

Free initial wave packets and the long-time behavior of the survival and nonescape probabilities

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The behavior of both the survival $S(t)$ and the nonescape $P(t)$ probabilities at long times for the one-dimensional free-particle system is shown to be closely connected to that of the initial wave packet at small momentum. We prove that both $S(t)$ and $P(t)$ asymptotically exhibit the same power-law decrease at long times, when the initial wave packet in momentum representation behaves as k^m with $m=0$ or 1 at small momentum. On the other hand, if the integer m becomes greater than 1, $S(t)$ and $P(t)$ decrease in different power laws at long times.

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The study of the space-time evolution of the wave packets is very significant for understanding the scattering phenomena and attracting many researchers in the various fields. It is then helpful to have the complete information about the free-particle system. For the one-dimensional case, if the Gaussian wave packet is chosen as the initial one, the wave packet $\psi(x,t)$ decreases asymptotically as $t^{-1/2}$ at long times. However, it has been recently found that the maximum of wave packet does not necessarily behave as $t^{-1/2}$ for non-Gaussian initial wave packet. In fact, a slower decrease than $t^{-1/2}$ can be found for the power-law tail wave packet [1–3], and a faster decrease than $t^{-1/2}$ can occur for the wave packet which vanishes at zero momentum [4]. These facts remind us of a naive question of how the characteristics of the initial wave packet affect the long-time behavior of the wave packet or related quantities such as the survival $S(t)$ and nonescape $P(t)$ probabilities. The former stands for the probability of a state still being in the initial state at a later time t . It is widely used for the decaying systems (see, e.g., Refs. [5–8], and references therein). The latter is the probability to find a particle in a specific region under consideration at a later time t . It is also used for the decaying systems (see, e.g., Refs. [7–10]). Such a question for $S(t)$ was answered in the following sense. For a one-dimensional free-particle system, it was shown that $S(t)$ behaves asymptotically like t^{-2m-1} , when the initial wave packet in momentum representation behaves like k^m near the zero momentum $k=0$ with an arbitrary nonnegative integer m [11]. Hence, as is pointed out in Ref. [4], the small-momentum behavior of initial wave packet plays a crucial role in determining the long-time behavior of the survival probability. However, such strict structures for the wave packet and the nonescape probability have not been clarified completely.

In this work, we consider the asymptotic behavior of a free wave packet $\psi(x,t)$ at long times for the one-dimensional case, assuming as in Ref. [11] that the initial wave packet behaves like k^m at small momentum. The asymptotic behavior is evaluated at every position x unlike the studies in Refs. [1–4]. This advantage enables us to discuss whether the asymptotic behavior of the wave packet has the position dependence. In addition, we are able to calculate

explicitly the asymptotic form of not only $S(t)$ but also $P(t)$ at long times [12]. We then examine and clarify the difference between the long-time behaviors of the $S(t)$ and $P(t)$, according to the small-momentum behavior of the initial states. Remark that a comparison between the long-time behaviors of $S(t)$ and $P(t)$ was already made in Ref. [7] for the potential systems in another context, though the analysis therein was correct for $S(t)$, but not for $P(t)$. The correct result for $P(t)$ turned out to be the t^{-3} behavior (see, Ref. [13], and references therein).

For the one-dimensional free-particle system with the Hamiltonian $H_0 = -(\hbar^2/2M)d^2/dx^2$, we here define the survival probability $S(t)$ of the initial state (wave packet) ψ as

$$S(t) := |\langle \psi, e^{-itH_0/\hbar} \psi \rangle|^2 = \left| \int_{-\infty}^{\infty} \overline{\psi(x)} \psi(x,t) dx \right|^2, \quad (1)$$

where $\psi(x,t) = (e^{-itH_0/\hbar} \psi)(x)$ and the bar ($\bar{}$) denotes complex conjugate. $\psi(x)$ is assumed to be square integrable. $S(t)$ is the probability that the state at a later time t is found in the initial one. We also define the nonescape probability $P(t)$ as the probability that a particle initially prepared in the state ψ is found in a bounded interval $[a,b]$ on the line at a later time t :

$$P(t) := \int_a^b |\psi(x,t)|^2 dx. \quad (2)$$

In order to estimate the asymptotic behavior of $\psi(x,t)$, we first refer to the explicit solution to the Schrödinger equation,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} e^{-i\hbar k^2/2Mt} \hat{\psi}(k) dk, \quad (3)$$

$$= \left(\frac{M}{2\pi i \hbar t} \right)^{1/2} \int_{-\infty}^{\infty} e^{iM|x-y|^2/2\hbar t} \psi(y) dy, \quad (4)$$

where $k = p/\hbar$ and the $\hat{\psi}(k)$ is the initial state in momentum representation. To see the long-time behavior of the solution, one can consider the asymptotic expansion of the integral in

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Eq. (3), using the phase stationary method [14] as used in Ref. [2,4] or making an integration by parts for the Fourier integral [15]. Then the differential coefficients of $\hat{\psi}(k)$ at $k=0$ naturally appear. However, to take into account the x dependence in the asymptotic behavior of $\psi(x,t)$, it may be convenient for us to start with Eq. (4). Indeed, expansion of the exponential function in Eq. (4) immediately leads to the asymptotic behavior of $\psi(x,t)$ with the x dependence. It reads

$$\psi(x,t) \sim \sum_{j=0}^{\infty} \frac{(-1)^{j-1} \Gamma(j+1/2)}{\pi(i\hbar t/2M)^{j+1/2}} (G_{2j}\psi)(x), \quad (5)$$

where G_j is the integral operator [16] defined by

$$(G_j\psi)(x) := -\frac{1}{2(j!)} \int_{-\infty}^{\infty} |x-y|^j \psi(y) dy. \quad (6)$$

Here, we assume the exchange of the order of summation and integration to be allowed. Note that $(G_{2j}\psi)(x)$ in Eq. (5) can be described in terms of the differential coefficient of $\hat{\psi}(k)$ at $k=0$, similar to the result reached from Eq. (3). This is seen from the following formal expansion of $\hat{\psi}(k)$:

$$\begin{aligned} \hat{\psi}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-iky} \psi(y) dy \sim \sum_{j=0}^{\infty} \frac{(-ik)^j}{\sqrt{2\pi} j!} \int_{-\infty}^{\infty} y^j \psi(y) dy \\ &= \sum_{j=0}^{\infty} \frac{k^j}{j!} \hat{\psi}^{(j)}(0), \end{aligned} \quad (7)$$

where $\hat{\psi}^{(0)}(0) = \hat{\psi}(0)$. This implies that

$$\hat{\psi}^{(j)}(0) = \left. \frac{d^j \hat{\psi}(k)}{dk^j} \right|_{k=0} = \frac{(-i)^j}{\sqrt{2\pi}} \int_{-\infty}^{\infty} y^j \psi(y) dy. \quad (8)$$

Then, we can rewrite $(G_{2j}\psi)(x)$ in Eq. (6) for $j=2j$ as

$$(G_{2j}\psi)(x) = -\frac{\sqrt{2\pi}}{2[(2j)!]} \sum_{n=0}^{2j} \binom{2j}{n} i^n \hat{\psi}^{(n)}(0) (-x)^{2j-n}. \quad (9)$$

Substituting Eq. (5) into Eqs. (1) and (2), we can obtain the asymptotic behaviors of $S(t)$ and $P(t)$ at long times as

$$S(t) \sim \left| \sum_{j=0}^{\infty} \frac{(-1)^{j-1} \Gamma(j+1/2)}{\pi(i\hbar t/2M)^{j+1/2}} \langle \psi, G_{2j}\psi \rangle \right|^2, \quad (10)$$

and

$$P(t) \sim \int_a^b \left| \sum_{j=0}^{\infty} \frac{(-1)^{j-1} \Gamma(j+1/2)}{\pi(i\hbar t/2M)^{j+1/2}} (G_{2j}\psi)(x) \right|^2 dx, \quad (11)$$

respectively. In Eq. (10), $\langle \psi, G_{2j}\psi \rangle$ is also described in terms of the differential coefficients $\hat{\psi}^{(j)}(0)$ as

$$\langle \psi, G_{2j}\psi \rangle = \frac{(-1)^{j-1} \pi}{(2j)!} \sum_{n=0}^{2j} \binom{2j}{n} \overline{\hat{\psi}^{(2j-n)}(0)} \hat{\psi}^{(n)}(0). \quad (12)$$

We now consider such a special case that the initial wave packet $\psi(x)$ satisfies

$$\hat{\psi}(k) = O(k^m) \text{ as } k \rightarrow 0, \quad (13)$$

where $m=1,2,\dots$. We notice from Eq. (7) that the condition (13) is equivalent to the condition

$$\hat{\psi}^{(j)}(0) = 0, \quad \text{for } j=0,1,\dots,m-1. \quad (14)$$

Note that the condition (14) causes the $S(t)$ to behave like t^{-2m-1} . To confirm this assertion, it suffices to show that the condition (14) implies the next condition

$$\langle \psi, G_{2j}\psi \rangle = 0, \quad \text{for } j=0,1,\dots,m-1, \quad (15)$$

and vice versa [11]. In fact, substitution of Eq. (15) into Eq. (10) surely leads to $S(t) \sim t^{-2m-1}$. We briefly show the equivalence between the conditions (14) and (15). The fact that Eq. (14) implies Eq. (15) follows straightforwardly from Eq. (12). Conversely, if Eq. (15) holds, we have from $\langle \psi, G_0\psi \rangle = 0$ that $\hat{\psi}^{(0)}(0) = 0$ [see Eq. (12)]. Then, we also have from $\hat{\psi}^{(0)}(0) = 0$ and $\langle \psi, G_2\psi \rangle = 0$ that $\hat{\psi}^{(1)}(0) = 0$ [see Eq. (12) again]. In the same way, we can recursively show Eq. (14), and the proof is completed. Under the condition (14), we see that the first nonvanishing term $\langle \psi, G_{2m}\psi \rangle$ in the summation in Eq. (10) is reduced to

$$\langle \psi, G_{2m}\psi \rangle = \frac{(-1)^{m-1} \pi}{(m!)^2} |\hat{\psi}^{(m)}(0)|^2. \quad (16)$$

Then, we obtain the asymptotic behavior for $S(t)$ as [11]

$$S(t) = \frac{\Gamma(m+1/2)^2}{(m!)^4 (\hbar t/2M)^{2m+1}} |\hat{\psi}^{(m)}(0)|^4 + O(t^{-2m-2}). \quad (17)$$

Note that this formula is also seen to be valid for $m=0$. Let us now examine how the same condition (13) [or (14)] affects the asymptotic behavior of $\psi(x,t)$. Under the condition (14), we see that Eq. (9) reads

$$(G_{2j}\psi)(x) = 0 \quad \text{for all } x \in \mathbb{R}, \quad (18)$$

where $j=0,1,\dots,\bar{m}-1$. The $\bar{m}-1$ is the largest integer satisfying $2(\bar{m}-1) \leq m-1$, and the \bar{m} turns out to be

$$\bar{m} = \begin{cases} m/2 & \text{for even } m, \\ (m+1)/2 & \text{for odd } m. \end{cases} \quad (19)$$

Equation (18) consequently implies that the asymptotic expansion (5) for the wave packet reads

$$\psi(x,t) = \frac{(-1)^{\bar{m}-1} \Gamma(\bar{m} + 1/2)}{\pi(i\hbar t/2M)^{\bar{m}+1/2}} (G_{2\bar{m}}\psi)(x) + O(t^{-\bar{m}-3/2}), \quad (20)$$

as $t \rightarrow \infty$. One also see that this formula is valid for $m=0$. By using Eq. (14), the first nonvanishing term $(G_{2\bar{m}}\psi)(x)$ can be reduced to a simple expression as

$$(G_{2\bar{m}}\psi)(x) = \frac{-\sqrt{2\pi}i^m}{2(m!)} \hat{\psi}^{(m)}(0), \quad (21)$$

for even m , or

$$(G_{2\bar{m}}\psi)(x) = \frac{-\sqrt{2\pi}i^{m+1}}{2[(m+1)!]} [\hat{\psi}^{(m+1)}(0) + i(m+1)x\hat{\psi}^{(m)}(0)], \quad (22)$$

for odd m . Substituting Eq. (20) into Eq. (2), we can also derive the asymptotic behavior for $P(t)$:

$$P(t) = \frac{\Gamma(\bar{m} + 1/2)^2}{\pi^2(\hbar t/2M)^{2\bar{m}+1}} \int_a^b |(G_{2\bar{m}}\psi)(x)|^2 dx + O(t^{-2\bar{m}-2}), \quad (23)$$

as $t \rightarrow \infty$. The above formula is also expressed in terms of the differential coefficients $\hat{\psi}^{(j)}(0)$, by using Eq. (21) [or Eq. (22)].

It is worth noting that, in the case of m being odd, there is a possibility to find a special position, denoted by ξ_0 , where $(G_{2\bar{m}}\psi)(x)$ in Eq. (22) vanishes. This means that at this position, the $\psi(x,t)$ follows the power law in the next order. However, this matter may be regarded as an exception, because a point in the entire line has only zero measure. From Eq. (22), ξ_0 is given by

$$\xi_0 = i\hat{\psi}^{(m+1)}(0)/[(m+1)\hat{\psi}^{(m)}(0)], \quad (24)$$

and must be real. We can find such a ξ_0 for the initial wave packet, e.g., $N_m k^m e^{-a_0^2(k-k_0)^2/2 - ix_0 k}$, where $a_0 > 0$, $k_0, x_0 \in \mathbb{R}$, and N_m being the normalization constant. In this case, the ξ_0 is given by $x_0 + ia_0^2 k_0$. Then, it becomes real if and only if $k_0 = 0$, which leads to $\xi_0 = x_0$, the center of the initial wave packet. Note that such a special position in Eq. (24), if any, does not have an influence on the asymptotic form of $P(t)$, because $P(t)$ is obtained by the integral of $|(G_{2\bar{m}}\psi)(x)|^2$.

Let us now consider and compare the long-time behaviors of $S(t)$ and $P(t)$. We see from Eq. (19) that m and \bar{m} are different when $m \geq 2$, and this fact directly affects the long-

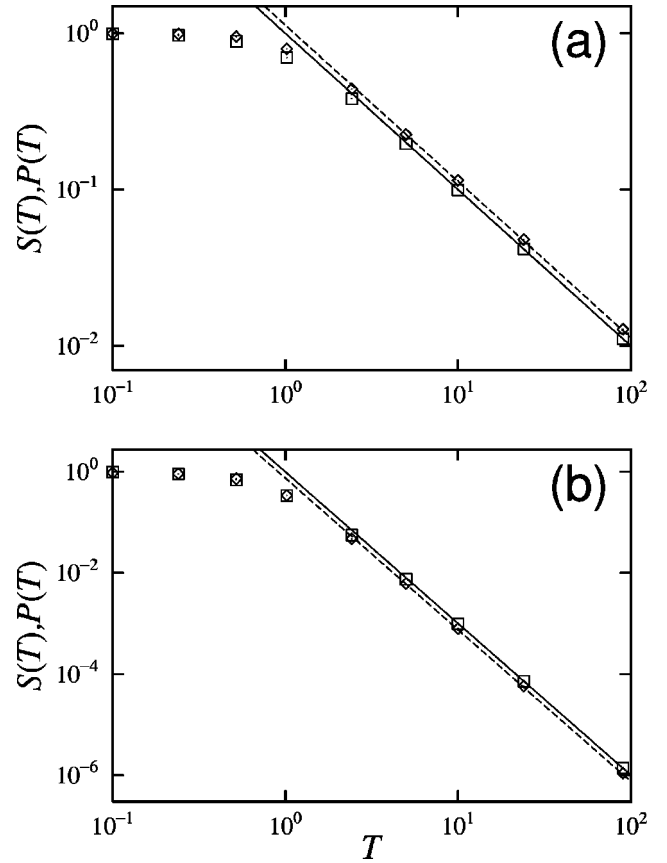


FIG. 1. (a) $S(T)$ and $P(T)$ (square and diamond, respectively) of the wave function ϕ_0 in Eq. (25), and their asymptotes predicted by Eqs. (17) and (23) (solid and dashed lines, respectively), where $T = \hbar t/2Ma_0^2$ is the reduced time. In this case, $S(T)$ and $P(T)$ show the same power decay behavior like T^{-1} at long times. (b) $S(T)$ and $P(T)$ of the wave function ϕ_1 , and their asymptotes. The notations and symbols are the same as those in (a). $S(T)$ and $P(T)$ exhibit the same power decay; however, they behave like T^{-3} instead of T^{-1} . Here, we set $k_0 = 0.0$ and $x_0 = 0.0$, in ϕ_0 and ϕ_1 , and $a/a_0 = -2.0$ and $b/a_0 = 2.0$ in $P(T)$'s.

time behaviors of $S(t)$ and $P(t)$. When the initial state ψ satisfies $\hat{\psi}(k) = O(k^m)$ with an arbitrary integer $m \geq 2$, $S(t)$ goes asymptotically like t^{-2m-1} , whereas $P(t)$ like t^{-m-1} for even m or like t^{-m-2} for odd m . For a large m , $S(t)$ decreases much faster than $P(t)$. We also see that $\bar{m} = m+1$ for odd m . This means that, in the case of an odd integer m , unlike $S(t)$, $P(t)$ decreases in the same power law under both the conditions; $\hat{\psi}(k) = O(k^m)$ and $\hat{\psi}(k) = O(k^{m+1})$.

To illustrate the difference in the long-time behaviors of $S(t)$ and $P(t)$, we choose three initial wave functions $\phi_0(x)$, $\phi_1(x)$, and $\phi_2(x)$, defined by

$$\hat{\phi}_m(k) = N_m k^m e^{-a_0^2(k-k_0)^2/2 - ix_0 k}, \quad \text{for } m=0,1,2. \quad (25)$$

These are the same ones considered after Eq. (24). They behave like $\hat{\phi}_m(k) = O(k^m)$ for small k . Figure 1 shows the

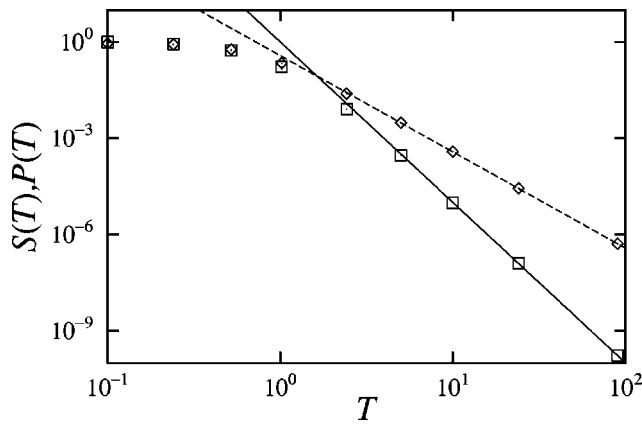


FIG. 2. $S(T)$ and $P(T)$ of the wave function ϕ_2 , and their asymptotes, where $T = \hbar t / 2Ma_0^2$. The same notations and symbols as in Fig. 1 are used. In this case, $S(T)$ and $P(T)$ exhibit different power decays at long times. The former behaves like T^{-5} , while the latter like T^{-3} . Here, we set $k_0 = 0.0$ and $x_0 = 0.0$, in ϕ_2 , and $a/a_0 = -2.0$ and $b/a_0 = 2.0$ in $P(T)$.

time evolution of $S(t)$ and $P(t)$, and their asymptotic forms predicted by Eqs. (17) and (23). The initial states ϕ_0 and ϕ_1 are used in Figs. 1(a) and 1(b), respectively. It is clearly seen that in Fig. 1(a), $S(t)$ and $P(t)$ behave asymptotically like t^{-1} at long times, and in Fig. 1(b) like t^{-3} . In these cases, the difference between the behaviors of $S(t)$ and $P(t)$ is not found. On the other hand, we notice that in Fig. 2 $S(t)$ and $P(t)$ for the initial state ϕ_2 differ asymptotically at long times. The former behaves asymptotically like t^{-5} , however, the latter behaves like t^{-3} . In our calculation, we have chosen a set of parameters $k_0 = 0.0$ and $x_0 = 0.0$ for the three initial states, and $a/a_0 = -2.0$ and $b/a_0 = 2.0$ for the interval $[a, b]$ for $P(t)$. Then, as is seen from Figs. 1 and 2, $P(0) \sim 1$, i.e., the initial states are well localized in the interval.

In conclusion, we have considered for every position the long-time behavior of the wave packet moving freely in one dimension, according to the characteristics of the initial wave packet at small momentum. We have then found that the asymptotic power of t obeyed by the wave packet is constant everywhere, at most excluding one position ξ_0 . We also have obtained the asymptotic behavior of the nonescape probab-

ility at long times, and compared that of the survival and non-escape probabilities. It is of interest that they can decrease in the different power laws depending on the initial states, in spite of the apparent similarity between their physical meanings. Our derivation can be easily extended to an arbitrary dimension, by starting with Eq. (4) in a corresponding dimension. In these analyses, we assume that the exchange of the order of summation and integration is admitted in the formal expansions in Eqs. (5) and (7). Indeed, this assumption can be rigorously guaranteed, when we make the same discussion with the finite series involving an appropriate remainder, instead of Eqs. (5) and (7). In any such procedure, to keep the validity of the formula, e.g., Eq. (20), what should be satisfied at least is that all of the differential coefficients $\hat{\psi}^{(j)}(0)$ with j up to m (or $m+1$) are finite for even m (or odd m). See Eq. (21) [or Eq. (22)]. It should be noted that this condition also implicitly implies that $\lim_{k \rightarrow +0} \hat{\psi}^{(j)}(k) = \lim_{k \rightarrow -0} \hat{\psi}^{(j)}(k)$ for $j = 0, 1, \dots, m$ (or $m+1$). These conditions are satisfied by those ψ 's which are rapidly decreasing functions as in Eq. (25). However, such a circumstance is not always valid for an arbitrary initial wave packet, e.g., the wave packet with the power-law tail [1–3] or that treated in Ref. [4]. The former causes $|\hat{\psi}(0)| = \infty$ and the latter causes $\lim_{k \rightarrow +0} \hat{\psi}^{(m)}(k) \neq \lim_{k \rightarrow -0} \hat{\psi}^{(m)}(k)$. It is then significant to consider how our results are modified for such initial wave packets. Furthermore, it is important to extend our consideration to the potential systems. In particular, it is relevant to examine in that case the possible influence of the characteristics of the initial states on the long-time behavior of the survival and nonescape probabilities. In fact, such an attempt has not been done in previous investigations. An extension may be realized by starting, instead of Eq. (5), with the asymptotic expansion of the wave packet at long times for the short-range potential systems, attained by several methods (see, for example, Refs. [7,8,10,17], and references therein).

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