Letter

Time evolution of a decaying quantum state: Evaluation and onset of nonexponential decay

Markus Nöth *
Mathematisches Institut, Ludwig-Maximilians-Universität München, Theresienstr. 39, D-80333 München, Germany

(Received 5 June 2022; accepted 22 December 2022; published 15 February 2023)

The method developed by van Dijk, Nogami, and Toyama for obtaining the time-evolved wave function of a decaying quantum system is generalized to potentials and initial wave functions of noncompact support. The long time asymptotic behavior is extracted and employed to predict the timescale for the onset of nonexponential decay. The method is illustrated with a Gaussian initial wave function leaking through Eckart's potential barrier on the half-line.

DOI: 10.1103/PhysRevC.107.L021602

Introduction. Quantum tunneling, the phenomenon of a particle traversing a potential barrier higher than its kinetic energy, has received a great deal of attention since the early works of Gamow [1]. Despite the time and effort spent on this issue (see [2–5] for important contributions to the discussion and reviews and [6] for a recent experiment), there still remain open questions about tunneling. One reason for this is that while tunneling is fundamentally a process in time, much of the analysis has been restricted to static aspects of the relevant setups. While important properties of tunneling systems such as exponential decay rates describing a decaying system for intermediate times can be found in such an analysis, a more thorough understanding seems desirable.

For this reason studying the time dependent wave function describing the tunneling particle is essential to complete the picture. For the setup of a decaying quantum state a great deal of progress in this direction has been achieved by van Dijk, Nogami, and Toyama [7–10]. For a precursor to the technique see [11]; however, please note that the discussion of the power law for the long time limit of the survival and nonescape probabilities of [11] is erroneous cf. [12]. In [7–10] a representation of the time dependent wave function well suited for studying early, intermediate, and late times is identified. This makes it well suited for analytic as well as numerical endeavors. The method was only applied to compactly supported potentials and initial wave functions. The compact support of the initial wave function played an important role, as will be explained below. In this article I extend this method and apply it to a Gaussian initial wave packet leaking out of Eckart's potential barrier; neither of which has a compact support. The necessary modification of the technique is introduced first.

Following a reminder of the tricks employed and the generalization of the present work I analyze the late-time asymptotics. While the power-law for the decay of the wave function

$$|\psi(r,t)| \overset{t\to\infty}{\to} \frac{|\psi_\infty(r)|}{t^{3/2}}, \tag{1}$$

in the generic case is well known, I derive a simple and fairly general expression for the constant involved cf. [13]. Furthermore, an estimate of the time t_{alg} after which the transition from exponential to algebraic decay takes place is given in Eq. (28). This result should be compared to the one for the survival amplitude by [14]. For a complicated barrier it may not be feasible to apply the full technique while the expressions for $|\psi_\infty(r)|$ and t_{alg} can be evaluated more easily and may therefore be of greater importance when comparing with experiments.

Recap and extension. Consider the Schrödinger equation (setting $\hbar = 2m = 1$)

$$i\partial_t\psi = -\partial_r^2\psi + V\psi, \tag{2}$$

for the scalar wave function ψ subject to the potential V and boundary condition $\psi(0,t) = 0$ for all t, chosen such that there are no bound states.[1] This theoretical setup may describe the radial part of a system describing α decay with zero angular momentum [15] or it may describe the motion of an ion along the axis of a quantum optical trap inducing a back wall [16,17] and an extra trapping potential V. The Jost solutions $f(k,r)$ of Eq. (2) will prove to be useful. They are the generalized eigenfunctions of the Hamiltonian of Eq. (2) of energy k^2 that satisfy

$$\lim_{r\to\infty} e^{-ikr} f(k,r) = 1. \tag{3}$$

Jost solutions exist for potentials V such that $\int_0^\infty dr\, r|V(r)| < \infty$. For fixed real r the Jost solution $f(k,r)$ is analytic on $\{\mathrm{Im}(k) \geqslant 0 \wedge k \neq 0\} \subset \mathbb{C}$ and fulfills $\overline{f(k,r)} = f(-\bar{k},r)$ [18, Thm XI.57]. Furthermore, I assume that 0 is not an eigenvalue or resonance of the Hamiltonian involved, which is typically true.

The generalized eigenfunction $u(k,r)$ of the same energy satisfying the proper boundary condition at the origin and the additional normalization

$$u(k,0) = 0, \quad u'(k,0) = 1, \tag{4}$$

*noeth@math.lmu.de

[1] See [9] for how to modify the technique in the presence of bound states.

where the prime denotes a derivative with respect to the second argument, is given by

$$u(k, r) = \big(f(k, 0)f(-k, r) - f(-k, 0)f(k, r)\big)\frac{1}{2ik}. \tag{5}$$

Furthermore, $u(k, r)$ is real for real r and k and even in k and for r fixed $u(k, r)$ is an entire function of k [18, Thm XI.56]. The solutions u form a complete set and are normalized to [7]

$$\int_0^\infty \overline{u(k, r)}u(k', r)dr = \frac{\pi}{2k^2}|f(k, 0)|^2\delta(k - k'), \tag{6}$$

for $k, k' > 0$. Expanding any solution $\psi(x, t)$ of Eq. (2) results in

$$\psi(r, t) = \frac{2}{\pi}\int_0^\infty \frac{k^2}{f(k, 0)f(-k, 0)}C(k)e^{-ik^2t}u(k, r)dk \tag{7}$$

with

$$C(k) = \int_0^\infty u(k, r)\psi(r, 0)dr, \tag{8}$$

where I eliminated complex conjugates by the above mentioned properties of u and f. Because of the symmetry properties of the integrand I split u up as in Eq. (5) to obtain

$$\psi(r, t) = \int_{-\infty}^\infty e^{-ik^2t+ikr}\frac{C(k)}{i\pi}\frac{k\, e^{-ikr}f(-k, r)}{f(-k, 0)}dk, \tag{9}$$

where I added an additional plane wave so that the last factor approaches a finite limit for $r \to \infty$. Next I introduce an auxiliary factor $h(k)$

$$\psi(r, t) = \frac{1}{i\pi}\int_{-\infty}^\infty e^{-ik^2t+ikr}h(k)\overbrace{\frac{k\, C(k)e^{-ikr}f(-k, r)}{h(k)f(-k, 0)}}^{=:g(k,r)}dk,$$

to achieve the following properties:

(i) The fraction $g(k, r)$ is still meromorphic in k.

(ii) The expansion of $g(k, r)$ by the Mittag-Leffler [19] theorem is of the form

$$g(k, r) = \sum_n \frac{a_n(r)}{k - k_n}, \tag{10}$$

where a_n are the residues of g at its poles k_n. A sufficient criterion for Eq. (10) is that $g(k, r)$ falls off at infinity in the complex k plane (excluding small circles around the poles) and the sum in Eq. (10) converges uniformly on compact sets.

(iii) The integral that remains after the exchange of the integral and sum which is of the form

$$\frac{1}{i\pi}\int_{-\infty}^\infty \frac{e^{-ik^2t+ikr}h(k)}{k - k_n}, \tag{11}$$

may be evaluated in closed form.

In [7–10], the initial wave functions $\psi(r, 0)$ under consideration vanish for any $r > R$ for some $R > 0$, this results in growth of the fractions of Eq. (9) like $e^{-\mathrm{Im}(k)R}$ in the negative imaginary direction. The choice $h = e^{ikR}$ exactly cancels this growth so that Mittag-Leffler can be applied.

The central innovation of the current paper is a different choice of h so as to allow for more generality:

$$h_\alpha(k) = e^{i\alpha k^2} + e^{-i\alpha k^2} + e^{-\alpha k^2}, \tag{12}$$

where $\alpha > 0$ is a free parameter.

To give an idea of which initial wave functions can be treated with this method a quick estimate of the growth of $C(k)$ in the imaginary direction may be helpful. From general scattering theory it is known that the eigenfunctions u generically grow exponentially in the complex plane see [20, equation (12.8)], [21, equations (6.4.13) and (6.4.17)]:

$$|u(k, r)| \leqslant \frac{c_1}{|k|}e^{|\mathrm{Im}(k)|r}. \tag{13}$$

Assuming that $\psi(r, 0) = \mathcal{O}(e^{-c_2r^{c_3}})$ for some $c_2 > 0, c_3 > 1$ for $r \to \infty$ big enough enables a stationary phase argument which yields

$$|C(k)| \leqslant c_4 e^{(c_2c_3)^{\frac{-1}{c_3-1}}(|\mathrm{Im}(k)|)^{\frac{c_3}{c_3-1}}(1-1/c_3)}. \tag{14}$$

If this growth can be controlled by a Gaussian the choice (12) will work for some $\alpha > 0$. Hence for any initial wave function with $c_3 \geqslant 2$ the method will succeed.

The choice (12) results in the following expression for the wave function:

$$\psi(r, t) = \sum_n a_n(r)\sum_{\gamma\in\{\alpha,\pm i\alpha\}} M(k_n, r, \gamma + it), \tag{15}$$

where M is given by

$$\begin{aligned} M(k, r, \beta) &= \int_{-\infty}^\infty \frac{dp}{i\pi}\frac{e^{-\beta p^2+irp}}{p - k} \\ &= e^{ikr-\beta k^2}[\mathrm{sgn}(\mathrm{Im}(k)) + \mathrm{erf}((r + 2ik\beta)/(2\sqrt{\beta}))] \end{aligned} \tag{16}$$

and is closely related to the Moshinsky function [22]. In order to apply the method one has to include all the poles of g, including the zeros of h_α, which are located close to the three sets

$$\Big\{\pm e^{-\frac{3\pi i}{8}}\sqrt{\pi(2n - 1)/(\sqrt{2}\alpha)}|n \in \mathbb{N}\Big\}, \tag{17}$$

$$\Big\{\pm e^{\frac{3\pi i}{8}}\sqrt{\pi(2n - 1)/(\sqrt{2}\alpha)}|n \in \mathbb{N}\Big\}, \tag{18}$$

$$\{\pm\sqrt{\pi(2n - 1)/(2\alpha)}|n \in \mathbb{N}\}. \tag{19}$$

Late time asymptotics. Besides the apparent use of the representation (15) to calculate $\psi(r, t)$ numerically with a small error for early as well as for late times it is also useful for theoretical considerations which will be illustrated next. I will discuss the late time asymptotics of a decaying quantum system recovering the well-known result

$$\psi(r, t) \xrightarrow{t\to\infty} \frac{\psi_\infty(r)}{t^{3/2}}, \tag{20}$$

valid for generic wave functions. Please note, that for special initial wave functions a different power law may apply [23]. The asymptotic behavior (20) was, e.g., also obtained by [4,9,13] for rigorous bounds see [21,24,25]. The amplitude $\psi_\infty(r)$ will be obtained for any system to which the method presented in this article is applicable and to arbitrary accuracy in the expansion (15). This expression is simpler than the one of [13]. For t large relative to r and α, I employ the asymptotic expression for erf [26, pp. 109–112][2]

$$\operatorname{erf}(\pm z) = \pm 1 - \frac{e^{-z^2}}{\sqrt{\pi}} \sum_{k=0}^{M} \frac{(-1)^k \left(\frac{1}{2}\right)_k}{(\pm z)^{2k+1}} + \mathcal{O}(e^{-z^2} z^{-2M-3}), \tag{21}$$

valid for $|\mathrm{ph}(\pm z)| < \frac{3}{4}\pi$, where the phase of k_n decides which of the two expansions is to be used and $(c)_k$ is the Pochhammer symbol. Taking $\gamma \in \{\alpha, \pm i\alpha\}$ and using Eq. (21) I get

$$\begin{aligned} &M(k_n, r, \gamma + it) \\ &\approx e^{ik_n r - (it+\gamma)k_n^2}(\mathrm{sgn}(\mathrm{Im}(k_n)) + \nu) \\ &- \frac{\sqrt{it+\gamma}\, e^{\frac{-r^2}{4(it+\gamma)}}}{\sqrt{\pi}\left(\frac{r}{2} + ik_n(it+\gamma)\right)} \left(1 - \frac{(it+\gamma)/2}{\left(\frac{r}{2} + ik_n(it+\gamma)\right)^2}\right) \end{aligned} \tag{22}$$

with $\nu = -1$ for $k_n = |k_n| e^{i\varphi}$ and $-\frac{1}{4}\pi \leqslant \varphi \leqslant \frac{3}{4}\pi$ and $\nu = 1$ otherwise. I omitted errors of order $\mathcal{O}(t^{-5/2})$. There are several remarks in order:

(i) Except for the case $k_n \in \mathbb{R}$ the first summand in Eq. (22) is either identically zero or decays exponentially in time for their respective region of φ and may therefore be absorbed into the error.

(ii) For a $k_n \in \mathbb{R}$, the first term is oscillatory. However, in this case $h_\alpha(k_n) = 0$ as the Jost solution $f(-k, 0)$ has no zeros and $C(k)$ no poles on the real line. Hence the first term of Eq. (22) vanishes in the sum over $\gamma \in \{\alpha, \pm i\alpha\}$.

(iii) The complicated fractions involving k_n, r, and t may be represented by a series in inverse powers of t, which will also be a series in inverse powers of k_n. Exploiting the absence of a constant term in Eq. (10) one may insert $k = 0$ into Eq. (10) and its derivatives to obtain

$$0 = \sum_n \frac{a_n(r)}{k_n}, \tag{23}$$

$$\frac{C(0)}{3} \frac{f(0, r)}{f(0, 0)} = -\sum_n \frac{a_n(r)}{k_n^2}, \tag{24}$$

$$\frac{C(0)}{3} \partial_k \left. \frac{e^{-ikr} f(-k, r)}{f(-k, 0)} \right|_{k=0} = -\sum_n \frac{a_n(r)}{k_n^3}. \tag{25}$$

This yields a simpler expression for the asymptotically late wave function.

As a next step I employ the binomial series to express the fractions in Eq. (22) and sum over the three possibilities of $\gamma \in \{\alpha, \pm i\alpha\}$ and over all poles k_n, this results in

$$\psi_\infty(r) = -\frac{C(0)}{2\sqrt{i\pi}} \partial_k \left. \frac{f(-k, r)}{f(-k, 0)} \right|_{k=0}. \tag{26}$$

[2]Formulated in terms of lower incomplete Γ function.

Corrections to Eq. (20) are of order $\mathcal{O}(t^{-5/2})$. If $C(0) = 0$ the decay of $\psi(r, t)$ for large t will be faster, as observed in [23]. Higher orders can be worked out analogously to extract an asymptotic series for $\psi(r, t)$ in $1/\sqrt{t}$, which implies a series of the same kind for

$$P(t) = \int_0^\rho |\psi(r, t)|^2 dr, \tag{27}$$

the probability of finding the particle inside the trapping region of length ρ. The use of the binomial series is only justified for late times, where what "late" means depends on r. This onset of the algebraic decay can be estimated by equating the exponential term with slowest decay of Eq. (22) with the term (26), yielding

$$t_{\mathrm{alg}} = \frac{-3/2}{|\mathrm{Im} k_0^2|} W_{-1}\left(\frac{-|\mathrm{Im} k_0^2|}{3/2^{1/3}} \left| \frac{\psi_\infty(r) \partial_{k_0} f(-k_0, 0)}{k_0 C(k_0) f(-k_0, r)} \right|^{2/3}\right), \tag{28}$$

where W_{-1} is the -1 branch of the Lambert W function and k_0 is the wave vector belonging to the slowest exponential decay, i.e., the zero of $f(-k, 0)$ in the fourth quadrant of the complex plane closest to the origin.

Besides Eq. (27) the survival probability

$$S(t) = \left| \int_0^\infty \psi^*(r, 0) \psi(r, t) dr \right|^2, \tag{29}$$

is often used to study decaying quantum states. The long time limit of $S(t)$ can be found plugging in Eqs. (7) and (6):

$$S(t) = \left| \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{k^2 C'(k) C(k)}{f(k, 0) f(-k, 0) h_\alpha(k)} e^{-ik^2 t} h_\alpha(k) dk \right|^2 \tag{30}$$

with

$$C'(k) = \int_0^\infty u(k) \psi^*(r) dr. \tag{31}$$

So that Mittag-Leffler can be applied again to obtain

$$S(t) = \left| \sum_n b_n \sum_{\gamma \in \{\alpha, \pm i\alpha\}} M(k_n, 0, \gamma + it) \right|^2. \tag{32}$$

Using the same expansion and manipulations as for the the long time limit of ψ then yields

$$S(t) \xrightarrow{t\to\infty} \frac{1}{t^3} \frac{|C(0)|^4}{4\pi (f(0, 0))^4}, \tag{33}$$

showing that S has the same power law as P and also decays faster if $C(0) = 0$. Evaluating expansions (15) and (32) without closed form expressions for f is difficult, this is not the case for Eqs. (26) and (33). They may be evaluated numerically for any potential V such that the growth conditions on the Jost solution f and the integrals over the initial wave function C are fulfilled. Hence these considerations of late times may be of some use to test nonrelativistic models of α decay when compared to experiment.

Applications to Eckart's potential.

Eckart's potential

$$V(r) = \frac{A e^{r-\rho}}{(1 + e^{r-\rho})^2}, \tag{34}$$

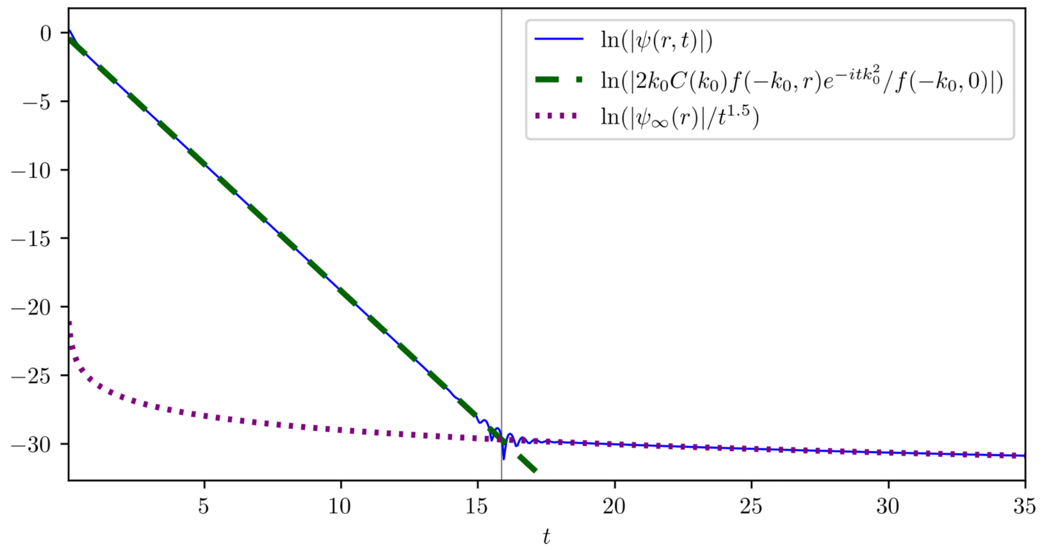

FIG. 1. Numerical logarithmic comparison of $|\psi(r,t)|$, $|\psi_\infty(r)|/t^{1.5}$ and the slowest exponential decay corresponding to the zero k_0 of $f(-k,0)$ closest to the origin in the fourth quadrant. The thin vertical line marks t_{alg}. The parameters are $A = 49.25$, $\rho = 1$, $r = 0.5$ and $\alpha = 1.25$. To compute $\psi(r,t)$ all summands of (15) corresponding to poles $|k_n| < 120$, which results in approximately 28000 summands. The code that produced this figure can be found in Ref. [27], it uses mpmath [28].

where $\rho \in \mathbb{R}$ and $A \in \mathbb{R}$ are free parameters together with the initial wave function

$$\psi_0(r) = \frac{2^{5/2}}{\rho^{3/2}\sqrt[4]{\pi}} r e^{-2(\frac{r}{\rho})^2} \tag{35}$$

provides a nice example for which an exponential choice of h would not suffice. This potential has been used to study tunneling [30] from the perspective of theoretical physics as well as from the perspective of chemistry [31]. The associated Jost solution is given by [4,32]

$$f(k,r) = e^{-ikr}\,{}_2F_1\left(\frac{1}{2} - i\delta, \frac{1}{2} + i\delta; 1 + 2ik; \frac{1}{1 + e^{r-\rho}}\right) \tag{36}$$

with $\delta = \sqrt{A - 1/4}$, where ${}_2F_1$ is the Gauss hypergeometric function.

In this setup the Mittag-Leffler theorem implies Eq. (10):

$$g(k,r) = \frac{kC(k)e^{-ikr}f(-k,r)}{h_\alpha(k)f(-k,0)} = \sum_n \frac{a_n(r)}{k - k_n}. \tag{37}$$

The main reason why my choice of h_α works while an exponential one does not is as follows.

The generalized Fourier transform of of the initial wave function, $C(k)$, satisfies the bound

$$|C(k)| \leqslant \frac{\sqrt{2}\sqrt{\rho}c_1}{|k|\sqrt[4]{\pi}} + 4c_1\sqrt[4]{\pi}\rho^{3/2}e^{\rho^2|\text{Im}(k)|^2}, \tag{38}$$

which can be derived using Eq. (13). The $\leqslant$ becomes $\approx$ for $|k|$ large enough and $k \notin \mathbb{R}$. This can be compensated for by my choice of h_α for α big enough, while clearly an exponential h does not suffice.

A detailed estimate on the real line shows

$$C(k) = \mathcal{O}(k^{-6}), \quad k \to \infty \tag{39}$$

implying that the sum (15) converges. In order to evaluate Eq. (15), the pole structure of g should be studied. Here, in addition to the artificial poles close to Eqs. (17), (18), and (19) there are poles due to the Jost solution f. It has poles at $k = in/2$ for $n \in \mathbb{N}$, however the poles cancel in the expression for g, as they appear in the numerator as well as the denominator. The function $f(-k,0)$ has zeros for complex k, symmetric about the imaginary axis. I conjecture the right arm of which approaches

$$k_n = \frac{n - \frac{1}{4} + \frac{i}{2\pi}\ln(e^{\pi\delta} + e^{-\pi\delta})}{i + \frac{\rho}{\pi}} \tag{40}$$

for large n. This conjecture is supported by numerical evidence, but I do not have a proof yet.

In Fig. 1 all of the above is used to check numerically how accurately t_{alg} reflects the transition from exponential to algebraic decay for the arbitrary choice $r = 1/2$. The behavior seen in Fig. 1 is consistent with the analysis in [9].

In Fig. 2 the evaluation of Eq. (15) is compared with the well-established Crank-Nicolson method at an early ($t = 3$) and moderately late ($t = 100$) time. One can see clearly that the two methods agree reasonably well at early times and the absolute value of $|\psi|$ still agrees at $t = 100$ while substantial phase difference has accumulated leading a large difference.

Conclusion. In the present paper I have generalized the method of van Dijk, Nogami, and Toyama [7–10] to a large class of noncompactly supported potentials and initial wave functions which includes Gaussian initial states. This method

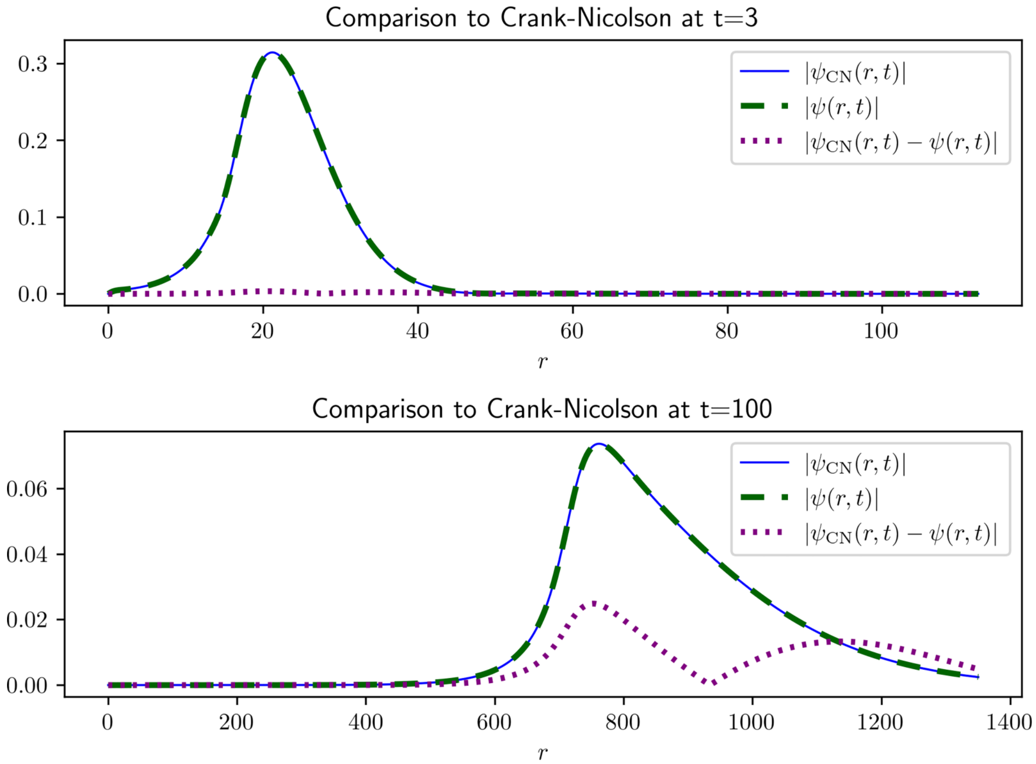

FIG. 2. Comparison of evaluation of Eq. (15) with $A = 49.25$, $\rho = 1$, and $\alpha = 1.25$ with the Crank-Nicolson (CN) method at $t = 3$ and $t = 100$. All poles with $|k_n| \leqslant 120$ are taken into account for Eq. (15). The discretization parameters for CN are $\Delta r = 0.01953125$ and $\Delta t = \Delta r^2/4$, the length of the simulation box is $L = 650$ for $t = 3$ and $L = 4480$ for $t = 100$. The CN method is implemented in Julia [29], the code that produces this figure can also be found in Ref. [27].

was used to derive the asymptotic amplitude $|\psi_\infty(r)|$ as well as estimate the onset of algebraic decay $t_{\rm alg}$ characteristic of large times. Finally, the method was applied to a Gaussian wave packet leaking through Eckart's potential against a hard-backwall potential barrier.

Acknowledgments. I wholeheartedly thank C. Bild for meticulously checking my calculations as well as S. Das for helpful discussions.

This article reflects the author's personal work and does not represent scientific standpoints of the author's employer.

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