AAPT PHYSICS EDUCATION | AMERICAN JOURNAL of PHYSICS

A simple example to introduce continuum discretization

A. Riera

Citation: American Journal of Physics **59**, 62 (1991); doi: 10.1119/1.16688
View online: http://dx.doi.org/10.1119/1.16688
View Table of Contents: http://scitation.aip.org/content/aapt/journal/ajp/59/1?ver=pdfcov
Published by the American Association of Physics Teachers

Articles you may be interested in

A Simple Example of Radioactive Dating
Phys. Teach. **52**, 115 (2014); 10.1119/1.4862120

Mass as a Form of Energy in a Simple Example
Phys. Teach. **51**, 546 (2013); 10.1119/1.4830069

Discrete and continuum descriptions of matter
Phys. Today **56**, 10 (2003); 10.1063/1.1554120

Simple demonstrations for introducing spatial coherence
Am. J. Phys. **64**, 1257 (1996); 10.1119/1.18388

Simple experiment to introduce the photomultiplier
Am. J. Phys. **44**, 649 (1976); 10.1119/1.10327

This article is copyrighted as indicated in the article. Reuse of AAPT content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 157.92.4.72 On: Tue, 19 Jan 2016 17:48:10

measurements," in *The Electromagnetic Interaction in Nuclear Spectroscopy*, edited by W. D. Hamilton (North-Holland, Amsterdam, 1975), pp. 474–475.
[14] C. M. Lederer and V. S. Shirley, *Table of Isotopes* (Wiley, New York, 1978), 7th ed.
[15] S. Fraga, J. Karwoski, and K. M. S. Saxena, *Handbook of Atomic Data* (Elsevier, New York, 1976).
[16] J. P. Desclaux, "Relativistic Dirac–Fock Values, $1 \leqslant Z \leqslant 120$," At. Data Nucl. Data Tables **12** (1973).
[17] Reference 4, pp. 351–361.
[18] B. L. Cohen, *Concepts of Nuclear Physics* (McGraw-Hill, New York, 1971), p. 309.

A simple example to introduce continuum discretization

A. Riera
Departamento de Química, C-XIV, Universidad Autónoma de Madrid, Canto Blanco, 28049-Madrid, Spain

(Received 2 October 1989; accepted for publication 29 January 1990)

Expansions in terms of L^2 integrable functions, such as Slater or Gaussian orbitals, or Hermite functions, are usually employed to describe bound states of atomic and molecular systems. A less familiar property of these expansions is that they can accurately reproduce continuum wave functions in selected regions of configuration space, yielding a procedure that is widely used in the calculation of probabilities of predissociation and ionization, as well as of unimolecular and bimolecular reactions. In the present work it is argued that the essentials of this procedure can be introduced with a modicum of theory through an extremely simple example, which lends itself to further numerical experimentation.

I. INTRODUCTION

Any introductory course on *Quantum Mechanics* includes a part on approximation methods, since the number of problems that can be treated analytically is very limited. Among these methods, linear variational theory occupies a deserved leading place for approximating bound-state energies and wave functions of atomic and molecular systems. What is less well known is that expansions in terms of, say, Slater or Gaussian orbitals, or Hermite functions, can also be used to represent accurately unbound states in selected regions of configuration space. This approximation method is usually called continuum discretization because it discretizes the true continuum spectrum of the Hamiltonian. As will be mentioned in Sec. II, it is widely used in the calculation of probabilities of predissociation, ionization, unimolecular, and bimolecular reactions. In Sec. III, an example in terms of standard one-dimensional square wells is presented that contains all pertinent features of discretization and that may be used to introduce the method using the elementary theory of any standard quantum mechanics course. Once these features have been grasped, the example can be made more sophisticated so as to approach, as much as desired, the characteristics of more "real life" problems.

II. CONTINUUM DISCRETIZATION

A recurrent theme in the literature is the representation of continuum wave functions by linear combinations of L^2 integrable functions. A typical example arises in the calculation of matrix elements of the type

$$\langle \chi | V | \psi_E \rangle, \tag{1}$$

where χ describes a bound state, V is an interaction term, and ψ_E is a δ-function normalized eigensolution of a Hamiltonian operator:

$$H\psi_E = E\psi_E; \quad \langle \psi_E | \psi_{E'} \rangle = \delta(E - E'). \tag{2}$$

For instance, in the Feshbach theory,[1] this operator is a projected Hamiltonian, and χ and ψ_E are closed and open channel components; in the study of photoionization phenomena, V is the dipole moment operator, χ and ψ_E are the initial (discrete) and final (continuum) states of the system, etc. Expression (1) is to be calculated for a given open channel or continuum energy $E = E^d$.

To construct the bound-state wave function χ, one may employ a Ritz variational treatment in an appropriate L^2 integrable basis (LIB). Obviously, evaluation of (1) is simplified when an LIB expansion is also employed for the continuum wave function ψ_E. This procedure is employed in many calculations, and in different fields, but is not discussed in textbooks, possibly due to the fact that the method is related to advanced topics such as Stieltjes imaging techniques,[2–5] or to the stabilization of resonances.[6] And the point is of pedagogical importance: One usually assumes that LIB expansions obtained with the Ritz variational procedure yield a good representation for the lower energy states, an increasingly worse one for higher excited

 © 1990 American Association of Physics Teachers

This article is copyrighted as indicated in the article. Reuse of AAPT content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 157.92.4.72 On: Tue, 19 Jan 2016 17:48:10

ones, and a meaningless one for states whose energy lies in a continuum—since, unlike LIB functions, continuum wave functions oscillate indefinitely in at least one direction of configuration space, and represent dissociating states. Hence, there is no *a priori* reason to expect a relation between the exact continuum wave functions and the corresponding "approximate," or discretized, ones obtained in the variational procedure.

However, Hazi and Taylor[7] found that these "approximate" wave functions turn out to agree remarkably well with the exact ones, although only within a domain D of configuration space and up to an overall normalization factor. Even more noteworthy, the agreement is reached with quite small bases. Clearly, provided that the domain D contains the region where the bound-state function χ of (1) takes nonnegligible values, and that one can find the renormalization factor, we can calculate (1) to any accuracy, irrespective of the fact that exact and discretized continuum wave functions can be totally different outside D. The size of this domain results from the choice of basis, and depends on the kind of application, being of atomic or molecular dimensions in the calculation of lifetimes, and much larger when phase shifts or cross sections are to be evaluated from the asymptotic form of the wave functions. A detailed explanation of why an LIB is capable of reproducing continuum wave functions may be found in Refs. 8 and 9. We now introduce, with the help of an example, the main features of discretization and the reason why the method works.

III. EXAMPLE

We consider the continuum formed by the eigensolutions of the Schrödinger equation for an electron moving along one dimension and bouncing on an infinite potential wall. Employing atomic units ($e = m_e = \hbar = 1$), the Hamiltonian, and δ-function normalized solutions to this problem are

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + V(x), \tag{3}$$

$$V = \begin{cases} \infty, & x<0, \\ 0, & x\geqslant 0, \end{cases} \tag{4}$$

$$\psi_E = \begin{cases} 0, & x<0, \\ (2/\pi k)^{1/2}\sin kx; \quad k=(2E)^{1/2}, & x\geqslant 0. \end{cases} \tag{5}$$

We then define an LIB by enclosing the system in a box by means of an infinite wall situated at a distance $x = a$: the (unit-normalized) eigenfunctions

$$\phi_n = \begin{cases} 0, & x<0, \\ (2/a)^{1/2}\sin k_n x, & 0\leqslant x\leqslant a, \\ 0, & x>a, \end{cases} \tag{6}$$

with

$$k_n = n\pi/a = (2E_n)^{1/2}; \quad E_n = n^2\pi^2/2a^2 \tag{7}$$

describe bound states of the electron, unlike those of Eq. (5). We then apply a standard linear variational procedure to the Hamiltonian (3)–(4) in an LIB of N chosen functions (6). Now, since the Hamiltonian matrix is diagonal in this representation, the "approximate" solutions obtained are precisely the wave functions (6) and the energies (7): We have discretized the continuum spectrum by placing a wall at a distance a. We now see that, for $k = k_n$, and inside the domain $D = [0,a]$, exact (5) and discretized (6) wave functions are identical except for a normalization factor. This feature is easily explained: They are proportional because they fulfill the same differential equation and initial condition; they are not identical because the discretized one is normalized to unity while the continuum one fulfills Eq. (2). Also, the feature is unrelated to the form chosen for the potential $V(x)$ in Eq. (4): It is clear that for any other choice of V, if we define the LIB set by placing a wall at $x = a$, strict proportionality between continuum and discretized wave functions will hold for $x < a$.

The previous reasoning also shows why discretization works for more common LIB sets, such as those built from Slater, Gaussian, or Hermite functions. Indeed, a possible further development of the problem is to (numerically) diagonalize the Hamiltonian in bases of one-dimensional analogs of these functions such as $\{x\exp(-\alpha_0\beta^n x/a)\}$, $\{x^n\exp(-x/a)\}$, $\{x\exp(-\alpha_0\beta^n x^2/a)\}$, $\{x^n \times\exp(-x^2/a)\}$, $(x\geqslant 0)$; α_0, β are real constants to be chosen by trial and error; $n = 1,2,3,...$; and a is a "size" factor. Since these functions decrease exponentially, a variational expansion in terms of them is, in a loose sense, equivalent to enclosing the system in a box: Instead of a sharp wall at $x = a$, we then have a diffuse boundary region. For x less than the boundary region, proportionality between continuum and discretized wave functions obtains; for x inside this region the exponential decrease of the discretized wave function spoils the proportionality; and for x larger than the boundary position continuum and discretized functions are unrelated. Illustrations of this behavior may be found in Refs. 7 and 9.

Once it is seen that the method works, there remains the problem of obtaining a discretized continuum wave function of any given energy [e.g., $E = E^d$ as in Eq. (1)]. For this purpose, one can introduce a nonlinear parameter in the basis, and then use inverse interpolation to *select* the appropriate basis. In our example, it suffices to choose the value of a in Eqs. (6) and (7):

$$a = n\pi(E/2)^{1/2} \tag{8}$$

and such that $[0,a]$ contains the domain where we wish the approximation to hold. The same procedure (varying the value of a) may be employed for the other bases mentioned. We notice that this inverse interpolation can be performed for more than one index n, yielding approximations ϕ_{n-1}, ϕ_n, etc., where ϕ_n differs from ϕ_{n-1} by reproducing one extra half-wavelength[7] of ψ_E, and so on. In practice, this yields an excellent means of testing the goodness of discretization techniques: When using different approximations ϕ_n [e.g., in Eq. (1)] one should obtain the same results to the accuracy required.

The last question is, can one find the renormalization factor that relates exact and discretized wave functions?[9] The honest answer is that, in the general case, one probably cannot, especially when the continuum presents a sharp resonant structure, the LIB set is small, and (as usual) the exact wave function is unknown. Nevertheless, one can see how to determine the renormalization factor for a resonance-free continuum such as that of Eqs. (3) and (4), starting with the case where $D = [0,a]$ is so large that discretization yields a quasicontinuum. The projector for the discretization basis is

$$P = \sum_{n=1}^{N} |\phi_n\rangle\langle\phi_n| = \sum_{E_n} \Delta E_n \frac{\Delta n}{\Delta E_n}|\phi_n\rangle\langle\phi_n|. \tag{9}$$

This article is copyrighted as indicated in the article. Reuse of AAPT content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 157.92.4.72 On: Tue, 19 Jan 2016 17:48:10

We see that, if we define:

$$\bar{\phi}_n = \rho^{1/2}(E_n)\phi_n, \tag{10}$$

where ρ is the density of states[10] of the quasicontinuum:

$$\rho(E_n) = \frac{dn}{dE_n} = \left(\frac{dE_n}{dn}\right)^{-1} = \frac{a^2}{n\pi^2}. \tag{11}$$

We then have the formal limit:

$$P = \sum_{E_n} \Delta E_n |\bar{\phi}_n\rangle\langle\bar{\phi}_n| \underset{\substack{D\to\infty \\ N\to\infty}}{\to} \int dE\, |\psi_E\rangle\langle\psi_E| \tag{12}$$

and from Eqs. (5) and (6) $\overline{\phi_n}$ exactly coincides with ψ_{En} within D and vanishes outside this domain, so that the renormalization factor is given by $\rho^{1/2}$. We stress the fact that ρ is devoid of physical significance and is a property of the basis set. As D (i.e., a) is progressively enlarged, $\rho\to\infty$, and the amplitude of each unit-normalized discretized wave function ϕ_n tends to 0, such as to keep the values of the renormalized one $\overline{\phi_n}$ identical to those of ψ_{En}, within D.

One may then remark that in many applications D is small, of atomic or molecular dimensions, so that the eigenvalues (7) are widely spread and discretization does not yield a quasicontinuum. Several procedures can then be employed[2–7,9] to *approximately* solve the problem. My personal bias is that the simplest one is to employ $\rho^{1/2}$ as a renormalization factor, where $\rho(E_n)$ is evaluated by Eq. (11), by considering $E(n)$ as an interpolation function of E_n vs n. In the present example, this procedure permits us to produce exactly the continuum wave functions ψ_{En} within D, however small this domain may be; in other cases, the agreement is only approximate. As may be expected, construction and differentiation of an interpolating function $E(n)$ is a procedure that must be handled with care; in practice, this means that some requirements are placed on basis sets such that the discretized spectrum obtained $\{E_n\}$ is sufficiently smooth[9]—a property that can always be ascertained *a posteriori*.

ACKNOWLEDGMENT

This research has been partially supported by the DGICYT project No. PB87-0112.

[1] H. Feshbach, "A unified theory of nuclear reactions," Ann. Phys. **5**, 357–389 (1958); "A unified theory of nuclear reactions II," Ann. Phys. **19**, 287–313 (1962).

[2] E. J. Heller and X. Yamani, "New L^2 approach to quantum scattering: Theory," Phys. Rev. A **9**, 1201–1208 (1974).

[3] W. P. Reinhardt, "L^2 discretization of atomic and molecular electronic continua:Moment, quadrature and J-matrix techniques," Comput. Phys. Comm. **17**, 1–21 (1979).

[4] J. T. Broad, "Weyl's theory in an L^2-basis Gauss quadrature of the spectral density," Phys. Rev. A **26**, 3078–3092 (1982).

[5] M. R. Hermann and P. W. Langhoff, "Explicit Hilbert space representation of Schrödinger states: Definitions and properties of Stieltjes–Tchebycheff orbitals," J. Math. Phys. **24**, 541–547 (1983).

[6] H. S. Taylor, "Models, interpretation and calculations concerning resonant electron scattering processes in atoms and molecules," Adv. Chem. Phys. **18**, 91–147 (1970).

[7] A. U. Hazi and H. S. Taylor, "Stabilization method of calculating resonance energies: Model problem," Phys. Rev. A **1**, 1109–1120 (1970).

[8] A. Macías and A. Riera, "On the detection and representtion of resonance by the method of stabilization," J. Phys. (Paris) **46**, 535–543 (1985).

[9] A. Macías, F. Martín, A. Riera, and M. Yáñez, "A practical solution of the 'unknown normalization' problem," Int. J. Quantum Chem. **33**, 279–300 (1988).

[10] S. Flügge, *Practical Quantum Mechanics* (Springer-Verlag, New York, 1970).

Test of the adiabatic approximation in quantum mechanics: Forced harmonic oscillator

Y. Nogami

Department of Physics, McMaster University, Hamilton, Ontario L8S 4M1, Canada

(Received 30 August 1989; accepted for publication 26 March 1990)

The accuracy of the adiabatic approximation in quantum mechanics is examined by applying it to the forced harmonic oscillator for which the time-dependent Schrödinger equation can be solved exactly. Nonadiabatic transitions caused by the external force that varies in time is focused on. A peculiar situation is illustrated such that, no matter how rapid and large the variation of the external force may be, all nonadiabatic transitions vanish exactly as $t\to\infty$.

I. INTRODUCTION

Consider a quantum mechanical system whose Hamiltonian H contains a time-dependent parameter $f(t)$. This parameter could, for example, represent an external electric field that varies in time. If the time variation of $f(t)$ is slow, i.e., if the variation of $f(t)$ does not cause a substantial variation of H in a time interval of the order of the natural period of the system with constant f, then the adiabatic approximation is expected to hold.

In his interesting book,[1] Peierls examines the adiabatic approximation for the forced harmonic oscillator. After

© 1990 American Association of Physics Teachers

This article is copyrighted as indicated in the article. Reuse of AAPT content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 157.92.4.72 On: Tue, 19 Jan 2016 17:48:10