Initial wave packets and the various power-law decreases of scattered wave packets at long times

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The long time behavior of scattered wave packets $\psi(x, t)$ from a finite-range potential is investigated, by assuming $\psi(x, t)$ to be initially located outside the potential. It is then shown that $\psi(x, t)$ can asymptotically decrease in the various power laws at long time, according to its initial characteristics at small momentum. As an application, we consider the square-barrier potential system and demonstrate that $\psi(x, t)$ exhibits the asymptotic behavior $t^{-3/2}$, while another behavior like $t^{-5/2}$ can also appear for another $\psi(x, t)$.

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A long time deviation from the exponential decay law is predicted in unstable quantum systems such as an $\alpha$-decaying nucleus [1]. These systems are often modeled in the systems of a particle in a short range potential. In this approach, a nonexponential decay is generally found to follow a particular power law, $t^{-3/2}$ (see, e.g., Refs. 2, 3, 4, 5). On the contrary to the theoretical results, an experimental evidence still has not been discovered [6], which requires us to reexamine such a nonexponentially decaying behavior from every aspect. As far as the author knows, conventional studies are developed without taking into account of the characteristics of the initial wave packets. A consideration for them may lead to a discovery of other aspects of the subjects. Indeed, as for the free particle system, the various power decreases of wave packets, not restricted to $t^{-3/2}$, have recently been demonstrated and shown to be characterized by the behavior of initial wave packets at small momentum [7, 8, 9, 10].

In this paper, we analytically prove that the wave packet $\psi(x, t)$ scattered from a finite-range potential can asymptotically behave like $t^{-3/2}$ at long times, where $j = 1, 2, \ldots$. By making an assumption that the $\psi(x, t)$ is initially located outside the potential, these various power behaviors can be characterized by the initial characteristics of the $\psi(x, t)$ at small momentum, like for the free particle case [8, 9, 10]. The validity of our analysis is numerically confirmed, through the application to the system with a square barrier potential.

For a one-dimensional system with a potential $V(x)$, the Hamiltonian $H$ is defined as $H \equiv H_0 + V$, where $H_0 \equiv -(h^2/2M)d^2/dx^2$ being the free Hamiltonian. For simplicity, we use the unit such that $h = 1$ and $2M = 1$ throughout the paper. Although we confine ourselves to the one dimensional case, the following discussion can be extended to that in an arbitrary dimension in principle. The potential $V(x)$ is assumed to have a finite-range, i.e.,

$$V(x) = 0 \quad \text{for} \ |x| > R, \quad (1)$$

for a positive number $R$. We only consider the systems without bound states. This restriction however is easily moderated. By using the eigenfunction expansion, the wave packet $\psi(x, t)$, evolving from the initial state (wave packet) $\psi(x)$, is expressed as

$$\psi(x, t) = (e^{-itH}\psi)(x) = \int_{-\infty}^{\infty} e^{-it\tilde{E}} \varphi(x, \tilde{E}) \tilde{\psi}(\tilde{E}) d\tilde{E}, \quad (2)$$

where the $\tilde{\psi}(\tilde{E})$, determining the initial energy-distribution, is defined by

$$\tilde{\psi}(\tilde{E}) \equiv \int_{-\infty}^{\infty} \varphi^*(y, k) \psi(y) dy. \quad (3)$$

The functions $\varphi(x, k)$ ($k \in \mathbb{R} \setminus \{0\}$) are stationary scattering solutions of the time-independent Schrödinger equation,

$$[H_0 + V] \varphi(x, k) = k^2 \varphi(x, k). \quad (4)$$

More precisely, they must satisfy the Lippmann-Schwinger equations in one dimension [11],

$$\varphi(x, k) = \frac{e^{ikx}}{\sqrt{2\pi}} + \frac{1}{2i|k|} \int_{-\infty}^{\infty} e^{\pi|k||x-y|} V(y) \varphi(y, k) dy. \quad (5)$$

Either solution of the above equation with (+) or (−) sign is accepted for $\varphi(x, k)$ in Eq. (9). Notice that, being integral equations, the Lippmann-Schwinger equations already incorporate the boundary conditions, unlike Eq. (4). We here choose the equation with (+) sign. Then, $\varphi(x, k)$ for positive $k$ and for negative $k$ are solutions of Eq. (4) to the cases of an incident plane wave from the left and from the right of the potential, respectively.

We first derive an asymptotic expansion of $\psi(x, t)$ at long times. The integral in Eq. (2) is changed to a Fourier-integral form over the energy variable $E = k^2$, i.e.,

$$\psi(x, t) = \frac{1}{2} \sum_{\sigma = \pm} \int_{0}^{\infty} E^{-1/2} \mathcal{F}_\sigma(x, E) e^{-itE} dE, \quad (6)$$

where $\mathcal{F}_\sigma(x, E)$ is a Fourier transform of $\varphi(x, \tilde{E})$, with

$$\mathcal{F}_\sigma(x, E) = \int_{-\infty}^{\infty} e^{i\sigma kx} \varphi(x, k) \tilde{\psi}(\tilde{E}) d\tilde{E}.$$
where $F_\pm(x, E) \equiv \varphi(x, \pm E^{1/2}) \tilde{\psi}(\pm E^{1/2})$. We may decompose $F_\pm(x, E)$ into the following forms,

$$F_\pm(x, E) = \pm E^{1/2} O_\pm(x, E) + E_\pm(x, E),$$  

where

$$O_\pm(x, E) = \sum_{r+s=\text{odd}} \frac{E^{(r+s-1)/2}}{r!s!} \partial_k^r \varphi(x, \pm 0) \tilde{\psi}(s)(\pm 0),$$  

as $E \to 0$. Both $\varphi(x, k)$ and $\tilde{\psi}(k)$ are assumed to be differentiable with respect to $k$ without the origin. Furthermore, we have used the notations $\partial_k^r \varphi(x, \pm 0) \equiv \lim_{k\to\pm 0} \partial_k^r \varphi(x, k)/\partial k^n$, and for any function of $k$, say, $f(k, f^{(n)}(\pm 0) \equiv \lim_{k\to\pm 0} \partial_k^n f(k)/\partial k^n$. Note that by setting $E \to 0$ into Eq. (9), $O_\pm(x, E)$ makes no singularity at $E = 0$ while $E^{-1/2} E_\pm(x, E)$ does not necessarily. Then, in taking such a singularity into account, the asymptotic form of the Fourier integral (9) may read formally as

$$\psi(x, x, t) \sim \frac{1}{2} \sum_{j=0}^{\infty} \frac{1}{(it+j+1)!} \sum_{\sigma = \pm} \sigma \partial_k E \varphi(x, \pm 0)$$

$$+ \frac{1}{2} \sum_{j=0}^{\infty} \frac{\Gamma(j+1/2)}{(jt+j+1/2) \sum_{\sigma = \pm} \partial_k E \varphi(x, \pm 0)},$$  

as $t \to \infty$, where $\lim_{E \to 0} \partial_k E \varphi(x, E) = 0$ and $\lim_{E \to \infty} \partial_k E \varphi(x, E) = 0$ were assumed. It is noted that we could also obtain the expansion [11] by different methods (see, Refs. [2, 3, 4, 5] and references therein).

As same as the results in Refs. [6, 7, 8, 9, 10, 12], we can expect from Eq. (10) that by specifying the low-energy behaviors of both $O_\pm(x, E)$ and $E_\pm(x, E)$ appropriately, $\psi(x, t)$ can asymptotically show the various power-decreases. This situation may be realized by such an initial wave packet $\psi(x)$ that satisfies

$$\tilde{\psi}^{(n)}(\pm 0) = 0 \quad \text{for } n = 0, 1, \ldots, m - 1,$$

with a certain integer $m$. In fact, let us first consider the case of $m$ being an even number given by $m = 2m_0$. In this case, $O_\pm(x, E)$ and $E_\pm(x, E)$ read

$$O_\pm(x, E) = E^{m/2} \varphi(x, \pm 0) \tilde{\psi}^{(m)}(\pm 0) + O(E^{(m+2)/2}),$$

$$E_\pm(x, E) = \frac{E^{m/2}}{m!} \varphi(x, \pm 0) \tilde{\psi}^{(m)}(\pm 0) + O(E^{(m+2)/2}),$$

as $E \to 0$, respectively. Then, substituting them into Eq. (10) leads to an expected result that

$$\psi(x, t) \sim \frac{1}{2} \sum_{j=0}^{\infty} \frac{1}{(it+j+1)!} \sum_{\sigma = \pm} \sigma \partial_k E \varphi(x, \pm 0)$$

$$+ \frac{1}{2} \sum_{j=0}^{\infty} \frac{\Gamma(j+1/2)}{(jt+j+1/2) \sum_{\sigma = \pm} \partial_k E \varphi(x, \pm 0)},$$

as $E \to 0$. Inserting them into Eq. (10) again, we obtain

$$\psi(x, t) \sim \frac{1}{2} \sum_{j=0}^{\infty} \frac{1}{(it+j+1)!} \sum_{\sigma = \pm} \sigma \partial_k E \varphi(x, \pm 0)$$

$$+ \frac{1}{2} \sum_{j=0}^{\infty} \frac{\Gamma(j+1/2)}{(jt+j+1/2) \sum_{\sigma = \pm} \partial_k E \varphi(x, \pm 0)},$$

as $E \to 0$. We have to give such initial wave packets $\psi(x)$ satisfying the formal condition [11]. Then, it seems practically advantageous to rewrite this condition in terms of the initial wave packet $\tilde{\psi}(k)$ in momentum (or $H_0$) representation. This can be achieved by assuming the $\psi(x)$ to be located in the left of the scattering potential $V(x)$, i.e.,

$$\psi(x) = 0 \quad \text{for } x \geq -R.$$  

This assumption will however be relaxed to that $\psi(x) = 0$ for $|x| \leq R$, in the discussions below. From the assumption [13], the $\tilde{\psi}(k)$ is expressed by the integral over the truncated interval ($-\infty, -R$),

$$\tilde{\psi}(k) = \int_{-\infty}^{-R} e^{-iky} \psi(y)dy = \int_{-\infty}^{-R} \frac{e^{-iky}}{\sqrt{2\pi}} \psi(y)dy.$$  

Meanwhile, the assumption [11] implies that $\varphi(x, k)$ for $x < -R$ is written by a superposition of plane waves

$$\varphi(x, k) = [g_+(k)e^{ik|x|} + g_-(k)e^{-ik|x|}] \sqrt{2\pi}.$$

Since we adopt Eq. (5) with (+) sign, we see that $g_+(k) = 1$ for $k > 0$ and 0 for $k < 0$. Substituting Eqs. [13] and [14] into Eq. (12), we obtain

$$\psi(x, t) \sim \frac{1}{2} \sum_{j=0}^{\infty} \frac{1}{(it+j+1)!} \sum_{\sigma = \pm} \sigma \partial_k E \varphi(x, \pm 0)$$

$$+ \frac{1}{2} \sum_{j=0}^{\infty} \frac{\Gamma(j+1/2)}{(jt+j+1/2) \sum_{\sigma = \pm} \partial_k E \varphi(x, \pm 0)}.$$
We obtain a desirable expression for \( \tilde{\psi}^{(n)}(\sigma) \) as a linear combination of \( \tilde{\psi}^{(l)}(\pm 0) \)'s,

\[
\tilde{\psi}^{(n)}(\sigma) = (\sigma 1)^n \delta_{\pm, \sigma} \tilde{\psi}^{(n)}(+0) + \sum_{l=0}^n \left( \begin{array}{c} n  \\ l \end{array} \right) (-\sigma 1)^{n-l} \tilde{\psi}^{(l)}(-0),
\]

where \( \sigma 0 \) stands for the limit symbol +0 or -0 for \( \sigma = + \) or - , respectively, and \( \delta_{\pm, \sigma} \) denotes Kronecker’s delta.

From this, one might expect that the condition (11) at low energy, which determines the asymptotic forms (14) and (17) with Eq. (21), by applying it to the system with the square barrier potential (2).

This condition indeed implies the condition (11). However, the converse does not necessarily hold. This incompatibility comes from the actual behavior of \( g^{-(n-l)}(\pm 0) \)'s.

Let us now demonstrate the asymptotic formulas (14) and (17) with Eq. (21), by applying it to the system with the square barrier potential \( V(x) \) given by Eq. (1) and

\[
V(x) = V_0 \quad \text{for } |x| \leq R,
\]

where \( V_0 (>0) \) is the height of the potential barrier. For this system, \( g_{-(k)} \) in Eq. (20) is given by (see, e.g., (13))

\[
g_{-(k)} = \begin{cases} \frac{\rho^2 + k^2}{2ik\rho} g(k) \sinh 2\rho R & \text{for } 0 < k < k_b \\ g(-k) & \text{for } -k_b < k < 0 \end{cases}
\]

where \( k_b = V_0^{1/2}, \rho = [k_b^2 - k^2]^{1/2} \), and

\[
g(k) \equiv \left[ \cosh 2\rho R + \frac{k^2 - \rho^2}{2ik\rho} \sinh 2\rho R \right]^{-1} e^{-2ikR}.
\]

The \( g(k) \) has the remarkable properties: \( \lim_{k \to 0} g(k) = 0 \) and \( \lim_{k \to \infty} g(\sigma k)/k = \sigma 2/(ik_b \sinh 2k_b R) \), to give

\[
g_{-(+0)} = -1, \quad g_{-(0)} = 0.
\]

This implies that incident plane waves with vanishing energy are totally reflected by the barrier. Since the \( \varphi(x, k) \) is continuous even at the barrier, we consequently see that

\[
\varphi(x, \pm 0) = 0 \quad \text{for } x \in \mathbb{R}.
\]

This is just the case without the zero-energy resonance (10). It is worth noting that if we assume that the initial wave packet \( \psi(x) \) is absolutely integrable, Lebesgue’s dominated convergence theorem leads to

\[
\tilde{\psi}(\pm0) = \int_{-\infty}^{\infty} \varphi^*(y, \pm0) \psi(y) dy = 0.
\]

Hence the condition (11) for \( m = 1 \) can be always satisfied for this system. This result implies the use of Eq. (17) with \( \overline{m} = 1 \), which leads to an estimation such that \( \psi(x, t) \) behaves as \( t^{-3/2} \), i.e.,

\[
\psi(x, t) \sim \frac{1}{2} \sqrt{\frac{3}{2\pi t}} e^{-\frac{x^2}{4t}}.
\]

However, the determination of the asymptotic behavior of \( \psi(x, t) \) may also need a consideration to the concrete behavior of the \( \psi(x) \). For definiteness, we here confine ourselves to deriving the behavior like \( t^{-5/2} \), and assume that the \( \psi(x) \) satisfies Eq. (13) and has a continuity at zero momentum:

\[
\tilde{\psi}^{(n)}(+0) = \tilde{\psi}^{(n)}(-0) \quad \text{for } n = 0, 1, 2, 3.
\]

This allows us to represent both \( \tilde{\psi}^{(n)}(+0) \) and \( \tilde{\psi}^{(n)}(-0) \) by the same symbol \( \tilde{\psi}^{(n)}(0) \). In this case, substitution of Eqs. (20) and (28) into (21) leads to a simple expression for \( \tilde{\psi}^{(1)}(0) \):

\[
\tilde{\psi}^{(1)}(0) = \tilde{\psi}^{(1)}(0) + 2\delta_{+, \sigma} \tilde{\psi}^{(1)}(0),
\]

where \( \tilde{\psi}^{(1)}(0) \) are straightforwardly evaluated as

\[
g_{-(+0)} = 2iR + 2(\cosh 2k_b R)/(ik_b \sinh 2k_b R), \quad g_{-(0)} = -2/(ik_b \sinh 2k_b R)
\]

Equation (11) implies the fact that if \( \psi(x) \) satisfies the condition (11) for \( m = 2 \), i.e.,

\[
\tilde{\psi}(0) = 0 \quad \text{and} \quad \tilde{\psi}^{(1)}(0) = 0,
\]

then, \( \tilde{\psi}^{(1)}(0) = 0 \) and the formula (20) is no longer effective. Note that this does not immediately mean the case of \( m = 2 \) in the condition (11) realized. Because, as is pointed out after Eq. (22), the system’s properties with Eqs. (30) and (34) causes \( \tilde{\psi}^{(2)}(0) = 0 \), even if \( \tilde{\psi}^{(2)}(0) \neq 0. \) See Eq. (21). Therefore, we should actually refer to the case of \( m = 3 \) in the condition (11). This time, the formula (17) (with \( \overline{m} = 2 \)) is used again to read

\[
\psi(x, t) \sim \frac{1}{2} \sqrt{\frac{5}{6\pi t^{5/2}}} \sum_{\sigma = \pm} \partial_\sigma \varphi(x, \sigma 0) \tilde{\psi}^{(3)}(\sigma 0).
\]

In this case, \( \tilde{\psi}^{(3)}(0) = 3g^{-(1)}(0) \tilde{\psi}^{(2)}(0) + 2\delta_{+, \sigma} \tilde{\psi}^{(3)}(0) \).

In order to illustrate the above analysis, we consider the long-time behavior of the nonescape probability \( P(t) \)

\[
P(t) = \int_a^b |\psi(x, t)|^2 dx,
\]

instead of \( \psi(x, t) \) itself. This is the probability of finding a particle, initially prepared in state \( \psi \), in a bounded interval \( I = [a, b] \) at a later time \( t \). By substituting Eq. (14) or (17) into the definition (30), the asymptotic behavior of \( P(t) \) directly reflects that of \( \psi(x, t) \). We have
FIG. 1: Nonescape probabilities $P(t)$’s for initial wave packets $\psi = \phi_0, \phi_1$, and $\phi_2$ and their asymptotes predicted by Eq. (29) or (35) (solid lines). For $\phi_0$ and $\phi_1$, $P(t)$ shows the well-known $t^{-2}$ behavior at long times (long-dashed and short-dashed lines), whereas $P(t)$ for $\phi_2$ exhibits another power-law behavior like $t^{-5}$ (a dotted-line).

restrict ourselves to the three wave packets $\phi_0(x), \phi_1(x),$ and $\phi_2(x)$, as the initial wave packets $\psi(x)$:

$$\hat{\phi}_m(k) = N_m k^m e^{-a_0^2(k-k_0)^2/2-ikx_0},$$

(37)

where $m = 0, 1, 2$, $a_0 > 0$, $k_0, x_0 \in \mathbb{R}$, and $N_m$ being the normalization constants. Note that the parameters $a_0$ and $x_0$ roughly indicate the width and the location of $\hat{\phi}_m(x)$, respectively. These wave packets are rapidly-decaying functions and satisfy the regularity (30). Both $\phi_0(x)$ and $\phi_1(x)$ are chosen to confirm the asymptotic formula (35), while $\phi_2(x)$ satisfies the assumption (31) to realize the asymptotic formula (35). These wave packets do not satisfy the assumption (15). This situation however could be taken into account. In fact, if we take appropriate parameters $a_0$ and $x_0$ where the latter satisfies $|x_0| = -x_0 >> R$, the errors in $\hat{\phi}_m^0(\pm 0)$’s might be negligibly small (17).

Figure 1 shows the time evolution of $P(t)$, and the asymptotes predicted by Eq. (29) or (35), for the three initial wave packets $\phi_0(x), \phi_1(x)$, and $\phi_2(x)$. In our calculation, we have chosen a set of parameters $a_0 = 1.0, k_0 = 1.0$, and $x_0 = -20.0$ for the three initial wave packets. Then, every average momentum in these initial states is positive. We have also chosen in all these cases the potential range $R = 1.0$, which is much smaller than the location $|x_0| = 20.0$, and height $V_0 = 16.0$, which is greater than the expectation value of energy $\langle \phi_m, H_0 \phi_m \rangle$. The interval $I = [a, b]$ for the nescence probability is set around the initial location of the wave packet $x_0$, and we set $a = -22.0$ and $b = -18.0$. One may recognize three different regions in the figure: for small $t$, all $P(t)$’s decrease smoothly, and then, they partially revive before decreasing again. These regions reflect the motion of a wave packet, i.e., it leaves the interval $I$ for the barrier, returns to the interval after a collision with the barrier, and goes outside through the interval, respectively (18). It is clearly seen that, in the last region, $P(t)$’s for initial wave packets $\phi_0$ and $\phi_1$ approach to the asymptote parallel to the well-known $t^{-3}$. On the other hand, the behavior of $P(t)$ for the initial state $\phi_2$ is in quite agreement with the asymptote parallel to $t^{-5}$, other than $t^{-3}$.

To summarize, we have considered the finite-range potential-systems for one dimension and explicitly characterized the various power decreasing behaviors of the scattered wave-packets at long times, in terms of their position and momentum behavior at an initial time. Our results can also cover the free case of Refs. (4) (10) and that of Refs. (2) (3) with a slight modification. The power-law decrease of the potential systems at long times still has not been observed experimentally, however it may exhibit an interesting phenomenon, involving a peculiar structure where the characteristics of the initial state play a crucial role.

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We can find the wave packets that satisfy the assumptions (18) and (22) simultaneously, in \( C^\infty_0 \)-functions, e.g., \((m-1)\)-th derivative of the function defined by 
\[ \psi(x) = \exp\left[ -a_0^2 / \left[ d^2 - (x - x_0)^2 \right] \right] \] 
for \(|x - x_0| < d\) or 0 otherwise, where \(a_0 > 0\), \(d > 0\), \(x_0 < 0\), and \(x_0 + d < -R\).

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The errors for \( \phi_2 \) seem considerable, to make a small but non-vanishing coefficient of \( t^{-3/2} \) in the asymptotic expansion of \( \phi_2(x,t) \), unsuitably for the expected behavior (35). However, \( \phi_2(x,t) \) may still follow Eq. (35) at long times, until the term proportional to \( t^{-3/2} \) dominates.

One may notice that the situation considered here is just the same as in Fig. 18 in the textbook [15].