AAPT PHYSICS EDUCATION | AMERICAN JOURNAL of PHYSICS

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Citation: American Journal of Physics **45**, 569 (1977); doi: 10.1119/1.10942
View online: http://dx.doi.org/10.1119/1.10942
View Table of Contents: http://scitation.aip.org/content/aapt/journal/ajp/45/6?ver=pdfcov
Published by the American Association of Physics Teachers

Construction of some soluble quantal problems

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(Received 26 October 1976; revised 14 December 1976)

Solutions to the Schrödinger equation for two or more simple potentials are used to construct, in closed form, solutions for relatively complicated potentials.

It is always useful to generate new soluble problems through the superposition of problems that have been solved. In Newtonian mechanics, we have for conservative forces a superposition procedure known as *Bonnet's theorem,* expressed as follows in Whittaker's *Dynamics*[1]:

> If a given orbit can be described in each of n given fields of force, taken separately, the velocities at any point P of the orbit being $v_1, v_2, \ldots, v_n$, respectively, then the same orbit can be described in the field of force which is obtained by superposing all these fields, the velocity at the point P being $(v_1^2 + v_2^2 + \cdots + v_n^2)^{1/2}$.

The proof is simple: At any point, in each of the separate force fields, the normal force is given by $F_j = mv_j^2/R$, where R is the local radius of curvature. In the superposed fields, $F = F_1 + F_2 + \cdots + F_n$, $mv^2/R = m(v_1^2 + v_2^2 + \cdots + v_n^2)/R$, and therefore $F = mv^2/R$, with the same R as for each separate field. Conservation of energy assures that the relation is maintained along the orbit. One should note that most of the orbits of the separate fields and of the combined fields have nothing in common; only a few are the same. Both Whittaker and Routh[1] present illustrative problems involving motion on an ellipse as a result of the simultaneous action of three forces: one inverse square force from each focus of the ellipse, and a harmonic oscillator force from the center of the ellipse.

It is natural to ask whether anything similar exists in quantum mechanics. Of course, there one cannot superpose force fields and solutions in any way that parallels closely what can be done in classical mechanics: energy eigenfunctions are determined by the behavior of the potential energy function at all points. One can, however, make use of the following. Suppose that one has, for different potential energy functions $V_1, V_2, \ldots, V_n$, real eigenfunctions $\psi_1, \psi_2, \ldots, \psi_n$ that satisfy the same boundary conditions and that all have the same energy E:

$$(T + V_1)\psi_1 = E\psi_1,$$
$$(T + V_2)\psi_2 = E\psi_2,$$
$$\vdots$$
$$(T + V_n)\psi_n = E\psi_n.$$

Multiply the jth equation by C_j and add

$$(T + V)\psi = E\psi, \tag{1}$$

where

$$\psi = C_1\psi_1 + C_2\psi_2 + \cdots + C_n\psi_n \tag{2}$$

and

$$V = \frac{C_1V_1\psi_1 + C_2V_2\psi_2 + \cdots + C_nV_n\psi_n}{C_1\psi_1 + C_2\psi_2 + \cdots + C_n\psi_n}. \tag{3}$$

The essence of this construction is nothing but the trivial statement that, given ψ, one can solve Eq. (1) for V. However, this formulation suggests some useful applications. One could call it a quantal Bonnet's theorem: the connection between it and the classical Bonnet's theorem is admittedly tenuous because the structure is entirely different, but there is a similarity in motivation.

Consider first a three-dimensional double-well problem constructed from two harmonic oscillator solutions. In cylindrical coordinates, choose

$$V_1 = (K/2)\,[(z - l)^2 + R^2],$$
$$V_2 = (K/2)[(z + l)^2 + R^2].$$

Then

$$(T + V_1)\psi_1 = E\psi_1,$$
$$(T + V_2)\psi_2 = E\psi_2$$

are solved by

$$\psi_1 = \exp\{-(\alpha^2/2)[(z - l)^2 + R^2]\},$$
$$\psi_2 = \exp\{-(\alpha^2/2)[(z + l)^2 + R^2]\},$$

where

$$\alpha^2 \equiv (mK)^{1/2}/\hbar \quad \text{and} \quad E = 3\hbar^2\alpha^2/2m.$$

The even solution for the double-well problem,

$$\psi_e = \psi_1 + \psi_2,$$

is given by Eq. (2) with $C_1 = C_2 = 1$. The result satisfies Eq. (1),

$$(T + V_e)\psi_e = E\psi_e,$$

for a potential energy function of the form given by Eq. (3):

$$V_e = (V_1\psi_1 + V_2\psi_2)/(\psi_1 + \psi_2)$$
$$= (E/3)\{[(\zeta - \lambda)^2 + \rho^2]e^{+\lambda\zeta} + [(\zeta + \lambda)^2 + \rho^2]e^{-\lambda\zeta}\}(e^{+\lambda\zeta} + e^{-\lambda\zeta})^{-1}, \tag{4}$$

where $\rho \equiv \alpha R$, $\zeta \equiv \alpha z$, and $\lambda \equiv \alpha l$. Figure 1 shows, for $\rho = 0$, the V_e and ψ_e obtained with $\lambda = 1.5$, that is, for fair separation of the two component wells.

The odd solution

$$\psi_o = \psi_1 - \psi_2$$

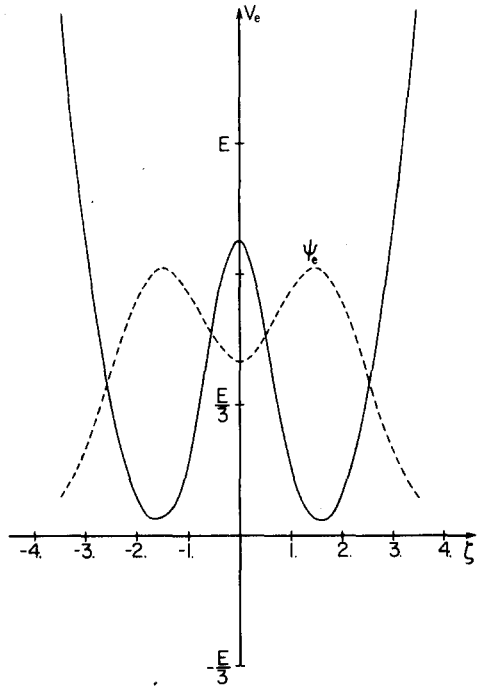

Fig. 1. The potential energy V_e of Eq. (4), for $\lambda = 1.5$, as a function of $\zeta = \alpha z$ along the $\rho = 0$ line joining the potential minima. The vertical scale is marked in multiples of $E/3$, the energy associated with the motion along one axis for completely separated wells. The dashed curve is the wave function $\psi_e(\zeta,\rho = 0)$ in arbitrary units.

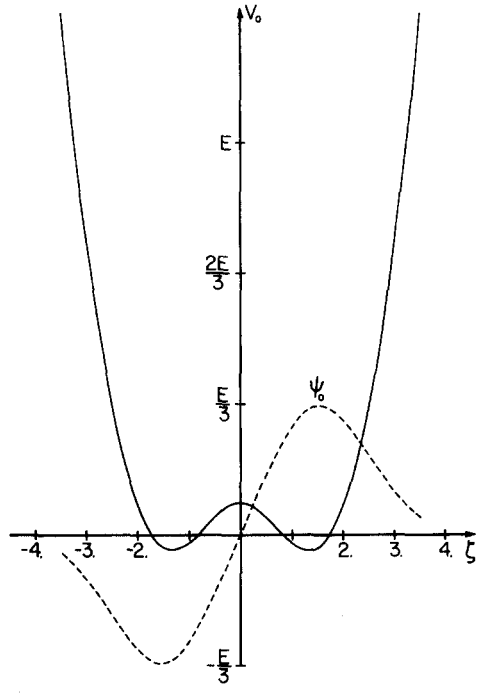

Fig. 2. The potential energy $V_o(\zeta,\rho = 0)$ of Eq. (5) for $\lambda = 1.5$. The dashed curve is the wave function $\psi_o(\zeta,\rho = 0)$ in arbitrary units.

satisfies

$$(T + V_o)\psi_o = E\psi_o$$

for

$$V_o = (V_1\psi_1 - V_2\psi_2)/(\psi_1 - \psi_2)$$
$$= (E/3)\{[(\zeta - \lambda)^2 + \rho^2]e^{+\lambda\zeta} - [(\zeta + \lambda)^2 + \rho^2]e^{-\lambda\zeta}\}(e^{+\lambda\zeta} - e^{-\lambda\zeta})^{-1}. \quad (5)$$

Figure 2 shows, for $\rho = 0$, V_o and ψ_o, also with $\lambda = 1.5$.

The shapes of V_e and V_o are similar, but V_o lies lower. The method fixes E to be the same throughout, and the interesting quantity is the location of the energy eigenvalue with respect to the potential energy curve. Figure 3 shows the difference between E and the minimum values of the potentials for the even and for the odd states. One thus obtains very easily for a three-dimensional example the familiar observation that in double wells even states become better bound as the distance between the wells is decreased, while odd states become less bound. Of course the comparison is not really direct because $V_e - V_{e,\min}$ and $V_o - V_{o,\min}$, the physically meaningful potentials seen by the even and the odd states, are different, especially near the origin. However, the difference between $V_e - V_{e,\min}$ and $V_o - V_{o,\min}$ is such as to bring the two curves of Fig. 3 closer together than they would be if the even and odd states saw the same potential. The quantity

$$(V_e - V_{e,\min}) - (V_o - V_{o,\min})$$

is positive over the most important region, from about $\zeta = -\lambda$ to $\zeta = +\lambda$, and never goes negative by as much as the difference between the two curves of Fig. 3.

Variations of this problem can be worked out readily. The wave function $C_1\psi_1 + C_2\psi_2$, with different magnitudes for C_1 and C_2, describes an unsymmetric double well. Three or more wells can be described by an extension of the sums. For example, an exact eigenstate in an infinite three-dimensional cubic lattice is given by

$$\psi = \sum_{s,t,u=-\infty}^{+\infty} \psi_{stu}$$

for

$$V = \sum_{s,t,u=-\infty}^{+\infty} \frac{V_{stu}\psi_{stu}}{\psi},$$

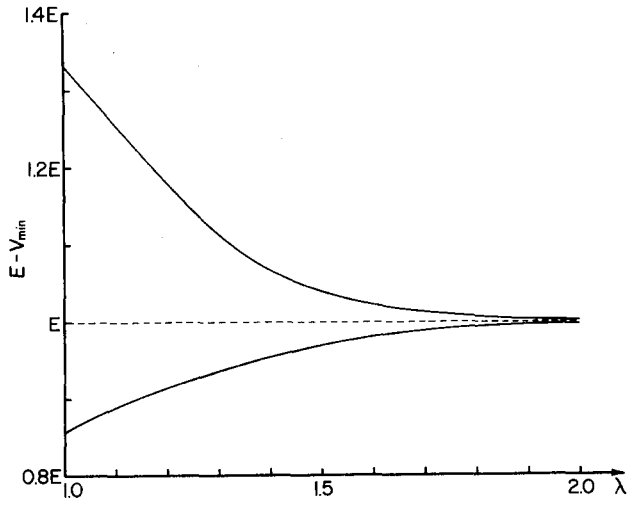

Fig. 3. The amount by which the energy eigenvalue lies above the minima of potential energy, as a function of the well separation $\lambda = \alpha l$. The results are not interesting for $\lambda \lesssim 1$; both V_e and V_o are defined so that they behave like V_1, not $2V_1$, when the wells coalesce.

where

$$\psi_{stu} = \exp\{-(\alpha^2/2)[(x - sl)^2 + (y - tl)^2 + (z - ul)^2]\}$$

and

$$W_{stu} = (K/2)[(x - sl)^2 + (y - tl)^2 + (z - ul)^2].$$

At any point, only a few near neighbors contribute appreciably to these sums because of the rapid decrease of the Gaussians.

Another class of applications involves the superposition of potential energy functions of different shapes. For example, an infinite well with an adjustable variation in the interior potential energy can be studied as follows. In spherical coordinates,

$$V_1 = 0, \quad r \le a,$$
$$= \infty, \quad r > a$$

has as its lowest state

$$\psi_1 = (a/r)\sin(\pi r/a), \quad E = \pi^2\hbar^2/(2ma^2).$$

Introduce a second potential

$$V_2 = Kr^2/2 - W.$$

Take as ψ_2 the lowest eigenfunction for V_2 which is zero at $r = a$ and which has the same energy E as ψ_1. Choose the two constants K and W to satisfy these two conditions. The function ψ_2 must then have the form $H_3(\alpha r)\exp(-\alpha^2r^2/2)/\alpha r$, or

$$\psi_2 = (1 - 2\alpha^2r^2/3)\exp(-\alpha^2r^2/2),$$

with

$$E = 7\hbar^2\alpha^2/2m - W, \quad \alpha^2 \equiv (Km)^{1/2}/\hbar.$$

The requirement $\psi_2(a) = 0$ is satisfied if $\alpha^2 = 3/2a^2$, $K = 9\hbar^2/4ma^4$, so that

$$\psi_2 = (1 - r^2/a^2)\exp(-3r^2/4a^2).$$

Now the wave function

$$\psi = C_1\psi_1 + C_2\psi_2$$
$$= C_1[\sin(\pi\eta)]/\eta + C_2(1 - \eta^2)\exp(-3\eta^2/4), \quad 0 \le \eta \le 1,$$
$$\psi = 0, \quad \eta > 1,$$

with $\eta = r/a$, is an exact solution for

$$V = (C_1V_1\psi_1 + C_2V_2\psi_2)/\psi$$
$$= E\frac{9\eta^2/4\pi^2 - 21/2\pi^2 + 1}{1 + BF(\eta)}, \quad 0 \le \eta \le 1, \qquad (6)$$
$$V = \infty, \quad \eta > 1.$$

Here

$$B \equiv \pi C_1/C_2$$

and

$$F(\eta) \equiv \frac{\sin(\pi\eta)\exp(3\eta^24)}{\pi\eta(1 - \eta^2)}$$

is a slowly varying function that increases from unity at $\eta = 0$ to 1.058 at $\eta = 1$. The potential energy V is therefore very nearly that of a harmonic oscillator with adjustable spring constant and with its origin shifted downward. If $B = 0$, ψ is exactly the harmonic oscillator wave function for $r \le a$. If $B = \infty$, the bottom of the well is flat and $\psi = \psi_1$. Any possibility between these limits can be obtained from a suitable choice of B. The energy eigenvalue is always $\pi^2\hbar^2/2ma^2$ with respect to the origin used in the specification of V_1 and V_2. Here also the physically important quantity is the amount by which the energy eigenvalue exceeds the minimum of V; that is,

$$E - V(0) = \frac{\pi^2\hbar^2}{2ma^2}\left(1 + \frac{21/2\pi^2 - 1}{1 + B}\right).$$

These examples illustrate the limitations and the strengths of the method. Since the potentials are made to fit given wave functions, a change in state forces a change in the potential; a set of different eigenstates in the same potential cannot be obtained. Also, the method yields a physically meaningful energy eigenvalue, $E - V_{\min}$, only if the potentials that are being combined have a finite minimum or other reference value, so that combinations of Coulomb potentials do not provide interesting applications. Nevertheless, it is useful to have exact solutions to a variety of relatively complicated problems, even if one only knows one state. Such solutions can be applied to specific problems and are also valuable for testing the accuracy of approximations. In addition, the method has a rather general pedagogic virtue. Introductory courses tend to be preoccupied with the question, "Given the potential, what is the wave function?" Research, however, frequently raises the question, "Given the wave function, what is the potential?" It is therefore desirable to call attention to elementary procedures for getting the potential from the wave function for systems of some complexity and physical interest.

[1] E. N. Whittaker, *A Treatise on the Analytical Dynamics of Particles and Rigid Bodies*, 4th ed. (Cambridge U. P., London, 1937; Dover, New York, 1944), Sec. 51. See also E. J. Routh, *A Treatise on Dynamics of a Particle* (Cambridge U. P., London, 1898; Dover, New York, 1960), Secs. 271–275. The theorem, although often attributed to Ossian Bonnet, was according to Whittaker first given by Legendre in 1817. I am not aware of any recent texts that discuss it. It is surprising that the theorem has become an arcanum; it can be used to discuss freshman questions such as, "What would happen if we had two suns, with one somehow fixed at each of the foci of the ellipse on which the Earth moves?"