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Diffusion-like solutions of the Schrödinger equation for a time-dependent potential well

Alberto Devoto† and Bojan Pomorišac‡

† Dipartimento di Scienze Fisiche, Università di Cagliari and Istituto Nazionale di Fisica Nucleare, Sezione di Cagliari, Via Ada Negri 18, I-09127 Cagliari, Italy
‡ Department of Chemistry and Physics, Salem State College, Salem, MA 01970, USA

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Abstract. We discuss a method of solution of the time-dependent Schrödinger equation for a time-dependent potential well. We obtain a simple solution for a well changing linearly with time and a solution for a well changing as the square root of time and as the square root of second degree polynomial in t. The quasi-energy spectra of these solutions are continuous. We use one of the solutions found to check the validity of the adiabatic approximation.

In the present work we study the quantum problem of a particle in a time-dependent square well with rigid walls. This is a prototype of a problem in which all the complications are introduced by the boundary conditions, while the equation without boundary conditions is readily solvable. One would like to solve the equation

$$\frac{\partial\Psi(x,t)}{\partial t}=\frac{i\hbar}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} \tag{1}$$

subject to the boundary conditions

$$\Psi(L(t)/2,t)=\Psi(-L(t)/2,t)=0. \tag{2}$$

Both walls of the well oscillate symmetrically about $x=0$ and parity is a good quantum number. It is straightforward to show using (1) and (2) that the norm of the solution of (1) is constant. Henceforth we will ignore the normalization constant.

One can readily write a solution to equation (1) without boundary conditions using the Fourier transform:

$$\Psi(x,t)=\int \exp[i(kx-\hbar k^2t/2m)]g(k)\,dk. \tag{3}$$

Here we assume that all the integrals in the expression for Ψ and $\partial\Psi/\partial t$, $\partial^2\Psi/\partial x^2$ exist. The nature of $g(k)$ determines the quasi-energy spectrum (i.e. the spectrum of the evolution operator)—the delta function singularities (or poles in the complex k integration plane) correspond to the discrete spectrum, while the integration over continuous k corresponds to continuous spectrum. With appropriate integration, even (odd) functions of x are automatically obtained using an even (odd) $g(k)$.

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One can write the solution of (1) in a different form; one can use the analogy between the Schrödinger equation and the diffusion equation [1] and, using the usual solution of the diffusion equation [2], write the solution of (1) in the form

$$\Psi(x, t) \sim 1/\sqrt{t} \exp\left[\frac{im}{2\hbar}\frac{x^2}{t}\right] \qquad t>0 \tag{4}$$

or more generally

$$\Psi(x, t) = \int \frac{f(x_0, t_0)}{\sqrt{t-t_0}} \exp\left[\mathrm{i}\frac{m}{2\hbar}\frac{(x-x_0)^2}{(t-t_0)}\right] \mathrm{d}x_0\, \mathrm{d}t_0. \tag{4a}$$

Here we assume that the function f is restricting the integral over t_0 to the region $t_0 < t$, so that the integral of the appropriate derivatives exists. Note that for any solution of (1) $\Psi(x, t)$, the integral over t_0 and x_0 of $\Psi(x-x_0, t-t_0)$ with an appropriate weight function is also a solution. Let us rewrite the solution (3) in a form similar to (4). Consider, for example, the fixed potential well $L(t) = L_0 =$ constant and an even wavefunction of fixed energy:

$$\begin{aligned} &\tfrac{1}{2}\exp\left(\mathrm{i}\frac{mx^2}{2\hbar t}\right)\int_{-\infty}^{+\infty} \mathrm{d}k \exp\left(-\mathrm{i}\frac{\hbar k^2 t}{2m}\right) \\ &\qquad \times\left[\delta\left(k+\frac{mx}{\hbar t}-\frac{2n+1}{L_0}\pi\right)+\delta\left(k-\frac{mx}{\hbar t}-\frac{2n+1}{L_0}\pi\right)\right] \\ &\quad = \cos\left(\frac{2n+1}{L_0}\pi x\right)\exp\left[-\mathrm{i}\frac{\hbar t}{2m}\left(\frac{2n+1}{L_0}\pi\right)^2\right]. \end{aligned} \tag{5}$$

The same solution can be obtained integrating

$$\exp\left(-\mathrm{i}\frac{\hbar t}{2m}k^2\right)\frac{\cos(kx)}{\cos(kL_0/2)}$$

over an appropriate contour in the complex k plane (for positive t the contour goes above the poles over the negative real k axis, below all poles except the nth pole over the positive real k axis, over the imaginary k axis and the contour is closed over negative $\mathrm{Im}(k)$ for positive $\mathrm{Re}(k)$, and over positive $\mathrm{Im}(k)$ for negative $\mathrm{Re}(k)$). The delta functions in (5) represent only the pole contribution of the integral of the type (3) and we see that the quasi-energy spectrum is discrete. Of course, all the parts of the complex k plane integral, e.g. the integral over imaginary $k = \mathrm{i}y$,

$$\int_{-\infty}^{+\infty} \exp\left(\mathrm{i}\frac{\hbar t}{2m}y^2\right)\frac{\cosh(yx)}{\cosh(yL_0/2)}\,\mathrm{d}y \qquad |x| \leq \frac{L_0}{2}$$

are solutions of (1); however, the pole contributions give the solutions satisfying the boundary conditions (2).

To rewrite the solutions (3) in a form analogous to (4), we assume that the function $g(k)$ is analytic in a neighbourhood of $k = 0$ (the case where this is not true is discussed later) and write

$$\begin{aligned} \Psi(x, t) &= \int_{-\infty}^{+\infty} g(k)\exp\left(-\mathrm{i}\frac{\hbar t}{2m}k^2 + \mathrm{i}kx\right)\mathrm{d}k \\ &= g(-\mathrm{i}\partial/\partial x)\int_{-\infty}^{+\infty}\exp\left(-\mathrm{i}\frac{\hbar t}{2m}k^2+\mathrm{i}kx\right)\mathrm{d}k \\ &= \frac{1-\mathrm{i}}{2}g(-\mathrm{i}\partial/\partial x)\sqrt{\frac{\pi m}{\hbar t}}\exp\left(\mathrm{i}\frac{mx^2}{2\hbar t}\right). \end{aligned} \tag{6}$$

Here it is assumed that the integral in (3) is over the whole real k axis, and the integral becomes the usual Fresnel integral. In this case the solutions of the form (3) are obtained by a particular combination of derivatives with respect to x of the diffusion-like solution (4). Of course, every derivative of a solution of (1) is also a solution. The function $g(-\mathrm{i}\partial/\partial x)$ is defined through a power series. The boundary conditions (2) read

$$g(-2\mathrm{i}\partial/\partial L)\sqrt{\frac{\pi m}{\hbar t}}\exp\left(\mathrm{i}\frac{m}{2\hbar t}\frac{L^2(t)}{4}\right)=0. \tag{7}$$

If the function $g(k)$ has a power series expansion

$$g(k)=\sum_{n=0}^{\infty}c_n k^n$$

the boundary condition at $x=L(t)/2$ can be written in terms of the Hermite polynomials H_n

$$\sum_{n=0}^{\infty}c_n(\mathrm{i}\rho(t))^n H_n(\rho(t)L(t)/2)=0 \qquad \forall t \tag{8}$$

where $\rho(t)\equiv\sqrt{-\mathrm{i}m/2\hbar t}$; (the boundary condition at $x=-L(t)/2$ leads to a similar equation). The solution of (8) is a non-trivial problem, the equation is an identity with respect to the variable t. This equation can be solved if $L(t)$ is a linear function of t using the generating function for the Hermite polynomials; however it is instructive to solve this case directly from (3) and (2):

$$\begin{aligned}0&=\int_{-\infty}^{+\infty}\exp(\mathrm{i}kL(t)/2-\mathrm{i}\hbar tk^2/2m)g(k)\,\mathrm{d}k\\&=\int_{-\infty}^{+\infty}\exp\left[\mathrm{i}k(L_0+at)/2-\mathrm{i}\frac{\hbar t}{2m}k^2\right]g(k)\,\mathrm{d}k\\&\quad+\int_{-\infty}^{+\infty}\exp\left[-\mathrm{i}k(L_0+at)/2-\mathrm{i}\frac{\hbar t}{2m}k^2\right]g(k)\,\mathrm{d}k\end{aligned} \tag{9}$$

where $L(t)$ is assumed to be a linear function, and $g(k)$ is assumed even—the case of odd $g(k)$ is analogous. We can perform an inverse Fourier transform with respect to time multiplying by $\exp(-\mathrm{i}\omega t)$ and integrating over $\mathrm{d}t$, using

$$\delta(f(x))=\sum_i\frac{1}{|f'(x_i)|}\delta(x-x_i)$$

where x_i's are the zeros of $f(x)$; after some manipulation we obtain

$$\exp\left[\mathrm{i}\left(\frac{ma}{2\hbar}+y\right)L_0/2\right]g\left(\frac{ma}{2\hbar}+y\right)+\exp\left[\mathrm{i}\left(\frac{ma}{2\hbar}-y\right)L_0/2\right]g\left(\frac{ma}{2\hbar}-y\right)=0 \tag{10}$$

where y is a variable depending on ω. It is easy to solve this equation for $L_0=0$ (the more general case is then obtained with a change of variable from x to $x-x_0$). In this case, the function $g(ma/2\hbar+y)$, an even function of the whole argument, is an odd function of y. There is an infinite number of solutions

$$g(k)=\cos\left(\frac{2n+1}{ma}\pi\hbar k\right)$$

which enables us to perform the integral in (3) and, shifting t into $t+t_0$, one obtains the solution of (1):

$$\Psi_e(x,t)=\frac{1}{\sqrt{t+t_0}}\exp\left\{\frac{im}{2\hbar(t+t_0)}\left[x^2+\left(\frac{2n+1}{ma}\pi\hbar\right)^2\right]\right\}\cos\left[\frac{2n+1}{a(t+t_0)}\pi x\right]. \qquad (11)$$

It can be verified that this is the solution of (1) by direct substitution of (11) into (1). Here n is an arbitrary integer, and it is obvious that the boundary conditions $\Psi=0$ for $x=\pm a(t+t_0)/2$ are satisfied. The analogous odd wavefunction is of the form

$$\Psi_o(x,t)=\frac{1}{\sqrt{t+t_0}}\exp\left\{\frac{im}{2\hbar(t+t_0)}\left[x^2+\left(\frac{2n}{ma}\pi\hbar\right)^2\right]\right\}\sin\left[\frac{2n}{a(t+t_0)}\pi x\right] \qquad (11a)$$

where n is again an arbitrary integer. Different initial conditions can be fitted by taking linear combinations of Ψ_e and Ψ_o with different n's. One can also shift x into $x-x_0$ in (11) and (11a) to obtain functions satisfying asymmetric boundary conditions at $x=x_0\pm a(t+t_0)/2$. A similar solution has been found by different methods by Doescher and Rice [3].

Analogously one can solve the three-dimensional spherically symmetric well with the boundary conditions: $\Psi(r=at,\theta,\phi)=0$. It can be shown that the radial part of the wavefunction is given by

$$R_l(r,t)=\frac{1}{r\sqrt{t}}\exp\left[\mathrm{i}\frac{m}{2\hbar}\frac{r^2+\delta^2}{t}\right]f_l\left(\frac{m\delta r}{\hbar t}\right) \qquad (12)$$

where the function $f_l(z)$ satisfies the equation

$$f_l''(z)-l(l+1)f_l(z)/z^2+f_l(z)=0$$

that is, $f_l(z)$ is z times the spherical Bessel function y_l, and the constant δ is determined by the condition $f_l(m\delta a/\hbar)=0$.

Let us now discuss the case where the function $g(k)$ is not analytic at $k=0$. Assume, for example, that the function is of the form $k^\alpha\phi(k)$ where $\phi(k)$ is analytic at zero. Looking at the form of the integral $\int k^{\nu-1}\exp(-\beta k^2-\gamma k)\,\mathrm{d}k$ [4] (with β with a positive real part) suggests a trial solution of (1) of the form

$$\Psi(x,t)=t^{-\delta}\exp(-\eta x^2/t)D_\nu(\gamma x/\sqrt{(t)})$$

where the D_ν are parabolic cylinder functions [5]. Replacing this form in (1) and shifting the variables x and t one finds the following solution:

$$\Psi(x,t)=(t-t_0)^{-(\nu+1)/2}\exp\left[\frac{im}{4\hbar}\frac{(x-x_0)^2}{t-t_0}\right]y_\nu\left(\sqrt{\frac{m}{\mathrm{i}\hbar(t-t_0)}}(x-x_0)\right) \qquad (13)$$

where the functions $y_\nu(z)$ are: $D_\nu(z)$, $D_\nu(-z)$, $D_{-\nu-1}(\mathrm{i}z)$, $D_{-\nu-1}(-\mathrm{i}z)$, and their linear combinations (conveniently, one may choose even or odd combinations). Here, one chooses ν so as to fit a particular boundary condition; for example to fit a condition

$$\Psi(x=x_0+\sqrt{\mathrm{i}\hbar(t-t_0)/m},t)=0$$

one may choose $\nu=2$ for an even function. We see that the function that describes a potential well changing as the square root of t is considerably more complicated than the linearly changing well (11). In addition to shifting x into $x-x_0$, integrating over x_0 and t_0 with a suitably chosen weight function, differentiating with respect to x (differentiation with respect to t is proportional to repeated x differentiation), one can create new solutions of (1) by integrating and differentiating with respect to ν. For example, differentiation with respect to ν of (13) will produce a solution of the form (3) with $g(k)$ having a logarithmic singularity at zero.

Note that the explicit solutions (i.e. (11) and (13)) that we discussed arise from integration over continuous k, these solutions therefore, as expected, have a continuous quasi-energy spectrum, in contrast to (5).

However, in all the ways of modification of solutions of (1) that we mentioned, there is not a single one that transforms the boundary conditions in a simple way. One would like to find a change of variables $x \to f_1(x, t)$, $t \to f_2(x, t)$ that, while leaving (1) unchanged (except, perhaps, by an overall multiplication by a function) would simply transform the boundary conditions. Unfortunately, it is straightforward to show that the only change of this sort is $x \to ax + b$, $t \to a^2 t$.

We now examine the general conditions necessary for this type of solution. We look for solutions of the following form:

$$\Psi(x, t) = h(x, t) f\left(\frac{\varphi(x)}{g(t)}\right). \tag{14}$$

The function f takes into account the boundary conditions (for example we may choose $g(t) = \varphi(L(t)/2)$ and require that $f(\pm 1) = 0$, for φ odd, or $f(1) = 0$ for φ even). Substituting (14) into (1) and demanding the cancellation of the terms containing f' leads to following equation for $h(x, t)$

$$\ln h(x, t) = -\tfrac{1}{2} \ln \varphi'(x) - \frac{1}{2\mathrm{i}\beta}\left(\frac{\mathrm{d} \ln g(t)}{\mathrm{d}t}\right) \int^x \frac{\varphi(s)}{\varphi'(s)} \mathrm{d}s + K(t) \tag{15}$$

where $\beta = \hbar/2m$ and K is an arbitrary function of time. If, furthermore,

$$\left(\frac{1}{h(x, t)} \frac{\partial^2 h(x, t)}{\partial x^2} - \frac{1}{\mathrm{i}\beta} \frac{\partial \ln h(x, t)}{\partial t}\right) \frac{g^2(t)}{\varphi'^2(x)} = \Phi\left(\frac{\varphi(x)}{g(t)}\right) \tag{16}$$

where Φ is function *only* of the ratio $\varphi(x)/g(t)$, then f satisfies the equation

$$f''(y) + \Phi(y) f(y) = 0.$$

Combining (15) and (16), one obtains, after some manipulations

$$\Phi\left(\frac{\varphi(x)}{g(t)}\right) = \left[-\tfrac{1}{2} S(x) + K_2(t) + \frac{1}{\mathrm{i}\beta} \frac{\mathrm{d} \ln g(t)}{\mathrm{d}t} \frac{\varphi(x)\varphi''(x)}{\varphi'^2(x)} - \frac{1}{4\beta^2}\left(\frac{\mathrm{d} \ln g(t)}{\mathrm{d}t}\right)^2 \times \left(\frac{\varphi(x)}{\varphi'(x)}\right)^2 - \frac{1}{2\beta^2}\left(\frac{\mathrm{d}^2 \ln g(t)}{\mathrm{d}t^2}\right) \int^x \frac{\varphi(s)}{\varphi'(s)} \mathrm{d}s \right] \frac{g^2(t)}{\varphi'^2(x)}. \tag{17}$$

Here $S(x)$ is the Schwarzian derivative of $\varphi(x)$

$$S(x) = \frac{\varphi'''(x)}{\varphi'(x)} - \frac{3}{2}\left(\frac{\varphi''(x)}{\varphi'(x)}\right)^2$$

and

$$K_2(t) = -\frac{1}{\mathrm{i}\beta}\left[\frac{1}{2} \frac{\mathrm{d} \ln g(t)}{\mathrm{d}t} + \frac{\mathrm{d}K(t)}{\mathrm{d}t}\right]$$

is an arbitrary function of t. Equation (17) can also be expressed in differential form: application of the operator

$$\left(\frac{\varphi(x)}{\varphi'(x)} \frac{\partial}{\partial x} + \frac{g(t)}{g'(t)} \frac{\partial}{\partial t}\right)$$

to the right-hand side of (17) must yield zero. Equations (15) and (17) are necessary conditions for ansatz (14) to work.

Using (14) we can find a third solution. If we assume $\varphi(x)=x$ and choosing $\mathrm{d}K(t)/\mathrm{d}t=-g'(t)/(2g(t))$, for

$$\Phi\left(\frac{\varphi(x)}{g(t)}\right)=-\frac{A_1}{4\beta^2}\left(\frac{x}{g(t)}\right)^2$$

with the help of equation (16) we find

$$g(t)=\sqrt{A_2(t+A_3)^2+A_1/A_2} \tag{18}$$

where A_1, A_2 and A_3 are arbitrary constants. In this case the function f satisfies

$$f''(y)-\frac{A_1}{4\beta^2}y^2f(y)=0$$

whose solution is

$$f(y)=\sqrt{y}\,\Upsilon_{1/4}\left(\sqrt{-\frac{A_1}{4\beta^2}}\,\frac{y^2}{2}\right). \tag{19}$$

Here Υ denotes a Bessel function of the first or second kind (J or Y) or a Hankel function ($H^{(1)}$ or $H^{(2)}$). The boundary condition requirement $f(\pm1)=0$ imposes some restrictions on the possible values of A_1. Then the wavefunction is given by

$$\Psi(x,t)=\frac{1}{\sqrt{g(t)}}\exp\left[\frac{\mathrm{i}}{4\beta}\frac{g'(t)}{g(t)}x^2\right]\sqrt{y}\,\Upsilon_{1/4}\left(\sqrt{-\frac{A_1}{4\beta^2}}\,\frac{y^2}{2}\right) \tag{20}$$

where $y=x/g(t)$, $g(t)$ is given by (18), and an overall normalization has been suppressed.

We would like to emphasize that this is one of the rare cases in quantum mechanics where one can follow the time development of a system having a time-dependent Hamiltonian. Therefore one has the possibility of checking some of the standard methods (for example the adiabatic approximation) used when dealing with time-dependent problems. The infinite potential well studied here is used in nuclear physics [6] and in modelling white dwarf stars (see e.g. Bransden and Joachain [7]). Therefore we use the spherically symmetrical solution (equation (12)); and we investigate the *limits of the adiabatic approximation when the radius of the potential well changes* with time. (The analogous one dimensional well has been studied in [8].)

We compute the total probability of excitation (due to the change of the radius) for a system initially in the ground state. Since this probability vanishes in the adiabatic approximation one has a quantitative estimate of its limits.

At time $t=0$ the radius of the well is $r_i=at_0$, where a is the expansion velocity, and the system is in the state

$$\Psi(r)=\frac{1}{r}\sqrt{\frac{2}{at_0}}\sin\left(\frac{\pi r}{at_0}\right) \tag{21}$$

which is the ground state of a spherical well of constant radius r_i. To find the exact solution of the time-dependent Schrödinger equation at time t with initial condition (21) we expand the wavefunction in terms of

$$R_0^{(p)}(r,t)=\frac{1}{r}\sqrt{\frac{2}{a(t+t_0)}}\exp\left(\mathrm{i}\frac{m}{2\hbar}\frac{r^2+\delta^2}{t+t_0}\right)\sin\left(p\frac{\pi r}{a(t+t_0)}\right). \tag{22}$$

Here $R_0^{(p)}$ is a solution of type (12) with $l=0$ and $\delta = p\pi\hbar/ma$, while p is an arbitrary positive integer. Thus the wavefunction at time t is

$$\Psi(r, t) = \sum_{p=1}^{\infty} a_p(\alpha) R_0^{(p)}(r, t). \tag{23}$$

The expansion coefficients a_p are given by

$$a_p(\alpha) = \frac{2}{\pi} \exp\left(-\mathrm{i}\frac{p^2}{4\alpha}\right) \int_0^{\pi} \exp(-\mathrm{i}\alpha\lambda^2) \sin(p\lambda) \sin(\lambda)\, \mathrm{d}\lambda. \tag{24}$$

The whole dependence of these coefficients on the parameters of the problem is contained in the dimensionless quantity

$$\alpha \equiv \frac{mar_i}{2\hbar\pi^2}. \tag{25}$$

When the size of the well is $r_f = a(t+t_0)$, the amplitude of finding the system in the ground state of the expanded well is

$$A_0 = \sum_{p=1}^{\infty} a_p(\alpha) a_p^*(\beta) \tag{26}$$

where * indicates complex conjugation and

$$\beta \equiv \frac{mar_f}{2\hbar\pi^2}. \tag{27}$$

We evaluated numerically A_0 for different values of the parameters α and β. In figures 1 and 2 we present the results for the probability of excitation: $P = 1 - |A_0|^2$, which vanishes in the adiabatic approximation, as a function of α and of $\beta/\alpha = r_f/r_i$. For the contracting well, as it can be seen from (26), one can read the results from the same graphs by changing the sign of α and taking the inverse of β/α; for example, the contraction for $\alpha = -1$ and $r_f/r_i = 0.9$ has the same probability of excitation as the

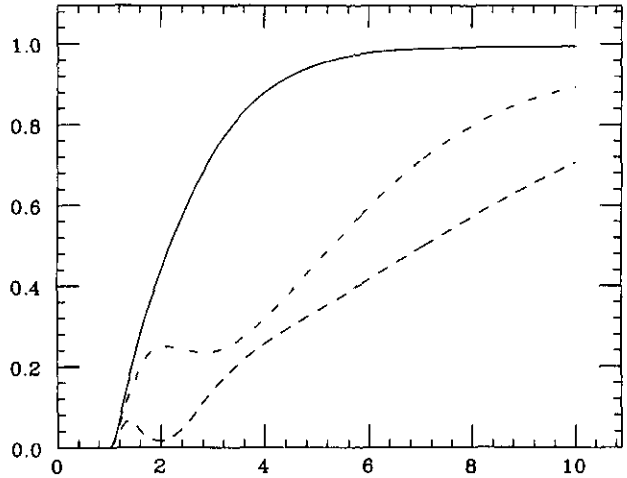

Figure 1. The probability of excitation for fixed α against r_f/r_i; full curve: $\alpha = 0.15$, chain curve: $\alpha = 0.10$, broken curve: $\alpha = 0.06$.

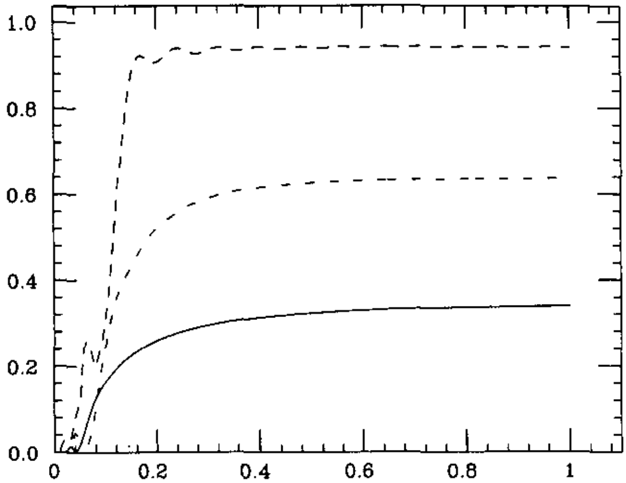

Figure 2. The probability of excitation for fixed r_f/r_i against α; full curve: $r_f/r_i=1.5$, chain curve: $r_f/r_i=2.0$, broken curve: $r_f/r_i=4.0$.

expansion with $\alpha=+1$ and $r_f/r_i=1/0.9$. In the numerical evaluation we kept up to fifty terms in the expansion of the wavefunction and we made sure that the sum of $|a_p|^2$ was equal to one to six significant figures. This also implies that for $\beta=\alpha$ the probability of excitation vanishes.

As it can be seen from the figures, the adiabatic approximation is valid only for a limited range of the parameters. The adiabatic limit corresponds to $a\to 0$, i.e. $\alpha, \beta\to 0$. In this limit, the asymptotic behaviour of A_0 is

$$A_0 \sim 1+\mathrm{i}(\beta-\alpha)\left(\frac{\pi^2}{3}-\frac{1}{2}\right)-\left(\frac{\alpha^2}{2}+\frac{\beta^2}{2}\right)\left(\frac{3}{2}-\pi^2+\frac{\pi^4}{5}\right)+\alpha\beta\left(\frac{\pi^2}{3}-\frac{1}{2}\right)^2$$
$$+\alpha\beta\sum_{p=2}^{\infty}\frac{64p^2}{(p^2-1)^2}\exp\left[\mathrm{i}\frac{p^2}{4}\left(\frac{1}{\beta}-\frac{1}{\alpha}\right)\right]. \tag{28}$$

The sum in this equation has an upper limit $64(\pi^2/12+\frac{1}{16})$, hence the probability of excitation goes to zero as a^2 in the adiabatic limit.

The dependence of the parameters α and β on the radius of the well is of interest. For example, for a nucleus of radius $r=5$ fm and for a velocity $a=0.01c$, the parameter $\alpha=1.2\times10^{-2}$, i.e., for non-relativistic speeds the adiabatic approximation is very good for a wide range of r_f/r_i. In contrast for a white dwarf of radius $r=10^4$ km, a in ms^{-1} is: $1.25\times10^{-9}\,\alpha$, i.e. for any reasonable velocity α is very large and the adiabatic approximation is not applicable. In conclusion, the range of applicability of this approximation depends crucially on the radius of the system.

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