## ARTICLES

# Dwell time and asymptotic behavior of the probability density

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The asymptotic long-time behavior of the probability density in a collision of a particle with several model potentials is analyzed. In all cases the observed dependence is an inverse cubic power of time. This assures the existence of the dwell time as a meaningful finite quantity.

In a recent publication[1] the decay of one-channel quantum states initially restricted to a finite spatial region $0 < r < R$ and interacting with a cutoff potential [i.e., $V(r) = 0$ for $r > R$] was examined. It was argued there that while the survival probability $|\langle\psi(t)|\psi(0)\rangle|^2$ behaves as $t^{-3}$ for long times, the nonescape probability

$$P(t) \equiv \int_0^R dr\, |\psi(r,t)|^2 \tag{1}$$

decays asymtotically as $t^{-1}$. In a general one-dimensional scattering or decay problem the asymptotic dependence of the probability of being in a given spatial region $[a, b]$ is important because a $t^{-1}$ behavior would make the *dwell time*

$$\tau(0,\infty) = \int_0^\infty dt \int_a^b dx\, |\psi(x,t)|^2 \tag{2}$$

an ill-defined (infinite) quantity. (We assume for simplicity that there are no bound states.) At a preparation time $t = 0$ the wave packet $\psi(x, 0)$ may or may not overlap with the potential as corresponds to a decay or a scattering problem, respectively. (Hereafter it is always assumed that $t > 0$ in all equations.) The concept of dwell time, as an average time spent by the particle between positions $a$ and $b$, has been central to the study of time-dependent aspects of wave-packet propagation and the temporal characterization of electronic devices,[2–5] so a careful examination of this matter is required. A second motivation to study the subject is that the observation of nonexponential decay in artificially built mesoscopic devices where different potential shapes can be obtained seems feasible.[6]

It is our aim here to present analytical and numerical evidence that, indeed, a $t^{-3}$ behavior can be expected quite generally for the probability density in one-dimensional collisions and partial waves in three-dimensional scattering.

A general understanding of the asymptotic behavior of the probability density is achieved from the expression for the propagator in terms of a contour integral in the complex momentum $q$ plane,

$$\langle x|e^{-iHt/\hbar}|x'\rangle = \frac{i}{2\pi}\int_C dq\, I(q) e^{-izt/\hbar}, \tag{3}$$

$$I(q) = \frac{q}{m}\left\langle x\left|\frac{1}{z-H}\right|x'\right\rangle, \tag{4}$$

where $z \equiv q^2/2m$ and the contour $C$ goes from $-\infty$ to $+\infty$, passing above all the singularities of the resolvent. In the absence of bound states $C$ goes simply above the real axis, which is the continuous spectrum of the Hamiltonian $H$; see Fig. 1. Due to the exponential $e^{-izt/\hbar}$ in (3) the large $t$ behavior is dominated by the region around the origin, which is associated with low momenta on the real axis. The origin is actually a saddle point for the steepest-descent path for this exponential factor that crosses the origin along the diagonal of the second and fourth quadrants; see contour $C'$ in Fig. 1. It is convenient to introduce the new variable

$$u = q/f, \quad f = (1-i)\sqrt{(m\hbar/t)}, \tag{5}$$

so that the exponential becomes $e^{-u^2}$ and $u$ remains real along the steepest-descent path.

The resolvent matrix element $\langle x|(z-H)^{-1}|x'\rangle$, which is defined for Im$q > 0$ (or first energy sheet), has to be analytically continued into the lower half $q$ plane (or second sheet of the complex $z$ plane) to allow for this type of analysis. Provided that the analytically continued function is analytical at the origin it has a Taylor series expansion

$$\langle x|(z-H)^{-1}|x'\rangle = a_0 + a_1 q + a_2 q^2 + \cdots, \tag{6}$$

with coefficients $a_i$ depending on $x$ and $x'$. But because of the (odd) $q$ factor in (4), the first term $a_0$ does not contribute to the integral (3). The asymptotic formula for the propagator comes, therefore, from the second term, and takes the form

 

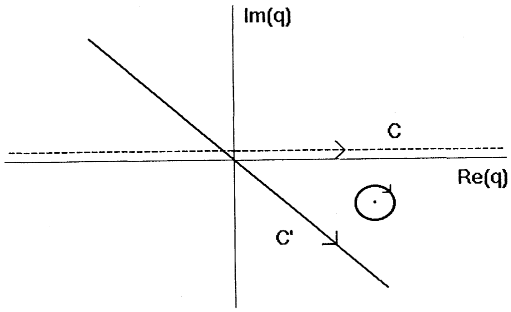


FIG. 1. Contour $C$ (dashed line) in the complex $q$ plane. The contour $C'$ results from deforming contour $C$ by a rotation by 45° and crossing a resonance pole.

$$\langle x|e^{-iHt/\hbar}|x'\rangle \sim \frac{i}{2m\pi}a_1 f^3 \int du\, u^2 e^{-u^2} = \frac{1-i}{2m\sqrt{\pi}}a_1 \left(\frac{m\hbar}{t}\right)^{3/2} . \quad (7)$$

This formal result depends on the validity of (6), and on the assumption that no additional contributions due to the deformation of the contour are to be considered asymptotically. In general the analytically continued matrix elements of the resolvent will have poles in the lower half $q$ plane that may be crossed when deforming the contour (see an example in Fig. 1) but these can only yield contributions that decay *exponentially* with time, so they are negligible at long times. It is then our objective to examine the factor $I(q)$ in the limit $q \to 0$ for several models. When $I(0)$ vanishes a $t^{-3}$ asymptotic behavior of the probability density will occur and dwell times will be well defined.

Based on the decomposition of the resolvent of $H$,

$$\frac{1}{z-H} = \frac{1}{z-H_0} + \frac{1}{z-H_0}V\frac{1}{z-H} \quad (8)$$

$$= \frac{1}{z-H_0} + \frac{1}{z-H_0}T(z)\frac{1}{z-H_0} , \quad (9)$$

in terms of the kinetic energy Hamiltonian $H_0$ and the parametrized transition operator $T(z) = V + V(z-H)^{-1}V$, the evolution operator $U \equiv e^{-iHt/\hbar}$ will be separated into "free" and "scattered" parts, $U = U_f + U_s$:

$$\langle x|U_f|x'\rangle \equiv \langle x|e^{-iH_0t/\hbar}|x'\rangle = \frac{i}{2\pi}\int dq\, e^{-izt/\hbar} I_f(q) , \quad (10)$$

$$I_f(q) = \frac{q}{m}\left\langle x\left|\frac{1}{z-H_0}\right|x'\right\rangle , \quad (11)$$

$$\langle x|U_s|x'\rangle \equiv \langle x|e^{-iHt/\hbar} - e^{-iH_0t/\hbar}|x'\rangle = \frac{i}{2\pi}\int dq\, e^{-izt/\hbar} I_s(q) , \quad (12)$$

$$I_s(q) = \frac{q}{m}\left\langle x\left|\frac{1}{z-H_0}T(z)\frac{1}{z-H_0}\right|x'\right\rangle . \quad (13)$$

Two different cases of one-dimensional motion will be discussed. First is the case in which the motion is allowed to cover the full line and second is the restriction to a half line. There is a basic difference in the asymptotic time dependence between these two cases for free motion while, at least for the potentials examined, the probability density for interacting motion commonly decays asymptotically as $t^{-3}$. For the latter to occur, $I(0)$ must vanish. This can arise either via a cancellation between free and scattering parts, i.e., $I_s(0) = -I_f(0) \neq 0$, or both terms can vanish separately, $I_s(0) = I_f(0) = 0$. The two possibilities are exemplified.

Consider first free motion on the full line. In this case $H_0$ is the kinetic-energy Hamiltonian for one particle moving in one dimension. Using the resolution of the identity in terms of momentum eigenstates and contour integration one finds the Green's function for free motion,

$$\left\langle x\left|\frac{1}{z-H_0}\right|x'\right\rangle = \frac{-im}{q\hbar}e^{i|x-x'|q/\hbar}, \quad (14)$$

so that $I_f(0) = -i/\hbar \neq 0$; see (11). As a consequence the asymptotic behavior of the probability density for free motion on the full line is $t^{-1}$. This is an important case in which Eq. (6) is *not* satisfied. Explicitly, by carrying out the integral in (3), the well-known propagator

$$\langle x|e^{-iH_0t/\hbar}|x'\rangle = \left(\frac{m}{iht}\right)^{1/2} e^{im(x-x')^2/2\hbar t} \quad (15)$$

is obtained, verifying an asymptotic $t^{-1}$ behavior of the probability density.

Next is the study of the scattering contribution to the propagator for a separable (noncutoff) potential,[7,8]

$$V = |\chi\rangle V_0\langle\chi| , \quad (16)$$

$$\langle p|\chi\rangle = \left(\frac{2a^3}{\pi}\right)^{1/2}\frac{1}{a^2+p^2}. \quad (17)$$

The $T(z)$ operator is known explicitly for this potential[9]

$$T(z) = |\chi\rangle\frac{V_0 q(q+ia)^2}{\mathcal{C}(q)}\langle\chi| , \quad (18)$$

$$\mathcal{C}(q) = q(q+ia)^2 - 2mV_0(q+2ia) , \quad (19)$$

which, using (13), gives for the scattering part of the propagator the factor

$$I_s(q) = \left\langle x\left|\frac{1}{z-H_0}\right|\chi\right\rangle\frac{V_0q^2(q+ia)^2}{m\mathcal{C}(q)}\left\langle\chi\left|\frac{1}{z-H_0}\right|x'\right\rangle. \quad (20)$$

The matrix elements depending on the coordinates in (20) can be evaluated by contour integration,

$$\left\langle x\left|\frac{1}{z-H_0}\right|\chi\right\rangle = \frac{-2mi}{q^2+a^2}\left(\frac{a^3}{\hbar}\right)^{1/2}\left[\frac{e^{i|x|q/\hbar}}{q} - \frac{e^{-a|x|/\hbar}}{ia}\right]. \quad (21)$$

[The matrix element depending on $x'$ is obtained from

(21) by taking its complex conjugate together with the replacements $-q^*$ by $q$ and $x$ by $x'$.] Substituting (20) in (12), the resulting integral has three simple poles at the roots of the cubic equation $\mathcal{C}(q) = 0$ and a double pole at $ia$. It can be explicitly evaluated by expanding $I(q)$ in partial fractions and recognizing the resulting integrals as $w$ functions[10] (for first-order poles) or as derivatives of $w$ functions (for second-order poles). For the present purpose it is sufficient to point out that, using (20) and (21), $I_s(0) = i/\hbar = -I_f(0)$, which exactly cancels the corresponding result for free propagation. For some initial wave packets analytical results can be obtained for the time-dependent wave function in terms of $w$ functions. In particular the Lorentzian momentum wave function

$$\langle p|\psi(0)\rangle = \left(\frac{2b^3}{\pi}\right)^{1/2} \frac{e^{-ix_c p/\hbar}}{b^2 + (p - p_b)^2} \tag{22}$$

allows an explicit analytical evaluation of $\langle x|\psi(t)\rangle$. Figure 2 shows the logarithm of the probability density at the point $x_c$, which is the central position of the packet at $t = 0$, versus the logarithm of time. The packet is initially on the left, $x_c < 0$, far from the potential barrier. An intermediate straight line of slope $-1$ denotes the asymptotic regime associated with free motion, and corresponds to a time regime where the effect of the potential is negligible. There is after that regime a complex oscillatory transient associated with the main passage of the reflected packet. Finally, the asymptotic $t^{-3}$ decay (slope $-3$ in the figure) is found. The two different asymptotic regimes, $t^{-3}$ or $t^{-1}$ for propagation with or without the potential, are also represented in Fig. 3, where the position chosen for the evaluation of the probability density is the potential center, $x = 0$. In addition, numerical calculations have been performed[11] for Gaussian wave packets colliding with square barriers, and the same asymptotic dependence $t^{-3}$ is found.

The next example is the $\delta$ function potential $\langle x|V|x'\rangle = V_0\delta(x)\delta(x - x')$. In this case one obtains,

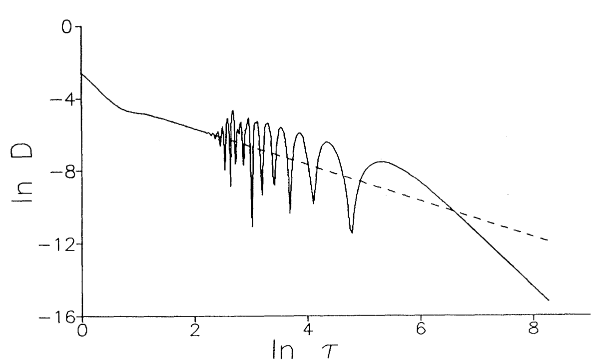


FIG. 2. $\ln D$, where $D \equiv (\hbar|\langle x_c|\psi\rangle|^2/a)$ versus $\ln\tau$, where $\tau \equiv ta^2/m\hbar$ for $x_c a/\hbar = -20$ (solid line). Barrier and state parameters are [see Eqs. (16), (17), and (22)] $mV_0/a^2 = 5$, $b/a = 1$, $p_c/a = 2$. The dashed line corresponds to the same state parameters but free propagation ($V_0 = 0$). Solid and dashed lines are indistinguishable in the scale of the figure until $\ln\tau \approx 2.5$.

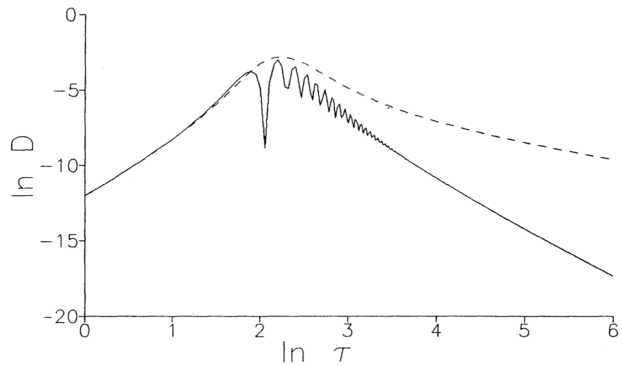


FIG. 3. $\ln D$, where $D \equiv (\hbar|\langle x = 0|\psi\rangle|^2/a)$ versus $\ln\tau$. Same barrier and initial state as in Fig. 2. The initial rise is associated with the approach of the packet to the barrier.

using (8),

$$T(z) = |0\rangle \frac{qV_0}{q + imV_0/\hbar}\langle 0|, \tag{23}$$

where $|0\rangle$ is the position ket associated with the origin, $\langle x|0\rangle = \delta(x)$. Using (13), (14), and (23) it is again found that $I_s(0) = i/\hbar = -I_f(0)$.

An example of a different nature is free motion restricted to the half line, i.e., to $r > 0$. This can be viewed as an $s$-wave partial wave of three-dimensional free motion or as one-dimensional motion restricted by an infinite barrier at the origin. [A distinction between radial motion and one-dimensional full line motion has been made by using $r$ for the radial coordinate versus $x$ as a general one-dimensional coordinate. The general discussion between Eqs. (2) and (13) applies to radial motion as well.] A convenient complete set of orthogonal functions is now given by

$$\langle r|p\rangle = \frac{2}{h^{1/2}}\sin(pr/\hbar), \;\; r > 0, \;\; p > 0\,, \tag{24}$$

which are the continuum eigenvectors of $H_0$, having eigenvalues $p^2/2m$, and normalized so that $\int_0^\infty \langle p|r\rangle\langle r|p'\rangle dr = \delta(p - p')$. The Green's function can be obtained by expanding $H_0$ in this basis:

$$\left\langle r\left|\frac{1}{z - H_0}\right|r'\right\rangle = \frac{mi}{\hbar q}[e^{i(r+r')q/\hbar} - e^{i|r-r'|q/\hbar}]. \tag{25}$$

[Note the additional amplitude in comparison to the result obtained for free motion on the full line (14).] $I_f$ is given, using (25), by

$$I_f(q) = \frac{i}{\hbar}[e^{i(r+r')q/\hbar} - e^{i|r-r'|q/\hbar}]\,, \tag{26}$$

which vanishes in the limit $q \to 0$ implying an asymptotic $t^{-3}$ behavior of the probability density in contrast with the $t^{-1}$ dependence for free motion on the full line. Explicitly, the corresponding propagator is given by

$$\langle r|U_f|r'\rangle = \left(\frac{m}{iht}\right)^{1/2}[e^{i(r-r')^2m/2t\hbar} - e^{i(r+r')^2m/2t\hbar}]. \quad (27)$$

The effect of a $\delta$ function potential at $r_0$ can be examined. The $T(z)$ operator is now

$$T(z) = |r_0\rangle \frac{qV_0}{q - imV_0[\exp(i2r_0q/\hbar) - 1]/\hbar}\langle r_0| \, , \quad (28)$$

and the scattering part of the propagator is determined by

$$I_s(q) = -\frac{mV_0}{\hbar^2}\frac{[e^{i(r_0+r)q/\hbar} - e^{i|r-r_0|q/\hbar}]}{q - imV_0[\exp(i2r_0q/\hbar) - 1]/\hbar} \times [e^{i(r_0+r')q/\hbar} - e^{i|r_0-r'|q/\hbar}]. \quad (29)$$

It is clear in this case that $I_s(0) = I_f(0) = 0$ so that the probability density will behave asymptotically as $t^{-3}$. This particular model was also examined by Nussenzveig.[12] This result agrees with Nussenzveig's but differs from Ref. 1. Nussenzveig, however, indicated that the physical mechanism to explain this behavior was free motion. The present analysis, based on a partition into free and scattering parts, demonstrates that this is not the case. In one-dimensional scattering on the full line, it is the combination of free and and scattering contributions that cancels the $t^{-1}$ term. In three dimensions, both free and scattering components have their asymptotically dominant terms of the same order, $t^{-3}$. Quite generally the resolvent will not have a singularity at zero energy. In one dimension there is indeed a single pole at the origin for free motion but a weak potential will shift this pole. For arbitrary values of potential strength, only in exceptional cases will a singularity occur at zero energy. In three-dimensional $s$-wave scattering the singularities at the origin are known as zero-energy resonances and can also be regarded as exceptional cases.[13]

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[11] The calculation has been carried out by expanding the evolution operator in a basis of eigenstates of $H$ and performing the integrals numerically. In particular, the following parameters have been used (in atomic units): The barrier is located between $x = 0$ and $x = 6$; barrier height $=0.85$; the packet is a minimum uncertainty Gaussian packet at time $t = 0$ centered at $x_c = -41$ and $p_c = 0.5$ with position variance $\delta^2 = 64$. The probability density is examined at points before, in, and after the barrier, $x = -5$, $x = 3$, and $x = 11$, respectively. The asymptotic behavior $t^{-3}$ is reached at $t > 100\,000$.

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