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Construction of exactly soluble double-well potentials

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Solving the tunneling problem in a double-well potential requires knowing the wave function not just of the ground state, but also of the first excited state. A method is described that allows one to construct potentials together with these two wave functions. No approximations are made. To illustrate the method several examples are given. These include potentials that either diverge for large $|x|$ or become asymptotically flat, with one or two wells, which may be symmetric or asymmetric.

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Double-well potentials have been used extensively to model a remarkable range of natural phenomena. This is, in part, because tunneling is a quite unbiquitous effect, but also because double-well potentials constitute a valuable testing ground for studying the transition between quantum and classical behavior, which is essential to a number of fundamental problems, including, for example, the quantum theories of measurement [1], friction and decoherence [2], and molecular structure [3–5].

Exact solutions are both desirable and rare; various kinds of semiclassical approximations have been the main tool in these studies [6]. A most remarkable feature of tunneling in double wells is the extreme sensitivity to perturbations [7–9]. In an even potential the eigenstates are delocalized: the probability amplitudes for the particle to be found on the left or on the right well are equal. The effect of even minute odd perturbations will be quite large, leading to eigenstates localized at one or the other well. This instability, the "flea-on-the-elephant" effect [9], makes the problem both interesting and difficult: the analysis requires a very careful control of the asymptotic behavior of tails of wave functions [8–11]. Of course, once the exact solutions of the unperturbed problem are available the effect of perturbations is easy to handle: this is precisely the textbook problem that perturbation theory for almost degenerate states is supposed to solve. This is one reason why such exact solutions are valuable.

Our problem is to solve the Schrödinger equation

$$\psi_n''(x)+[\epsilon_n-u(x)]\psi_n(x)=0 \tag{1}$$

for the two lowest states $n=0$ and 1, for a double-well potential $u(x)$. The potential and the energies have been scaled by $2m/\hbar^2$. Rather than following the usual approach, in which one starts from a given u to find ψ_n and ϵ_n, we will proceed backwards: given the "answer," find the "problem." For example, given a wave function ψ_0 and its energy ϵ_0, it is trivial to find the corresponding potential u by substituting into Eq. (1) [see Eq. (6) below]. For our present purposes this is not sufficient; we also need the first excited state ψ_1 and its energy ϵ_1.

First we show that given a certain function $\phi(x)$ and an energy splitting $\epsilon=\epsilon_1-\epsilon_0$, one can construct a potential u, together with its two lowest states ψ_0 and ψ_1 exactly. This is our main result. Then we discuss the choice of the function ϕ. If this method is to be useful one should be able to choose ϕ functions that lead to interesting potentials. In other words, one should identify features of ϕ that will lead to desirable properties of the potential, such as its having one or two wells, its being symmetric or not, and whether for large $|x|$ it diverges or becomes asymptotically flat. To illustrate the method, we offer specific examples. The first consists of an asymmetric double-well potential that is the superposition of two Morse potentials [12] (see Ref. [13] for the solution to the symmetric version of this potential using other methods). The second example is a symmetric, asymptotically flat, double-well potential that, for large well separations, becomes a superposition of two Eckart potentials [12]. For simplicity, here we will only deal with one-dimensional situations, but *this restriction is not essential.*

Consider the function ϕ such that

$$\psi_1=\phi\psi_0 \,. \tag{2}$$

Substitute Eq. (2) into Eq. (1) for $n=1$. Write down Eq. (1) for $n=0$, multiplied by ϕ. Subtracting these two equations one obtains

$$\psi_0'+\chi\psi_0=0 \,. \tag{3}$$

The function χ, given by

$$\chi=\frac{\phi''+\epsilon\phi}{2\phi'} , \tag{4}$$

where $\epsilon=\epsilon_1-\epsilon_0$, can be recognized as the superpotential, a function that has also been found useful in the context of supersymmetric quantum mechanics [14]. Incidentally, Eq. (4) provides a simple way to construct the superpotential χ for potentials for which ψ_0 and ψ_1 are known (this includes, of course, *all* soluble potentials). The remarkable feature of Eq. (3) is that it is easily integrable. The ground-state wave function is

$$\psi_0(x)=\psi_0(0)\exp\left[-\int_0^x\chi(x')dx'\right] , \tag{5}$$

where $\psi_0(0)$ is a normalization constant. Substituting $\psi_0(x)$ into Eq. (1) with $n=0$ determines the potential up to an additive constant:

$$u(x)=\frac{\psi_0''}{\psi_0}+\epsilon_0=\chi^2-\chi'+\epsilon_0 . \tag{6}$$

Let us summarize. Given ϕ and ϵ, first one calculates χ from Eq. (4), then ψ_0 and u from Eqs. (5) and (6), and finally, ψ_1 is obtained from Eq. (2). No approximations are made.

Now we proceed to the next stage: what ϕ should we choose? If we want ψ_0 and ψ_1 to be the ground and the first excited states, ϕ should have one node. Furthermore, if one desires an even potential, then ϕ should be odd. For example, $\phi=x$ leads, trivially, to a harmonic oscillator potential.

Suppose we want to construct a symmetric potential with two widely separated wells. Then ψ_0 and ψ_1 are approximately given by $\psi_{0,1}\propto f(x)\pm f(-x)$, where $f(x)$ is the ground state of one of the isolated wells, say, the one on the right. This suggests that we choose ϕ so that in the vicinity of the right well $\phi\approx$const, while in the vicinity of the left well $\phi\approx-$const. For example, choices of ϕ such as $\tanh(\beta x)$, $\tan^{-1}(\beta x)$, or $\text{erf}(\beta x)$ do lead to interesting double-well potentials. If we want an even potential with an *even* number of wells we may require that $x=0$ be a maximum of $u(x)$. Substituting

$$\phi(x)=\phi_1 x+\frac{1}{3!}\phi_3 x^3+\frac{1}{5!}\phi_5 x^5+\cdots$$

into Eqs. (4) and (6), the condition for $u''(0)<0$ is

$$(2\phi_3+\epsilon\phi_1)^2-\phi_1\phi_5<0 . \tag{7}$$

Let us pursue further the case of $\phi=\tanh(\beta x)$. It satisfies condition (7) and leads to a symmetric potential that is the sum of two Morse wells [13]

$$u(x)=U_M^L(x-x_L)+U_M^R(-x-x_R) . \tag{8}$$

The Morse potential with minimum $-U_0$ at $x=0$ is given by [12]

$$U_M(x)=U_0(e^{-4\beta x}-2e^{-2\beta x}) . \tag{9}$$

To illustrate our method in more detail we will consider a slight generalization leading to an asymmetric double well,

$$\phi=\alpha+\tanh(\beta x) . \tag{10}$$

The superpotential χ, given by Eq. (4), is

$$\chi(x)=-\beta\tanh(\beta x)+\frac{\epsilon}{4\beta}[\sinh(2\beta x)+2\alpha\cosh^2(\beta x)] , \tag{11}$$

the ground-state wave function Eq. (5) is

$$\psi_0(x)=\psi_0(0)\cosh(\beta x)\exp\left[-\frac{\epsilon}{4\beta^2}\left[\sinh^2(\beta x)+\alpha\beta x+\frac{\alpha}{2}\sinh(2\beta x)\right]\right] , \tag{12}$$

while ψ_1 is given by Eq. (2). The potential Eq. (6) is determined only up to an additive constant. If we choose the ground state energy to be

$$\epsilon_0=-\beta^2-\frac{\epsilon}{2}+\frac{\epsilon^2}{32\beta^2}(1-\alpha^2) , \tag{13}$$

then $u(x)$ is the sum of two Morse wells as in Eqs. (8) and (9), but now with different depths

$$U_0^{L,R}=4\beta^2\left[1\pm\frac{2\epsilon\alpha}{(4\beta)^2}\right]^2 . \tag{14}$$

The difference in depths, the asymmetry, is $v:=U_0^L-U_0^R=2\epsilon\alpha$. The minima of the wells are located at

$$x_{L,R}=\mp\frac{1}{2\beta}\ln\frac{(4\beta)^2\pm2\epsilon\alpha}{\epsilon(1\mp\alpha)} . \tag{15}$$

Notice that changing ϵ while keeping β and v fixed shifts the Morse wells without deforming them. In fact, it is instructive to invert Eq. (14) to exhibit explicitly the exponential dependence of ϵ on the well separation $X=x_R-x_L$,

$$\epsilon=\left[\frac{v^2}{4}+[(4\beta)^4-v^2]e^{-2\beta X}\right]^{1/2} . \tag{16}$$

Furthermore, substituting $\alpha=v/2\epsilon$ into Eq. (12) shows that, for sufficiently large X, a minute asymmetry v will

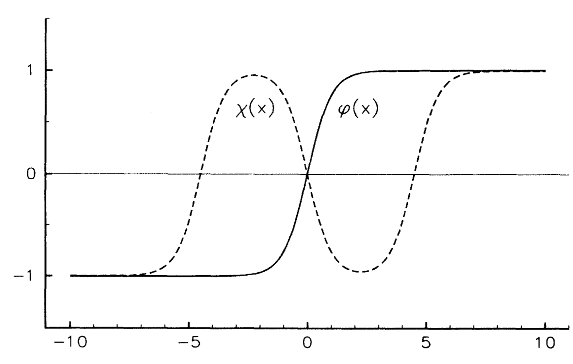

FIG. 1. The function $\phi(x)$, given by Eq. (18) for $a^2=1$ and $b^2=0.999$, and the corresponding superpotential $\chi(x)$.

induce a pronounced localization on one well or the other (the flea-on-the-elephant effect) [8,9]. By "minute" we mean $|v| \ll U_0$, but still much larger than the energy splitting in the symmetric case, $(4\beta)^2\exp(-\beta X)$. For large X this is not a restrictive condition at all.

The examples above involve potentials that diverge for large $|x|$. For potentials that asymptotically vanish we have $\psi_n \sim \exp(-\sqrt{-\epsilon_n}|x|)$, which implies that for large $|x|$

$$\phi \sim \exp[-(\sqrt{-\epsilon_0}-\sqrt{-\epsilon_1})|x|] \; . \tag{17}$$

For example, $\phi=\sinh(\alpha x)$ leads to the Eckart potential $u(x) \propto 1/\cosh^2(\alpha x)$ with the desired asymptotic behavior. However, it violates condition (7) and has only one well. To generate an asymptotically flat double well requires a ϕ that resembles a tanh for small x and satisfies (17) for large $|x|$. An acceptable choice is

$$\phi(x)=\frac{\sinh(ax)}{\cosh(bx)} \; , \tag{18}$$

where $a=\sqrt{-\epsilon_0}$ and $b=\sqrt{-\epsilon_1}$.

In Fig. 1 a plot of ϕ and of the superpotential χ is shown for $\epsilon_0=-1$ and $\epsilon_1=-0.999$. It is obvious from Eq. (5) that zeros of χ correspond to extrema of ψ_0. Thus the three zeros of χ are an indication that this potential has at least two wells.

The ground-state wave function and the corresponding potential are

$$\psi_0(x)=\psi_0(0)\frac{2ae^{ax}(1+e^{bx})}{(a+b)(e^{2ax}+e^{2bx})+(a-b)(e^{2(a+b)x}+1)} \tag{19}$$

and

$$u(x)=-2\frac{(a^2-b^2)[a^2\cosh^2(bx)+b^2\sinh^2(ax)]}{[a\cosh(ax)\cosh(bx)-b\sinh(ax)\sinh(bx)]^2} \; . \tag{20}$$

These are shown in Fig. 2. Equations (19) and (20) are exact, but it may be useful to note that as b tends to a, the two wells separate and tend to Eckart potentials $u_E(x)=-2a/\cosh^2[a(x-x_m)]$ centered at $x_m \approx \pm(1/2a)\ln[4a/(a-b)]$. This leads to the expected asymptotic exponential dependence of ϵ on the well separation $2x_m$.

A simple and useful expression for the wave function normalization is obtained as follows. For even potentials integration of Eq. (1) [15] leads to

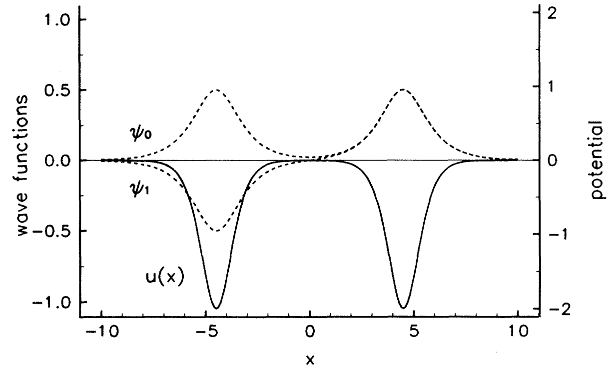

FIG. 2. The potential and the exact wave functions of the ground and first excited states for $\phi(x)$ given by Eq. (18) with $a^2=1$ and $b^2=0.999$.

$$\epsilon=\frac{\psi_0(0)\psi_1'(0)}{\int_0^\infty \psi_0\psi_1 dx} \tag{21}$$

exactly. When the wells are far apart we may approximate $\psi_1'(0) \approx \phi'(0)\psi_0(0)$ in the numerator and replace the integral in the denominator by $\frac{1}{2}$. This implies

$$\psi_0(0) \approx \left[\frac{\epsilon}{2\phi'(0)}\right]^{1/2} \; . \tag{22}$$

We have only dealt with tunneling in one-dimensional potentials, but the method presented here may be of use in a variety of other situations. For example, one may generalize to multidimensional potentials or one may be interested in single-well nontunneling potentials, where two exact eigenstates are needed. Notice, by the way, that there is no restriction to the two lowest-lying states; choosing ϕ with the appropriate numbers of zeros and poles will lead to a ψ_0 and ψ_1 that are the nth and the mth excited states. One field in which the ideas of this work are likely to be useful is supersymmetric quantum mechanics [14], where the superpotential χ, a quantity that has emerged so naturally here, is such a central concept. Another possible application, given the formal similarity between the Schrödinger and the diffusion equations, is in diffusion problems in nontrivial potentials [16].

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