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Novel Expression for the Wave Function of a Decaying Quantum System

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We report on a novel, practical method of determining the nonrelativistic wave function of a decaying quantum system at all positions and times. The system consists of a particle which is initially confined around the origin and leaks out tunneling through a potential barrier. We show that the wave function $\psi(r,t)$ of the particle can be expressed as a linear combination of Moshinsky functions, each of which is associated with a pole of the scattering **S** matrix of the system. The $\psi(r,t)$ so obtained is normalizable. In the light of this approach we reexamine the Gamow wave function, which is not normalizable. We elucidate the source of this difficulty.

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A complete description of the evolution of a decaying quantum system, such as an α-decaying nucleus, involves the determination of the time-dependent wave function. Early in the development of quantum physics approximate wave functions were used to study the decay rates [1]. One assumes that a particle is initially confined within a region around the origin and at a certain time, say $t = 0$, it begins to leak out by tunneling through a potential barrier. Many such models have been examined in the literature over the years, but the knowledge of the space-time evolution of the wave function $\psi(r,t)$ of the particle has been limited to that inside the boundary of the interaction region [2–5]. In fact, most of the studies deal with the exponential decay law and the deviation thereof at small and large times. For such analyses it is sufficient to know the $\psi(r,t)$ inside the interaction region. However, for the quantum mechanical study of the decaying particle as it emerges from the parent system and interacts with its environment, e.g., α particles with atomic electrons or detectors [6], one needs the explicit wave function *in the entire space.* We are not aware of any papers which have addressed this issue except for a recent one [7] in which $\psi(r,t)$ was determined by numerically solving the time-dependent Schrödinger equation. Such a numerical approach is computationally prohibitive as r and/or t become very large.

The purpose of this Letter is to show that the $\psi(r,t)$ of the model can be expressed as a linear combination of the Moshinsky functions [8], each of which is associated with a pole of the scattering **S** matrix of the interaction. In this way we can easily calculate the wave function accurately no matter how large r and/or t are. For simplicity we consider the S state but extension to other partial waves is not difficult. We also reexamine the so-called Gamow or resonance state that is discussed extensively in the literature [9,10]. Despite its merits the Gamow wave function is not a good wave function outside the decaying system. It grows exponentially and hence it is not normalizable. We will elucidate the source of this difficulty.

We assume a central potential $V(r)$ representing a repulsive barrier that supports one or more unstable bound states or resonances. For simplicity let us also assume that there is no stable bound state and that

$$V(r) = 0 \quad \text{for } r > R\,. \tag{1}$$

This excludes a Coulomb barrier such as an emitted α particle feels, but in principle the restriction on the potential can be relaxed to include such systems. It is also understood that $\int_0^\infty rV(r)\,dr$ is finite. To reduce notational complication we set $\hbar = 1$ and $2m = 1$ throughout. Thus we are interested in obtaining the solution $\psi(r,t)$ of the time-dependent Schrödinger equation for $t > 0$

$$i \frac{\partial \psi(r,t)}{\partial t} = \left[-\frac{\partial^2}{\partial r^2} + V(r) \right] \psi(r,t), \quad (2)$$

where $\psi(r,0)$, the initial state, is given. The $\psi(r,0)$ is confined to $r < R$ and is normalized to unity.

Let us write the stationary scattering solutions as

$$\phi(k,r,t) = e^{-ik^2 t} u(k,r), \quad (3)$$

$$u(k,r) = \frac{1}{2ik} [f(k) f(-k,r) - f(-k) f(k,r)], \quad (4)$$

where $k > 0$ and k^2 is the associated energy [11]. The function $u(k,r)$ is real, $u(k,0) = 0$, and $du(k,0)/dr = 1$. The $f(k,r)$ is the Jost solution, which becomes $f(k,r) = e^{-ikr}$ for $r > R$. The $f(k) \equiv f(k,0)$ is the Jost function, which is related to the scattering phase shift $\eta(k)$ and the **S** matrix by

$$f(k) = |f(k)| e^{i\eta(k)}, \qquad \mathbf{S}(k) = \frac{f(k)}{f(-k)}. \quad (5)$$

A useful relation is $f^*(-k^*, r) = f(k,r)$ [11].

The $u(k,r)$ form a complete orthogonal set with

$$\int_0^\infty u^*(k,r) u(k',r)\, dr = \frac{\pi}{2k^2} |f(k)|^2 \delta(k - k'), \quad (6)$$

where $k, k' > 0$. The wave function $\psi(r,t)$ can be expressed in terms of the stationary solutions as

$$\psi(r,t) = \frac{2}{\pi} \int_0^\infty \frac{k^2}{|f(k)|^2} C(k) e^{-ik^2 t} u(k,r)\, dk, \quad (7)$$

$$C(k) = \int_0^\infty u^*(k,r) \psi(r,0)\, dr. \quad (8)$$

The $C(k)$ differs from the $C(k)$ of Ref. [7] through a factor related to the normalization of $u(k,r)$. The $u(k,r)$ is an entire function of k and so is $C(k)$ [11]. Since $C(-k) = C(k)$ we can write the $\psi(r,t)$ as

$$\psi(r,t) = \int_0^\infty e^{-ik^2 t} [e^{ikr} g(k,r) + e^{-ikr} g(-k,r)]\, dk \quad (9)$$

$$= \int_{-\infty}^\infty e^{-ik^2 t} e^{ikr} g(k,r)\, dk, \quad (10)$$

$$g(k,r) = -\frac{i}{\pi} k C(k) \frac{e^{-ikr} f(-k,r)}{f(-k)}. \quad (11)$$

The $g(k,r)$ as a function of complex k has an infinite number of simple poles, which are due to the zeros of $f(-k)$, which in turn give rise to poles of the **S** matrix. The $g(k,r)$ has no other singularities for finite $|k|$. This follows from the fact that $f(k,r)$ is an entire function of k when the potential vanishes for $r > R$ [12]. In the absence of bound states, these poles are all in the lower half of the complex k plane, located symmetrically about the imaginary axis [12]. Let us denote the poles in the fourth quadrant with k_ν, $\nu = 1,2,3,\ldots$; $\mathrm{Re}(k_\nu)$ increases with increasing ν. We also denote the poles in the third quadrant with k_ν, but with $\nu = -1,-2,-3,\ldots$. Because of the symmetric locations of the poles, $\mathrm{Re}(k_\nu) = -\mathrm{Re}(k_{-\nu})$ and $\mathrm{Im}(k_\nu) = \mathrm{Im}(k_{-\nu}) < 0$.

If we assume that $g(k,r)$ has no essential singularity at infinity, the Mittag-Leffler theorem [13] allows us to expand $g(k,r)$ as

$$g(k,r) = \sum_\nu \frac{a_\nu(r)}{k - k_\nu}, \qquad \nu = \pm 1, \pm 2, \ldots, \quad (12)$$

where $a_\nu(r)$ is the residue of $g(k,r)$ associated with the pole at $k = k_\nu$. Note that if $r > R$, $e^{-ikr} f(-k,r) = 1$, and hence $a_\nu(r)$ becomes independent of r. No additional constant term occurs in this expansion because $g(0,r) = 0$, a condition which also leads to the residues satisfying the relation $\sum_\nu a_\nu(r)/k_\nu = 0$.

Equations (10) and (12) lead to the following simple expression for $\psi(r,t)$:

$$\psi(r,t) = -2\pi i \sum_\nu a_\nu(r) M(k_\nu, r, t), \quad (13)$$

where the summation is over $\nu = \pm 1, \pm 2, \ldots$. The $M(k,r,t)$ is the Moshinsky function defined by

$$M(k,r,t) = \frac{i}{2\pi} \int_{-\infty}^\infty \frac{e^{-ip^2 t} e^{ipr}}{p - k + i\epsilon}\, dp, \quad (14)$$

where $\epsilon > 0$ is infinitesimal. The ϵ is introduced when k is real, so that the wave function has the properties of an outgoing wave at $t = 0$. After the p integration, $M(k,r,t)$ becomes [8]

$$M(k,r,t) = \frac{1}{2} e^{-ik^2 t} e^{ikr} \operatorname{erfc}(y),$$

$$y = e^{-i\pi/4} \frac{r - vt}{2\sqrt{t}}, \quad (15)$$

where $v = 2k (= k/m)$ and $\operatorname{erfc}(y) = (2/\sqrt{\pi}) \times \int_y^\infty e^{-u^2}\, du$. Originally the Moshinsky function was defined for real k but the above formulas are valid for complex k with a negative imaginary part [14]. Depending on the model, $g(k,r)$ may actually have an essential singularity at infinity. Such cases can be handled by slightly modifying Eqs. (12) and (13) as we illustrate in an example below.

Among the poles, one of them, say k_1, may contribute dominantly to the integral. This occurs when the main constituent of the initial state of the system is a narrow resonance [3]. If we single out this pole contribution, we obtain the approximate solution

$$\psi_1(r,t) \equiv -2\pi i a_1(r) M(k_1, r, t). \quad (16)$$

Recall that $a_1(r)$ is a constant if $r > R$. The $\psi_1(r,t)$ is normalizable but it by itself is not normalized to unity.

Let us now turn to the Gamow wave function. The k integration of Eq. (9) can be rewritten in the form of an

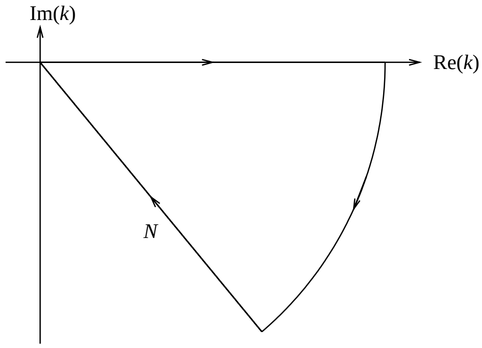

FIG. 1. The integration contour of Eq. (17) in the complex k plane. The path N is the contour part that is below the real axis so that all the poles in the fourth quadrant are included in the contour.

integral along a contour in the complex k plane as shown in Fig. 1 [3]. We choose the contour such that it contains all of the poles of $g(k,r)$ which are in the fourth quadrant. The $g(-k,r)$ has no poles in the lower half of the plane. Then Eq. (9) can be reduced to the form

$$\psi(r,t) = -2\pi i \sum_{\nu} b_{\nu}(r) - \int_N e^{-ik^2 t}[e^{ikr} g(k,r) + e^{-ikr} g(-k,r)]\, dk\,, \tag{17}$$

where the ν summation is for $\nu = 1, 2, \ldots$. Note that the residues $b_{\nu}(r)$ and $a_{\nu}(r)$ are different. The former is that of the integrand of Eq. (9), whereas the latter is that of $g(k,r)$. They are related by $b_{\nu}(r) = e^{-ik_{\nu}^2 t} e^{ik_{\nu} r} a_{\nu}(r)$. By taking only the dominant pole contribution we obtain the Gamow wave function

$$\psi_G(r,t) = -2\pi i b_1(r) = -2\pi i e^{-ik_1^2 t} e^{ik_1 r} a_1(r)\,. \tag{18}$$

Outside the barrier $\psi_G(r,t)$ is an outgoing wave. Because of the negative imaginary part of k_1 the amplitude of $\psi_G(r,t)$ grows exponentially as r increases since $a_1(r)$ approaches a constant value for large r. This wave function is not normalizable.

By comparing Eqs. (16) and (18) we see that the $M(k_1, r, t)$ of the former is replaced by a simple function of $e^{-ik_1^2 t} e^{ik_1 r}$ in the latter, or $\frac{1}{2}\operatorname{erfc}(y)$ is replaced by 1. Note the difference between the k integrations of Eq. (10) and that of Eq. (17). The former is a direct integration along the real axis over $(-\infty, \infty)$, whereas the latter is a contour integration in the complex k plane. Although we take account of only one dominant pole in the two methods of integration, $\psi_1(r,t)$ is a far better approximation than $\psi_G(r,t)$ to the actual wave function, and the former is not more difficult to obtain. One term of Eq. (13) corresponds to one pole term of Eq. (17) plus part of the integral along the segment N. The latter becomes important as r becomes comparable to or greater than vt. It is now clear what is responsible for the "exponential catastrophe" [10] of the Gamow wave function.

Let us illustrate the above analysis by considering a specific model. This model has been used by a number of authors [3–5,7,15] to study the exponential decay law and deviations from it. The potential is assumed to be

$$V(r) = (\lambda/R)\delta(r - R), \qquad \lambda > 0\,. \tag{19}$$

In numerical illustrations we set $R = 1$. For the strength of the potential we take $\lambda = 6$ and 100, which represent typical situations of fast- and slow-decay processes. For the wave function at $t = 0$ we assume

$$\psi(r,0) = \sqrt{\frac{2}{R}}\, \sin\!\left(\frac{\pi r}{R}\right)\theta(R - r)\,, \tag{20}$$

where $\theta(x) = 1$ (0) if $x > 0$ ($x < 0$).

For this model the $g(k,r)$ for $r > R$ is given by

$$g(k,r) = i\sqrt{2R}\, \frac{kRe^{-ikR}\sin kR}{k^2R^2 - \pi^2} \times [kR\cos kR + (\lambda - ikR)\sin kR]^{-1}. \tag{21}$$

The $g(k,r)$ for $r < R$ is obtained by multiplying the $g(k,r)$ of Eq. (21) with

$$e^{-ikr} f(-k,r) = 1 + (\lambda/2ikR)[e^{2ik(R-r)} - 1]\,. \tag{22}$$

The poles k_{ν} are the zeros of the equation $kR\cot kR + \lambda - ikR = 0$. The residues $a_{\nu}(r)$ of $g(k,r)$ are

$$a_{\nu}(r) = i\sqrt{2R}\, \frac{e^{-ik_{\nu}R}\sin k_{\nu}R}{k_{\nu}^2R^2 - \pi^2}\, \frac{k_{\nu} + (\lambda/2iR)[e^{2ik_{\nu}(R-r)} - 1]\theta(R - r)}{(1 + \lambda - ik_{\nu}R)\cos k_{\nu}R - (i + k_{\nu}R)\sin k_{\nu}R}\,. \tag{23}$$

The $g(k,r)$ has an essential singularity at infinity. When $r > R$, the singularity is due to the factor of e^{-ikR}. However, $e^{ikR} g(k,r)$ has no such singularity and hence the Mittag-Leffler theorem can be applied to it. This leads to

$$\psi(r,t) = -2\pi i \sum_{\nu} a_{\nu}(r) e^{ik_{\nu}R} M(k_{\nu}, r - R, t)\,, \tag{24}$$

for $r > R$. The $\psi(r,t)$ for $r < R$ can be obtained in a similar manner although it is somewhat more complicated.

Figure 2 shows the wave function for the fast-decay case, i.e., $\lambda = 6$. The graph shows $|\psi(r,t)|$ outside the potential region. The two conjugate-poles approximation (with the poles at k_1 and k_{-1}) is a good approximation up to $r/R \approx 15$. The one-pole approximation (k_1) is not quite

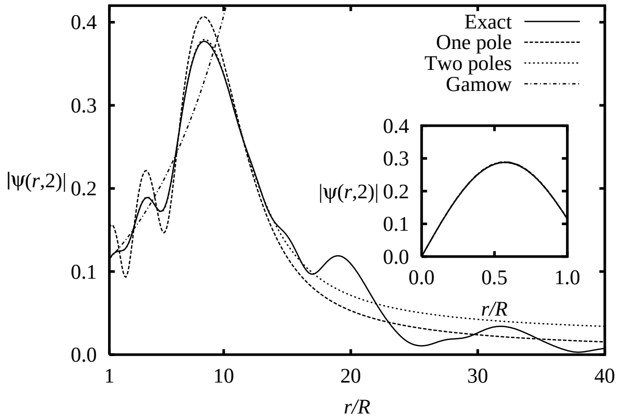

FIG. 2. The modulus of the wave function $|\psi(r,t)|$ for $\lambda = 6$ and $t = 2$. The solid line is for the complete calculation with all pole contributions obtained by using Eq. (13). The dashed or dotted lines show the result when the contribution of only one dominant pole or two conjugate poles is included. The Gamow wave function is shown as a dash-dotted line.

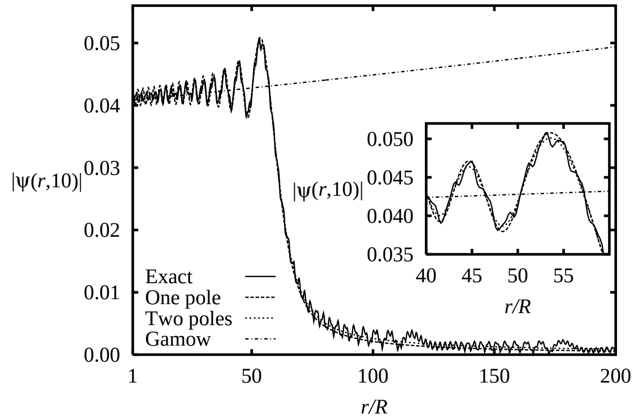

FIG. 3. The modulus of the wave function $|\psi(r,t)|$ for $\lambda = 100$ and $t = 10$, obtained by using Eq. (13). The solid line is for the complete calculation with all pole contributions. The dashed (dotted) line shows the result when only one (two) dominant pole(s) is (are) included. The dash-dotted line gives the Gamow wave function.

as good and gives a wave function that is not continuous at $r = R$. The Gamow wave function is obtained using Eq. (18) but scaled so that it has the exact amplitude at $r = R$. No such scaling is required for the one- and two-pole approximations when $\lambda = 6$. The inset shows the exact wave function and its approximations in the interior region of the potential where they are indistinguishable. The normalization of the wave function is not important to determine decay rates and hence all approximations would be useful for that. The wave function has a discontinuous slope at $r = R$ because of the δ-function potential. To obtain an accurate wave function for larger values of r/R many poles need to be included, but the effort required is not computationally prohibitive. We have also determined the wave function by solving Eq. (2) numerically and have confirmed the wave function [7].

For the slow-decay case we show the graph of the wave function when $\lambda = 100$ in Fig. 3. We note that, when $\lambda \gg 1$ and $\Gamma/k^2 \approx -4\,\mathrm{Im}(k_1)/v \ll 1$, where Γ is the decay constant, the wave function has a clear wave-front structure which travels outward at speed v. It drops sharply as r exceeds vt. Ahead of the main wave front, there are noticeable humps traveling at speeds $2v$, $3v$, etc. These are due to the admixture in the original state at $t = 0$ of higher-energy resonance states. The inset shows the details of the wave functions around the wave front. One can see that the exact wave function has considerably greater structure than the one- and two-pole approximations. Although no graph for the wave function inside the barrier is shown, the exact and the scaled Gamow wave functions are similar to those of Fig. 2 with much larger amplitudes. The one- and two-pole approximations, however, have much smaller amplitudes than the exact wave function and need to be scaled for the case of large λ.

In this Letter we considered the basic elements of determining the time-dependent wave function of a decaying system. The analysis can be generalized in several ways. Bound states can be included by generalizing Eq. (7) using the completeness relation which takes account of the bound states, and by giving due consideration to the bound-state zeros of the Jost functions. The condition of a finite range of the potential can be relaxed provided the Jost functions retain a structure involving simple poles only. The Jost solutions for various potentials are known [12] and the theory can be applied to such cases. The theory may be applied to higher partial waves but the corresponding Moshinsky functions need to be determined. Similarly, functions corresponding to the Jost solutions have been analyzed for the Coulomb potential [12], and hence these could be used to obtain a wave function of a particle tunneling through a Coulomb barrier.

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Note added in proof.—In order that Eq. (13) be compatible with the initial wave function of a finite extension, it has to be modified as was done in the illustration to obtain Eq. (24). This is related to the applicability of the Mittag-Leffler expansion to the function $g(k,r)$. A full account of the method will be published elsewhere.

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