho}_1 \cdot \nabla_{\boldsymbol{\rho}_1} u^2\left(x, \boldsymbol{\rho}_1\right) -$$

$$- \frac{n^2 L}{\varepsilon} \int d\boldsymbol{\rho}_1 \cos\left(\chi\left(\boldsymbol{\rho}_1\right) - \chi\left(\boldsymbol{\rho}_1 - \boldsymbol{\rho}\right)\right) \boldsymbol{\rho}_1 \chi\left(\boldsymbol{\rho}_1\right) \times$$

$$\left. \times \int d\boldsymbol{\rho}_2 \sin\left(\chi\left(\boldsymbol{\rho}_2\right) - \chi\left(\boldsymbol{\rho}_2 - \boldsymbol{\rho}\right)\right) \nabla_{\boldsymbol{\rho}_2} \chi\left(\boldsymbol{\rho}_2\right) \right\}. \quad (8)$$

In deriving this formula, we used integration by parts. As a result, all terms proportional to L in F_2 and F_3, Eq. (6), vanish.

It is convenient to rewrite Eq. (8) in another form. The differential in the momentum transfer $\mathbf{Q}$ cross section $d\sigma/d\mathbf{Q}$ of high-energy scattering on one atom, calculated in the semiclassical approximation with the first correction taken into account, satisfies the relation [10, 9]

$$\int d^2 Q \left(1 - e^{i\mathbf{Q}\cdot\boldsymbol{\rho}} \right) \frac{d\sigma}{d\mathbf{Q}} =$$

$$= \int d\boldsymbol{\rho}_1 \left[1 - \cos\left(\chi\left(\boldsymbol{\rho}_1\right) - \chi\left(\boldsymbol{\rho}_1 - \boldsymbol{\rho}\right)\right) + \right.$$

$$+ \frac{1}{\varepsilon} \int\limits_{-\infty}^{\infty} dx \sin\left(\chi\left(\boldsymbol{\rho}_1\right) - \chi\left(\boldsymbol{\rho}_1 - \boldsymbol{\rho}\right)\right) \times$$

$$\left. \times \boldsymbol{\rho}_1 \cdot \nabla_{\boldsymbol{\rho}_1} u^2\left(x, \boldsymbol{\rho}_1\right) \right]. \quad (9)$$

Using this relation, we obtain

$$\frac{dW}{d\Omega} = \frac{\varepsilon^2}{(2\pi)^2} \int d\boldsymbol{\rho}\, e^{-i\mathbf{q}\cdot\boldsymbol{\rho}} \times$$

$$\times \exp\left[-nL \int d^2 Q \left(1 - e^{i\mathbf{Q}\cdot\boldsymbol{\rho}} \right) \frac{d\sigma}{d\mathbf{Q}} \right] \times$$

$$\times \left\{ 1 - \frac{n^2 L}{\varepsilon} \int d\boldsymbol{\rho}_1 \cos\left(\chi\left(\boldsymbol{\rho}_1\right) - \chi\left(\boldsymbol{\rho}_1 - \boldsymbol{\rho}\right)\right) \boldsymbol{\rho}_1 \chi\left(\boldsymbol{\rho}_1\right) \times \right.$$

$$\left. \times \int d\boldsymbol{\rho}_2 \sin\left(\chi\left(\boldsymbol{\rho}_2\right) - \chi\left(\boldsymbol{\rho}_2 - \boldsymbol{\rho}\right)\right) \nabla_{\boldsymbol{\rho}_2} \chi\left(\boldsymbol{\rho}_2\right) \right\} \quad (10)$$

with the same accuracy as in Eq. (8). The leading term $dW_M/d\Omega$ in Eq. (10), corresponding to unity in braces, coincides with Molière's formula. The correction $dW_C/d\Omega$ describes the effect of the bulk density of the target and has not been known so far.

3. DISCUSSION

We discuss the magnitude and the structure of the correction obtained. At a fixed areal density nL (the number of target atoms per unit area), the correction behaves as n (or L^{-1}), and increases as L decreases. Estimations show that the relative magnitude of the correction is the largest when the leading contribution to the integral over $\boldsymbol{\rho}$ in Eq. (10) comes from the region $\rho \sim a$, where a is the screening radius of the atom, $a \sim a_B Z^{-1/3}$, a_B is the Bohr radius, and Z is the nuclear charge number. This condition is satisfied when $q \sim nLa$, where q is the momentum transfer. In this case, the correction has the relative order

$$\delta = \left(\frac{dW_M}{d\Omega} \right)^{-1} \frac{dW_C}{d\Omega} \sim \frac{Z\alpha n a^3}{\varepsilon a} R,$$

$$R = (Z\alpha)^2 nLa^2, \quad (11)$$

where $\alpha = 1/137$ is the fine structure constant. Using the estimates

$$(\varepsilon a)^{-1} \ll (ma)^{-1} \sim \alpha Z^{1/3} \ll 1,$$

$$Z\alpha n a^3 \lesssim Z\alpha a_B^{-3} \left(a_B Z^{-1/3} \right)^3 = \alpha \ll 1,$$

we obtain

$$\delta \lesssim 10^{-3} R \frac{m}{\varepsilon}.$$

The upper bound for δ increases with R. However, when $R \gg 1$, both the leading term and the correction are suppressed by the factor $\exp\left[-b\,R\right]$, where $b \sim 1$ is some numerical constant. Therefore, in the whole region interesting from the experimental standpoint, R is not too big and hence δ is very small.

To conclude, we have calculated the volume density correction to Molière's formula and estimated the magnitude of the correction. It turns out to be very small for all reasonable values of parameters. Therefore, Molière's formula remains very accurate even for a high density of the target.

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