Non-stationary scattering of wave-packets

D.R. Bitouk

Department of Physics, Moscow State University, Vorob'yevy Gory, Moscow, 117234, Russia

bitouk@theor.gpi.ru

M.V. Fedorov

General Physics Institute, 38, Vavilova St., Moscow, 117942, Russia

fedorov@theor.gpi.ru

Abstract: Potential scattering of free-electron wave packets is considered in the framework of non-stationary quantum-mechanical theory. The general expression for the average angle of scattering is obtained. The traditional quantum-mechanical plane-wave approximation and classical results are shown to be incorporated in the results derived.

OCIS codes: (290.0290) Scattering; (290.5850) Scattering, particles

References and links

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1. Introduction

Potential scattering of particles is a pretty well–known and studied phenomenon. Its new features can arise, when quantum-mechanical states of particles have the form of wave packets. Such a formulation is often mentioned in many papers and books [1], but, as far as we know, almost never is used as a practical instrument for calculation of experimentally measurable parameters. Meanwhile, the modern techniques of strong-field photoionization of atoms allows to produce very nice electron wave packets in a controllable way [2], and this is one of the motivations for re-considering seriously the problem of wave packet scattering. Another motivation is based on the observation that sometimes the classical and standard stationary quantum-mechanical theory of potential scattering give strongly different results. Indeed, if one calculates the average angle of scattering, $\overline{\theta}$, the classical mechanics [3] predicts that, in the approximation of small deviations, $\overline{\theta}$ is of the first order in the potential $U(\boldsymbol{r})$, $\overline{\theta} \sim U$. On the other hand, the first non-zero contribution to $\overline{\theta}$ determined by the standard stationary quantum-mechanical theory [4] is determined by the result of the first Born approximation, which is squared in U, $\overline{\theta} \sim U^2$. This is a direct contradiction between the predictions of the classical and standard quantum-mechanical theories, which,

#4586 - $15.00 US Received March 02, 1998; Revised April 28, 1998

as far as we know, has never been explicitly formulated and which requires explanations. The natural explanation to this controversy arises from the non-stationary quantum-mechanical theory of wave-packet scattering which is briefly described below. In this letter, the theory of potential scattering of wave-packets is briefly outlined. The lowest-order quantum-mechanical angle of scattering is found and its relationship and analogy with the predictions of the classical theory are established and discussed.

2. Non-stationary wave-packet quantum-mechanical theory of scattering

Inevitably, the theory of wave-packet scattering has to be constructed as a non-stationary theory. In principle, such a theory has to take into account irreversible spreading of wave packets. Moreover, the results obtained below can be referred as the transient ones and they are essentially different from the asymptotic results of the stationary theory. Non-stationary wave-packet theory of scattering is formulated as the initial-value problem, and this formulation is different from the usual *S*-matrix approach in the stationary theory of potential scattering.

In the non-stationary approach, an electron is assumed to be described quantum-mechanically by its wave function $\Psi(\boldsymbol{r}, t)$ obeying the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi(\boldsymbol{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r}) \right) \Psi(\boldsymbol{r},t) \tag{1}$$

with an initial condition $\Psi(\boldsymbol{r}, t{=}0) = \Psi^{(0)}(\boldsymbol{r})$, where $\Psi^{(0)}(\boldsymbol{r})$ is an unperturbed initial wave function of an electron (at $t = 0$). It is assumed that at $t{=}0$ an electron is located far from a target atom. The exact time-dependent wave function of an electron $\Psi(\boldsymbol{r}, t)$ can be expanded in a series (integral) of plane waves

$$\Psi(\boldsymbol{r},t) = \frac{1}{(2\pi\hbar)^{3/2}} \int d\boldsymbol{p}\, C_{\boldsymbol{p}}(t) \exp\left[\frac{i}{\hbar} \left(\boldsymbol{p}\cdot\boldsymbol{r} - E_{\boldsymbol{p}} t \right) \right] \tag{2}$$

where $E_{\boldsymbol{p}} = \boldsymbol{p}^2/2m$ is the free-electron energy corresponding to the momentum $\boldsymbol{p}$ and the probability amplitudes $C_{\boldsymbol{p}}(t)$ obey the equation

$$i\hbar \dot{C}_{\boldsymbol{p}}(t) = \int d\boldsymbol{p}'\, C_{\boldsymbol{p}'}(t) \tilde{U}(\boldsymbol{p}' - \boldsymbol{p}) \exp\left[\frac{i}{\hbar} \left(E_{\boldsymbol{p}} - E_{\boldsymbol{p}'} \right) t \right] \tag{3}$$

and the initial conditions

$$C_{\boldsymbol{p}}(t)\big|_{t=0} \equiv C_{\boldsymbol{p}}^{(0)} = \int d\boldsymbol{r} \exp\left(-\frac{i}{\hbar} \boldsymbol{p}\cdot\boldsymbol{r} \right) \Psi^{(0)}(\boldsymbol{r}). \tag{4}$$

In Eq. (3) and below, $\tilde{U}(\boldsymbol{q})$ is the Fourier-transform of the potential $U(\boldsymbol{r})$,

$$\tilde{U}(\boldsymbol{q}) = \frac{1}{(2\pi\hbar)^3} \int d\boldsymbol{r}\; U(\boldsymbol{r}) \exp\left(i \frac{\boldsymbol{q}\cdot\boldsymbol{r}}{\hbar} \right). \tag{5}$$

In the framework of perturbation theory with respect to the potential $U(\boldsymbol{r})$

$$C_{\boldsymbol{p}}(t) = C_{\boldsymbol{p}}^{(0)} + C_{\boldsymbol{p}}^{(1)}(t) + C_{\boldsymbol{p}}^{(2)}(t) + \ldots \tag{6}$$

where $C_{\boldsymbol{p}}^{(0)} = C_{\boldsymbol{p}}(0)$ and

$$C_{\boldsymbol{p}}^{(1)}(t) = -\frac{i}{\hbar} \int_0^t dt' \int d\boldsymbol{p}'\, C_{\boldsymbol{p}'}^{(0)} \tilde{U}(\boldsymbol{p}' - \boldsymbol{p}) \exp\left[\frac{i}{\hbar} \left(E_{\boldsymbol{p}} - E_{\boldsymbol{p}'} \right) t' \right] \tag{7}$$

#4586 - $15.00 US Received March 02, 1998; Revised April 28, 1998

Let us assume now that the initial electron wave function $\Psi^{(0)}(\boldsymbol{r})$ is characterized by a Gaussian distribution over momentum

$$C_{\boldsymbol{p}}^{(0)} = \frac{(\Delta r_0)^{3/2}}{\pi^{3/4}\,\hbar^{3/2}} \exp\left[-\frac{(\Delta r_0)^2}{2\hbar^2} (\boldsymbol{p} - \boldsymbol{p}_0)^{\ 2} - \frac{i}{\hbar}\, \boldsymbol{p}\cdot\boldsymbol{r}_0 \right], \tag{8}$$

where Δr_0 is the size of the unperturbed wave packet at $t = 0$, $\boldsymbol{p}_0$ is the momentum of the "center of mass", and $\boldsymbol{r}_0$ is its initial position. In the problem of scattering, in analogy with the classical picture, the component of the initial-position vector $\boldsymbol{r}_0$, perpendicular to $\boldsymbol{p}_0$, $\boldsymbol{r}_{0\perp}$, determines the impact parameter $\rho = |\boldsymbol{r}_{0\perp}|$.

The general consideration of this paper is valid for any Δr_0 and t, and it takes into account the spreading effects completely. However, some of our specific calculations below and the main qualitative conclusions are based on the assumption that the characteristic wave-packet spreading time

$$\Delta r(t) = \sqrt{(\Delta r_0)^2 + \left(\frac{\hbar t}{m\,\Delta r_0} \right)^2} \tag{9}$$

is much longer than any other characteristic times of the problem under consideration, $t_{spr} >> t_c$, where t_c includes both the interaction time and a time it takes for a scattered electron to reach the detector. From this point of view, the results obtained in the case of $t_{spr} >> t_c$ can be referred to as the transient ones and they can be essentially different from asymptotic long-time results occurring at $t_c >> t_{spr}$.

To find the average angle of scattering, let us use the following two-step procedure. First, let us average the well-defined quantum-mechanical operator $\hat{p}_x$ over the wave function Ψ ($\boldsymbol{r}$, t). The x–axis is assumed to be lying in the ($\boldsymbol{p}_0$, $\boldsymbol{r}_0$) plane perpendicular to $\boldsymbol{p}_0$ (directed along the z-axis). For spherically symmetric potentials $U(r)$, ($\boldsymbol{p}_0$, $\boldsymbol{r}_0$) is the scattering plane, i.e., the average transverse momentum $\overline{p}_y = 0$, where 0y is the third Cartesian axis perpendicular to both 0x and 0z. In terms of the probability amplitudes $C_{\boldsymbol{p}}(t)$, $\overline{p}_x$ is given by

$$\overline{p_x}(\rho) = \int p_x \left| C_{\boldsymbol{p}}(t) \right|^2 \frac{d\boldsymbol{p}}{(2\pi\hbar)^3}. \tag{10}$$

The ρ-dependent average angle of scattering $\overline{\theta}$ is determined as

$$\overline{\theta}(\rho) = \sin^{-1}\left(\frac{\left| \overline{p_x}(\rho) \right|}{p_0} \right) \approx \frac{\left| \overline{p_x}(\rho) \right|}{p_0}. \tag{11}$$

$\overline{\theta}(\rho)$ is the analogue of the classical angle of scattering [5] for an individual electron-atom pair of interacting objects.

By substituting into Eq. (10) the probability amplitude $C_p(t)$ (7), we get the first-order average angle of scattering of a wave packet by a single atom

$$\begin{aligned} \overline{\theta}^{(1)} &= \frac{1}{p_0} \left| \int p_x \left(C_{\boldsymbol{p}}^{(0)} C_{\boldsymbol{p}}^{(1)*} + C_{\boldsymbol{p}}^{(1)} C_{\boldsymbol{p}}^{(0)*} \right) \frac{d\boldsymbol{p}}{(2\pi\hbar)^3} \right| = \\ &= \frac{1}{\pi^{3/2} p_0} \left| \int_0^t dt' \frac{1}{[\Delta r(t')]^3} \int d\boldsymbol{r}\, \frac{\partial U}{\partial x} \exp\left\{ -\frac{(\boldsymbol{r} - \boldsymbol{r}_0 - \boldsymbol{v}_0 t')^2}{[\Delta r(t')]^2} \right\} \right|. \end{aligned} \tag{12}$$

#4586 - $15.00 US Received March 02, 1998; Revised April 28, 1998

This expression can be reduced to the "classical-like" form [3] with the effective potential U_{eff}

$$\bar{\theta}^{(1)} = \frac{1}{p_0}\left|\int_0^t dt'\left[\frac{\partial}{\partial x}U_{eff}(\boldsymbol{r},t')\right]_{\boldsymbol{r}=\boldsymbol{r}_0+\boldsymbol{v}_0t'}\right|. \tag{13}$$

The effective potential $U_{eff}(\boldsymbol{r}, t)$ is determined as [6]

$$U_{eff}(\boldsymbol{r},t) = \int d\boldsymbol{r}' U(\boldsymbol{r}+\boldsymbol{r}')\left|\Psi^{(0)}_{c.m.}(\boldsymbol{r}',t)\right|^2, \tag{14}$$

where $\left|\Psi^{(0)}_{c.m.}(\boldsymbol{r}',t)\right|^2$ is the squared absolute value of the zero-order electron wave function of the wave packet in its own center-of-mass frame

$$\left|\Psi^{(0)}_{c.m.}(\boldsymbol{r},t)\right|^2 = \frac{1}{\pi^{3/2}[\Delta r(t)]^3}\exp\left[-\frac{r^2}{[\Delta r(t)]^2}\right]. \tag{15}$$

Eq. (13) looks very similar to the classical angle of scattering, found in the approximation of small deviations [3]. Except for the replacement of $U(r)$ by $U_{eff}(\boldsymbol{r}, t)$, the only other difference between Eqs. (13) and the classical one concerns the limits of integration over t' : 0 and t instead of $-\infty$ and $+\infty$. But, as we assume that $t' = 0$ and $t' = t$ correspond to, respectively, some instants of time long before and long after scattering, these limits can be substituted by $-\infty$ and $+\infty$ to reduce formally Eq. (13) to the form of the classical expression. But of course, in fact, there is no complete identity between Eqs. (13) and the classical expression, and the difference between them is concentrated in the difference between $U(r)$ by $U_{eff}(\boldsymbol{r}, t)$. It should be noted that the effective potential identical to that of Eq. (14) has been introduced earlier in theory of atomic emission in a very strong laser field in the so-called Barrier-Suppression Wave-Packet-Spreading regime of ionization [6]. An origin of the effective potential has rather simple reasons and qualitative explanation. In the wave-packet state, the electron charge-density is spread around its "center of mass" in accordance with the distribution law $\left|\Psi^{(0)}_{c.m.}(\boldsymbol{r},t)\right|^2$ (15). If such a "charged cloud" interacts with other dot-like charges located at some point $\boldsymbol{r}'$, the total interaction energy is given by a sum (integral) of contributions from all the parts of the "electron cloud" [$U(\boldsymbol{r} - \boldsymbol{r}')$] with the weight function $\left|\Psi^{(0)}_{c.m.}(\boldsymbol{r},t)\right|^2$, in accordance with the definition (14). For the specific case of a pure Coulomb potential $U_C(r)=-\alpha/r$, the effective potential is known [6] to have the form

$$U_{eff}(r,t) = -\frac{\alpha}{r}\,\mathrm{Erf}\left(\frac{r}{\Delta r(t)}\right), \tag{16}$$

where Erf denotes the error function [7]. As at large arguments the error function approaches one, at large distances, $r >> \Delta r(t)$, the effective potential of Eq.(16) coincides with the Coulomb potential, $U_{eff}(\boldsymbol{r}, t) \approx -\alpha/r$. At small arguments, $x << 1$, $\mathrm{Erf}(x) \approx 2x/\sqrt{\pi}$ and, hence, at small distances, $r << \Delta r(t)$, $U_{eff}(\boldsymbol{r}, t)$ (15) approaches

$$U_{eff}(0,t) = -\frac{2\alpha}{\sqrt{\pi}\,\Delta r(t)}. \tag{17}$$

In contrast to the Coulomb potential, the effective potential $U_{eff}(\boldsymbol{r}, t)$ has no singularity at $r=0$ [6]. It is worth noticing that for an infinitely extended wave packet ($\Delta r \to \infty$), the effective potential $U_{eff}(\boldsymbol{r}, t)$ (16) turns zero identically. In the case of a pure Coulomb potential

#4586 - $15.00 US Received March 02, 1998; Revised April 28, 1998

$U_C(r)=-\alpha/r$, the effective potential $U_{eff}(r)$ is given by Eq. (16). With this effective potential and in the approximation of a non-spreading wave packet, $\Delta r(t) \approx \Delta r_0$, the final result appears to be given by a very simple and nice formula:

$$\bar{\theta}^{(1)} = \theta_{cl}^{(1)}\left[1-\exp\left(-\frac{\rho^2}{\Delta r_0^2}\right)\right], \tag{18}$$

where $\theta_{cl}^{(1)} = 2\alpha/\left(mv_0^2\rho\right)$ is the angle of scattering calculated from the classical theory and for the Coulomb potential.

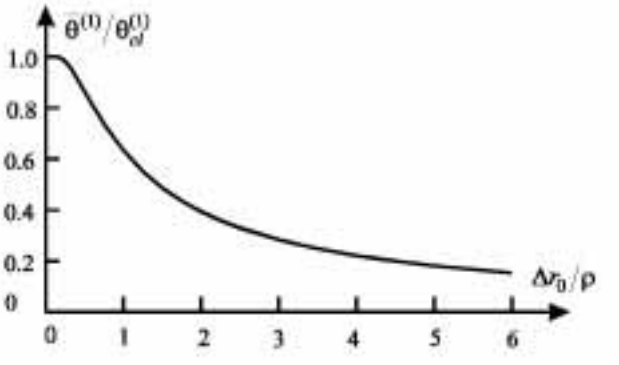

Fig 1. The first-order angle of scattering $\bar{\theta}^{(1)}(\Delta r_0)$ of the Gaussian wave packet scattered by a pure Coulomb potential.

In the limit of a narrow wave packet, $\Delta r_0 << \rho$, $\bar{\theta}^{(1)} = \theta_{cl}^{(1)}$. Appositely, in the limit of a very wide wave packet, $\Delta r_0 >> \rho$, the first-order quantum-mechanical angle of scattering quantum-mechanical angle of scattering $\bar{\theta}^{(1)}$ (18) falls as $1/\Delta r_0^2$:

$$\bar{\theta}^{(1)}\Big|_{\Delta r_0>>\rho} \approx \frac{\rho^2}{\Delta r_0^2}\,\theta_{cl}^{(1)}. \tag{19}$$

In the case of a short-range potential $U(r)$, the first-order angle of scattering can be shown to be independent of Δr_0 at small Δr_0 ($\Delta r_0 << d$, ρ) and coinciding with the corresponding classical expressions. In the limit of a large width of the wave packet, $\Delta r_0 >> \rho$ and $\Delta r_0 >> d$ (where d is the atomic size), the exponential factor on the right-hand side of Eq. (12) can be approximated by one to give

$$\bar{\theta}^{(1)}\Big|_{\Delta r_0>>\rho,\,d} = -\frac{8\rho}{mv_0^2\Delta r_0^4}\int_0^\infty r^2 dr\, U(r). \tag{20}$$

Eq. (20) shows that in the wide-packet limit, the first-order average angle of scattering as a function of Δr_0 falls as $1/\Delta r_0^4$, i.e., much faster than in the case of a pure Coulomb potential

$$\bar{\theta}^{(1)}\Big|_{\Delta r_0>>\rho,\,d} = \frac{8\alpha\rho\, d^2}{m\,v_0^2\Delta r_0^4} = \left(\frac{2\rho d}{\Delta r_0^2}\right)^2\theta_{cl}^{(1)}. \tag{21}$$

It should be noted that, whereas the general equations (12) and (13) for $\bar{\theta}^{(1)}$ are valid at any Δr_0, the specific results of Eqs. (18)-(21) are derived under the assumption of a non-spreading wave packet, $\Delta r(t) \approx \Delta r_0$. This assumption can be reformulated as the condition

#4586 - $15.00 US
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that the spreading time t_{spr} (9) is much longer than the time of scattering (interaction), t_{int}. The latter, for a short-range potential can be estimated as d/v_0 to give

$$t_{spr} >> t_{int} = \frac{md}{p_0}. \tag{22}$$

Both assumptions, $\Delta r_0 << d$ and $t_{spr} >> t_{int}$, can be rewritten in the form of the inequalities

$$(\lambda\!\!\!^{-}_{dB} d)^{1/2} << \Delta r_0 << d, \tag{23}$$

where $\lambda\!\!\!^{-}_{dB} = \hbar/mv_0$ is De-Broglie wavelength of an electron. These are the conditions under which the quantum-mechanical expression for the first-order angle of scattering $\bar{\theta}^{(1)}$ [(13) and (18)] coincide exactly with the corresponding classical expressions. For the long-range Coulomb potential, the quantum-mechanical expression for the ρ-dependent first-order angle of scattering (18) coincides with the classical one as long as $\Delta r_0 << \rho$. In this case the effective interaction time can be determined as ρ/v_0. The substitution of d by ρ in inequalities (23) determines the conditions under which spreading of the wave packet can be ignored and the wave packet itself can be considered as a narrow one for scattering by the long-range Coulomb potential:

$$(\lambda\!\!\!^{-}_{dB} \rho)^{1/2} << \Delta r_0 << \rho, \tag{24}$$

3. Discussion

It should be noted, that for the electron-atom scattering, probably, classical effects of the first-order in U are hardly observable, because it's rather difficult to construct a well localized and long-living electron wave packet with a size smaller than an atomic size. Such a wave packet would spread during a very short time on the order of the atomic time (~ 10^{-16} s). Vice-versa, in the case of scattering from a focused light field, such a situation is quite realistic, because the focal size is usually much larger than the atomic radius. For instance, for electrons with $v_0 \sim 10^8$ cm/s and for the focal waist $d \sim 10^{-2}$ cm, inequalities (24) give

$$10^{-2}\,\text{cm} << \Delta r_0 << 10^{-5}\,\text{cm}. \tag{25}$$

In principle, creation and control of such wave packets are realizable with the help of modern experimental techniques. For example, electron wave packets can be produced in a controllable way be means of photoionization or multiphoton ionization of atoms by a laser field. In the case of a not too strong laser field and short pulses, the energy width of wave packets is expected to be of the order of the inverse pulse duration τ, $\Delta E \sim 1/\tau$, whereas the mean energy is on the order of the light frequency ω. This corresponds to the uncertainty of the electron momentum $\Delta p \sim \tau^{-1} \omega^{-1/2}$ and the width of a packet in space $\Delta r \sim \tau \omega^{1/2}$. E.g., for $\omega \sim 0.1$ and $\tau \sim 10^5$ (~ 30 ps) we get $\Delta r \sim 10^5$ in atomic units or $\Delta r \sim 10^{-3}$ cm. This size falls into the range of parameters determined by inequalities (24). The spreading time of such a packet is of the order of 10^{-6} s. During this time an electron with a speed $v \sim \omega^{1/2} \sim 10^8$ cm/s crosses a very large distance about 1 m. A scheme of an experiment for observing scattering of wave packets by a focused light field can be similar to the well-known experiment [2] with two laser foci. In this experiment, electrons produced in one of the foci were scattered by the second one and the energy distribution of scattered electrons was investigated. Under similar conditions, by measuring the average angle of scattering for different relations between Δr_0 and the focal waist d, one has to find a big difference between the cases $\Delta r_0 < d$ and $\Delta r_0 > d$. A much larger classical angle of scattering has to be observed in the first of these two cases. Transition from the case $\Delta r_0 < d$ to $\Delta r_0 > d$ can be provided

#4586 - $15.00 US Received March 02, 1998; Revised April 28, 1998

either by changing the conditions of focusing in the second focus or by changing the pulse duration of the first laser, which is supposed to ionize atoms and to produce wave packets.

In addition to explanations given above, it may be reasonable to mention an alternative interpretation of the results derived. According to this interpretation, the non-zero first-order term $\bar{\theta}^{(1)} \neq 0$ (12) in the perturbation-theory expansion of the average angle of scattering arises owing to interference between the incoming and scattered parts of the wave function. Such interference exists only in the transient case when the initial size of the wave packet Δr_0 is much smaller than the size of a target d and the wave-packet spreading time is much longer than the time it takes for the scattered electron to reach the detector. These results can be essentially different from the asymptotic infinitely-long-time results. In terms of the interference interpretation, it is clear why $\bar{\theta}^{(1)}$ vanishes in the plane-wave limit. In this case simply there is nothing to interfere with for partial plane waves scattered at any non-zero angle with respect to the incident plane wave. To formulate explicitly the interference interpretation of the results described one has to investigate the structure of the wave function after scattering under these or other assumptions about its initial size, time of scattering, distance from the atom after scattering, etc.

The results obtained indicate a significant difference between two cases, which sometimes are referred to as equivalent ones: scattering of a stream of well-localized particles, which are incoherent to each other, and scattering of a particle, which has the wave function close to a single plane wave. According to our results, the average angle of scattering in these two cases is given either by the classical expression, or by the well-known result derived in the first Born approximation of the traditional quantum-mechanical theory of scattering, respectively.

It should be noted, finally, that the problem discussed can be related to even much more general and fundamental features of particles in beams. Indeed, practically under any conditions electrons have some degree of localization determined by the size of the their wave functions (wave packets). This is a quantum mechanical size, hardly recognizable in the routine experiments. In particular, in the case of electron beams, produced by electron guns, the only size, which is usually measured and mentioned, is the transverse size of the beam. The above-discussed quantum-mechanical size of electrons can be either equal or much smaller than the size of the beam. The quantum-mechanical size of wave packets remains a hidden parameter of electrons hardly ever seen and discussed. In our opinion, scattering of electrons by ponderomotive potentials of focused lasers and measuring, e.g., the verage angle of scattering can be used to measure the above-discussed quantum-mechanical size of electrons and to make conclusions on the size of the wave packets describing electrons in beams.

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