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Energy conservation in approximated solutions of multi-beam scattering problems

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Abstract

Scattering of particles by time-independent potentials is describable by wave solutions in the form of series expansion. As mathematically demonstrated here, such form of solutions when applied to multi-beam scattering phenomena can lead to energy violation where the incident and scattered numbers of particles are not preserved. In this work, we outline a general basic requirement for developing consistent solutions of time-dependent multi-beam scattering problems by extended potentials.

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1. Introduction

Elastic scattering of quantum particles by extended potentials is a well-known phenomenon in Physics. It is extremely important in Material Science where beams of particles, like photons and electrons, are used to probe the atomic structure of the matter. Such phenomena are describable by scattered waves – vectorial electromagnetic waves for photons and scalar wave functions for

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matter particles – written in the form of series expansions, for instance

$$\Psi(\boldsymbol{r}) = \psi_0(\boldsymbol{r}) + \psi_1(\boldsymbol{r}) + \psi_2(\boldsymbol{r}) + \cdots = \sum_{n=0}^{\infty} \psi_n(\boldsymbol{r}) \tag{1}$$

is the probability amplitude accounting for nth-order scattering events. The number of terms is related to the extension of the potential, which increases higher-order scattering probabilities. Eq. (1) stands for the general form of the Born approximation series of time-independent scattering potentials; and although it is conceptually simple and of practical usage, it is quite limited for describing multi-beam scattering problems. In particular, to describe the excitement of one beam when others are already excited since this situation would configure time-dependent scattering regime.

The first objective of this paper is to analytically demonstrate that phenomenological interpretation of multi-beam scatterings based on Eq. (1) leads to energy violation where the potential scatters more particles than exist in the incident beam. Consequently, series expansions should not be taken as a generally valid form of solution for quantitative and accurate description of this type of phenomenon; this remark does not depend on the number of terms considered in the series expansion. The second objective is to develop a general time-dependent solution of the phenomenon that preserves the number of particles entering and leaving the effective volume of the scattering potential.

2. Theory

In the standard Born approximation, as find in text books [1], $\psi_0(\boldsymbol{r})$ stands for the incident wave everywhere. It is a reasonable approach for perturbation theories where the scattered beams are much weaker than the incident one. However, for a general treatment considering very strong scattered beams, $\psi_0(\boldsymbol{r})$ has to be the incident wave inside the potential's range only; outside, it must give the probability amplitude for non-interacting particles, those passing through the potential without been scattered.

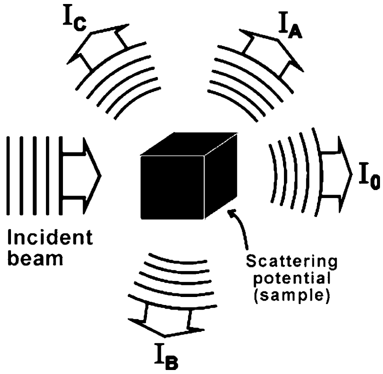

Fig. 1. General configuration of multi-beam elastic scattering of quantum particles (photons, electrons, neutrons, ions, etc.) by extended potentials (macroscopic samples). It is characterized by scattered waves, $\Psi_G(\boldsymbol{r})$, within distinct non-overlapping directions of the space. The power of the scattered beams, in number of particles per unit of time, are given by $I_G = \oint \Psi_G(\boldsymbol{r})\Psi_G^*(\boldsymbol{r})r^2\,d\Omega$ $(G = 0, A, B, \ldots)$ where the integral is carried out on any closed surface outside the potential's volume.

A multi-beam scattering configuration, as schematized in Fig. 1, occurs when Eq. (1) can be rewritten as

$$\Psi(\boldsymbol{r}) = \Psi_0(\boldsymbol{r}) + \Psi_A(\boldsymbol{r}) + \Psi_B(\boldsymbol{r}) + \cdots \tag{2}$$

since

$$\Psi_G(\boldsymbol{r}) = \sum_{n=0}^{\infty} \psi_{n,G}(\boldsymbol{r}), \quad G = 0, A, B, \ldots \tag{3}$$

and

$$\sum_G \psi_{n,G}(\boldsymbol{r}) = \psi_n(\boldsymbol{r}), \tag{4}$$

where $\psi_{0,0}(\boldsymbol{r}) = \psi_0(\boldsymbol{r})$. None contribution of the incident wave appears in the directions of the scattered ones, $\psi_{0,G\neq 0}(\boldsymbol{r}) = 0$, neither first-order scattering in the direction of the incident wave, $\psi_{1,0}(\boldsymbol{r}) = 0$. Moreover, to characterize a multi-beam scattering configuration, it is also necessary that

$$\oint \Psi(\boldsymbol{r})\Psi^*(\boldsymbol{r})r^2\,d\Omega = I_0 + I_A + I_B + \cdots = N_0, \tag{5}$$

where

$$I_G = \oint \Psi_G(\boldsymbol{r})\Psi_G^*(\boldsymbol{r})r^2\,d\Omega \tag{6}$$

provides the time average number of particles scattered within distinct non-overlapping solid angles. It guarantees that interference of probability amplitudes occurs exclusively among the series expansion terms of each $\Psi_G(\boldsymbol{r})$, Eq. (3). The integrals are carried out on any closed surface outside the potential's volume. Hereinafter, we will refer to I_G as the beam intensity.

Approximated solution in series expansions are always valid, in principle, for time-independent potentials, or stationary scattering regime. To use the same form of solution for describing the excitement of an extra beam, besides those already excited, further developments are necessary otherwise the incident and scattered numbers of particles are not preserved in the process. This point is demonstrated here by means of an example. Let us assume a small potential where third-order scatterings are negligible, as well as higher order ones, i.e. $\psi_{n\geqslant 3,G} \approx 0$. According to Born approximations, or similar method,

$$\Psi'_0(\boldsymbol{r}) = \psi'_0(\boldsymbol{r}) + \psi'^{(A)}_{2,0}(\boldsymbol{r}) \quad \text{and} \quad \Psi'_A(\boldsymbol{r}) = \psi'_{1,A}(\boldsymbol{r}) \tag{7}$$

are the scattered waves under a two-beam, I'_0 and I'_A, excitement condition. On the other hand, when another beam is excited, I_B for instance, the scattered waves are given by

$$\begin{aligned} \Psi_0(\boldsymbol{r}) &= \psi_0(\boldsymbol{r}) + \psi^{(A)}_{2,0}(\boldsymbol{r}) + \psi^{(B)}_{2,0}(\boldsymbol{r}),\\ \Psi_A(\boldsymbol{r}) &= \psi_{1,A}(\boldsymbol{r}) + \psi^{(B)}_{2,A}(\boldsymbol{r}),\\ \Psi_B(\boldsymbol{r}) &= \psi_{1,B}(\boldsymbol{r}) + \psi^{(A)}_{2,B}(\boldsymbol{r}). \end{aligned} \tag{8}$$

(A, B) superscripts are used on second-order waves to identify the first-order ones originating them. For instance, $\psi^{(A)}_{2,0}(\boldsymbol{r})$ stands for the rescattering of $\psi_{1,A}(\boldsymbol{r})$ towards the forward-transmitted wave, $\psi_0(\boldsymbol{r})$.

The number of particles entering and leaving the potential must be preserved under pure elastic scattering. It means that for an incident beam constant in time, $\mathrm{d}N_0/\mathrm{d}t = 0$ in Eq. (5), the total intensity of the scattered waves in Eqs. (7) and (8) are equal, i.e. $\mathrm{I}'_0 + \mathrm{I}'_A = \mathrm{I}_0 + \mathrm{I}_A + \mathrm{I}_B$, which leads to

$$\begin{aligned} &\oint \left\{ \left|\psi'_0 + \psi'^{(A)}_{2,0}\right|^2 + \left|\psi'_{1,A}\right|^2 \right\} r^2\,\mathrm{d}\Omega \\ &= \oint \left\{ \left|\psi_0 + \psi^{(A)}_{2,0} + \psi^{(B)}_{2,0}\right|^2 + \left|\psi_{1,A} + \psi^{(B)}_{2,A}\right|^2 + \left|\psi_{1,B} + \psi^{(A)}_{2,B}\right|^2 \right\} r^2\,\mathrm{d}\Omega. \end{aligned} \tag{9}$$

The challenge in describing the scattering of multiple beams by approximated solutions can be summarized in the above example, in how to go from Eq. (7) to Eq. (8) without violating the equality in Eq. (9). In more specific words, it is necessary to described not only how the extra terms in Eq. (8) are excited, but also how the terms already excited in Eq. (7) are affected by the excitement of the new beam, I_B in this case. For a qualitative description, one may assume that $\psi_0(\boldsymbol{r}) = \psi'_0(\boldsymbol{r})$, $\psi^{(A)}_{2,0}(\boldsymbol{r}) = \psi'^{(A)}_{2,0}(\boldsymbol{r})$ and $\psi_{1,A}(\boldsymbol{r}) = \psi'_{1,A}(\boldsymbol{r})$ and that the extra terms in Eq. (8) are switched on as the potential varies in time. However, in this phenomenological description the total number of scattered particles is not preserved; unless in the case of a very particular coincidence where $\psi^{(B)}_{2,G}(\boldsymbol{r})$ would provide destructive interference with the other terms of $\Psi_G(\boldsymbol{r})$ (G = 0 or A) so that these destructive interference would account for the exact number of particles in I_B. Although some phase relationships may exist among the scattered waves, they vary from one potential to another since the phases are intrinsically related to the internal three-dimensional structure of the scattering potentials – remember that three-dimensional holograms are made by recording the phases of the scattered light from the objects. Therefore, phase relationships among the series expansion terms are not responsible for the above equality, Eq. (9). In the next part of this paper, we present a general time-dependent solution, in the form of series expansion, for describing multi-beam scattering phenomena.

3. Discussions

Conservation of the number of scattered particles in approximated solutions is possible by taken into account the scattering probabilities of the particles when traveling through the potential.

By introducing $p_{H,G}(n,t)$ as the scattering probability from beam G to beam H after n scattering events, the population of particles in the beam H that have already been scattered (bounced) from one beam to another $n+1$ times is

$$P_H(n+1) = \sum_G p_{H,G}(n,t) P_G(n), \quad (10)$$

where $p_{H,G}(n,t) = 0$ for H = G and the time, t, dependence of these probabilities are determined by the potential, i.e. on how it varies in time until a multi-beam scattering configuration is achieved. Moreover, assuming a slow time variation to assure that at any time instant the populations are given by Eq. (10), the behavior of the populations as a function of n can be inferred by the sum of probabilities,

$$s_G(n) = \sum_H p_{H,G}(n). \quad (11)$$

When $s_G(n) = 1$ the n-bounced particles in the beam G have 100% probability to be scattered towards another beam before leaving the potential's range. Therefore, outside the potential, the total number of particles on beam G is calculated as

$$\mathtt{I}_G = \sum_n [1 - s_G(n)] P_G(n). \quad (12)$$

It implies that when $s_G(n) = 1$ none n-bounced particles are found on beam G. On the other hand, when $s_G(n) \ll 1$ the potential scatters a significant fraction of the population of n-bounced particles through beam G.

A direct comparison between Eqs. (6) and (12) leads to a straightforward conclusion that the $\Psi_G(\boldsymbol{r})$ waves, as given in Eq. (3), must be redefined outside the potential as

$$\Psi_G(\boldsymbol{r}) = \sum_{n=0}^{\infty} \sqrt{1 - s_G(n)}\, \psi_{n,G}(\boldsymbol{r}). \quad (13)$$

The physical meaning of $\sqrt{1 - s_G(n)}$ is clear. It reduces the probability amplitudes of scattering towards beam G when other beams are excited, i.e. when the particles on beam G, inside the potential, have a non-null probability of leaving the potential's volume via other beams. Let us use the three-beam configuration represented in Eq. (8) to demonstrated that the above form of solution, Eq. (13), can be used to described the excitement of the third beam and at the same time preserving the total number of scattered particles, N_0.

The small potential responsible for the scattered waves in Eq. (8) can be represented by a set of scattering probabilities, so that $s_0 = p_{A,0} + p_{B,0}$, $s_A = p_{0,A} + p_{B,A}$ and $s_B = p_{0,B} + p_{A,B}$ are supposed to be constant values as a function of n. Then, by upgrading the scattered waves in Eq. (8) according to the new definition given in Eq. (13), and replacing then into Eq. (6) we obtain

$$\begin{aligned} \mathtt{I}_0 &\simeq N_0(1 - p_{A,0} - p_{B,0} + p_{0,A}p_{A,0} + p_{0,B}p_{B,0}), \\ \mathtt{I}_A &\simeq N_0(p_{A,0} + p_{A,B}p_{B,0} - p_{0,A}p_{A,0} - p_{B,A}p_{A,0}), \\ \mathtt{I}_B &\simeq N_0(p_{B,0} + p_{B,A}p_{A,0} - p_{0,B}p_{B,0} - p_{A,B}p_{B,0}), \end{aligned} \quad (14)$$

where triple products of the $p_{H,G}$ probabilities are disregarded since $\psi_{n\geqslant 3,G} \approx 0$ for such a small potential.

According to the above intensities, Eq. (14), the total number of particles is always preserved, i.e. $\mathtt{I}_0 + \mathtt{I}_A + \mathtt{I}_B \simeq N_0$ independently of the excitement condition of these beams. When $p_{B,0} = p_{B,A} = 0$, beam B is not excited but the sum of intensities still provides the incident number of particles, $\mathtt{I}'_0 + \mathtt{I}'_A \simeq N_0$. If beam A is also switched off, $p_{A,0} = p_{A,B} = 0$, no particle-potential interaction occurs so that $\mathtt{I}''_0 = N_0$.

The proposed solution for the scattered waves, Eq. (13), allows a better understanding on the practical consequences of the number-of-particles balance, i.e. energy balance, among the scattered beams. General aspects of such consequences can be outlined by monitoring one beam,

$$\mathtt{I}_A(t) = \oint [1 - s_A(t)] \left| \psi_{1,A}(\boldsymbol{r}) + \psi_{2,A}^{(B)}(\boldsymbol{r},t) \right|^2 r^2\, \mathrm{d}\Omega, \quad (15)$$

while another beam, beam B, is excited as a function of time in the previously used example of a three-beam configuration. Although the excitement condition of beam A is kept unchanged in this hypothetical experiment, $s_A(t) = p_{0,A} + p_{B,A}(t)$ and $\psi_{2,A}^{(B)}(\boldsymbol{r},t)$ are affected by the time-dependence of the potential when exciting beam B.

$\psi^{(B)}_{2,A}(\boldsymbol{r},t)$ can enhance or reduce the intensity of beam A, Eq. (15), depending on its relative amplitude and phase regarding $\psi_{1,A}(\boldsymbol{r})$. However, besides the interference effects between the scattered waves, an intensity reduction always occurs owing to the enhancement of $p_{B,A}(t)$, and consequently of $s_A(t)$, as beam B is excited.

Note that neglecting $s_A(t)$ in Eq. (13) misleads the interpretation of $\mathtt{I}_A(t)$ towards weaker amplitudes of $\psi^{(B)}_{2,A}(\boldsymbol{r},t)$ as well as phase shifts to favor destructive interference. Moreover, the intensity reduction owing to $[1 - s_A(t)]$ term in Eq. (15) will be a dominant effect when the second-order wave is very weak, i.e. $\psi^{(B)}_{2,A}(\boldsymbol{r},t) \approx 0$. In multi-beam X-ray diffraction experiments such effect is known as *Aufhellung* [2,3] and, under the framework of the second-order approximation, induced phase shifts by the *Aufhellung* effect have already been reported [4].

4. Conclusions

In summary, multi-beam scattering configurations are mathematically defined. It demonstrates that the number of incident and scatted particles is not preserved when time-independent solutions in form of series expansion are extended to describe time-dependent scattering problems. Basic requirements of time-dependent solutions for extended potentials are pointed out and their consequences discussed. The proposed form of solution could also be used, in principle, to upgrade available solutions to account for the *Aufhellung* effect, commonly observed in multi-beam X-ray diffraction.

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References

[1] C. Cohen-Tannoudji, Quantum Mechanics, Wiley-Interscience, New York, 1977.
[2] E. Wagner, Phyz. Z. 21 (1923) 94.
[3] S.-L. Chang, Multiple Diffraction of X-rays in Crystals, Springer, Berlin, 1984.
[4] S.L. Morelhão, S. Kycia, Enhanced X-ray phase determination by three-beam diffraction, Phys. Rev. Lett. 89 (1) (2002) 015501.