Periodic boundary conditions and the one-dimensional hydrogen atom

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lines with constant scale speed c. The process of following a dot across the screen is a simple routine well suited to the capabilities of the microcomputer. The appropriate relativistic velocity components of the photons are computed using standard formulae[2] and are stored in a table in the program.

The second program, on the same disk, displays the electric field lines of a radiating dipole; see Fig. 3. There are 64 different high-resolution pictures stored in memory (the Apple's usual 48k memory is sufficient for this) and they are displayed at the rate of eight pictures per second.

These programs complement the short film, "Dipole Radiation."[3] They contain essentially the same kinds of information, but they give the user control of some of the parameters involved. They are useful for classroom demonstration and for individual study.

The programs are available from the author (send an ordinary 5-in. disk).

[1]R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics* (Addison-Wesley, Reading, MA, 1964), p. II-26-4.
[2]P. Lorrain and D. Corson, *Electromagnetic Fields and Waves* (Freeman, New York, 1970), 2nd ed., p. 216.
[3]R. H. Good, Am. J. Phys. **49**, 185 (1981).

Periodic boundary conditions and the one-dimensional hydrogen atom

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Periodic boundary conditions are usually introduced into quantum mechanics courses in two contexts. First, for a system in which the potential is periodic the wave function also exhibits periodicity. Second, in order to avoid the use of continuum wave functions it is convenient to introduce artificial "boundaries" so that the spectrum becomes discrete. The continuum is obtained again in the limit that the length of the period is made infinite.

In order to elucidate the dependence of the energy levels on the magnitude of the bounded region it is useful to examine cases where the original problem can actually be solved completely. The one-dimensional hydrogen atom with a δ-function interaction is such an example which may be useful for discussion in a quantum mechanics course.

The one-dimensional hydrogen atom with a δ-function potential has been the subject of a number of studies.[1] If the wave function satisfies periodic boundary conditions one may also determine the positive energy eigenfunctions and eigenvalues for a repulsive δ-function potential. These results are compared with those for the one-dimensional hydrogen atom in an infinite square well obtained by Lapidus.[2]

Consider an electron with mass m moving in a one-dimensional potential well

$$V(x) = -Ze^2\delta(x), \tag{1}$$

where $\delta(x)$ is the Dirac delta function. The Schrödinger equation

$$-(\hbar^2/2m)\psi'' + V(x)\psi = E\psi \tag{2}$$

has one negative energy solution,

$$\psi(x) = (1/a)^{1/2}\exp(-|x|/a), \tag{3}$$

with

$$E = -Z^2E_0 = -Z^2me^4/2\hbar^2, \tag{4}$$

where $a = \hbar^2/Ze^2m$.

The solution (3) is obtained by using the boundary condition $\psi(x)\to 0$ as $|x|\to\infty$. If the atom is enclosed between boundaries separated by a distance $2L$ the energy of the atom is significantly changed for $L\sim a$. The wave function satisfies the boundary conditions $\psi(L) = \psi(-L)$ and $\psi'(L) = \psi'(-L)$. In addition $\psi_+(0) = \psi_-(0)$ and $\psi'_+(0) - \psi'_-(0) = -(2/a)\psi(0)$ because of the δ function at the origin. The potential given in Eq. (1) is even; hence the energy eigenfunctions are also eigenfunctions of parity.

Making use of the above conditions, the negative energy eigenvalues are obtained from

$$\kappa a = \coth(\kappa L), \tag{5}$$

where $E = -\hbar^2\kappa^2/2m$, corresponding to the wave function

$$\psi_\pm(x) = \left(\frac{\kappa^2a^2 - 1}{L(\kappa^2a^2 - 1) + a}\right)^{1/2}\cosh\kappa(x\mp L). \tag{6}$$

For $L\to\infty$, $\coth(\kappa L)\to 1$. Then $\kappa = 1/a$ and one again obtains Eq. (4). For finite values of L the energy decreases without limit as $L\to 0$.

Recently Lapidus[2] has obtained the energy eigenfunctions and eigenvalues of the one-dimensional hydrogen atom in an infinite square well. In that case the bound state energy levels are obtained from the relations

$$\kappa a = \tanh(\kappa L). \tag{7}$$

In contrast to Eq. (5) the energy increases as L decreases and $E = 0$ when $L = a$. For $L < a$ the energy is positive and its value is obtained from the relation

$$\kappa a = \tan(\kappa L). \tag{8}$$

If the potential in Eq. (1) is replaced by a positive potential, the energy eigenvalues are positive. For the even parity wave functions one must replace Eq. (5) by

$$\kappa a = \cot(\kappa L), \tag{9}$$

corresponding to the wave functions

$$\psi_\pm(x) = \left(\frac{\kappa^2a^2 + 1}{L(\kappa^2a^2 + 1) + a}\right)^{1/2}\cos\kappa(x\mp L), \tag{10}$$

where $E = \hbar^2k^2/2m$.

The odd parity wave functions are obtained by noting that the wave functions must vanish at the origin. Thus the potential has no effect. The wave functions are given by

$$\psi(x) = L^{-1/2} \sin(n\pi x/2L), \tag{11}$$

and the energy eigenvalues are

$$E_n = n^2\pi^2\hbar^2/8mL^2. \tag{12}$$

For a positive δ-function potential the energy of the system enclosed in an infinite square well is again given by Eq. (8).

In the previous discussion the boundaries were placed symmetrically at $x = \pm L$. If the atom is located asymmetrically in an infinite square well the energy is a function of d the distance of the atom from the origin.[2] But this is not so for periodic boundary conditions; the energy is given by Eq. (5) or Eq. (9).

Finally we note that the problem of the one-dimensional hydrogen atom with periodic boundary conditions is actually identical to that of a particle constrained to move on a circular path with circumference $2L$, which may be solved simply by the replacement $x = R\theta$, $L = \pi R$, $k = \alpha/R$.

[1] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), p. 1644; A. A. Frost, J. Chem. Phys. **22**, 1613 (1954); I. R. Lapidus, Am. J. Phys. **37**, 930 (1969); **37**, 1064 (1969).

[2] I. R. Lapidus, Am. J. Phys. **50**, 563 (1982).

Comment on a paper by Leavitt and Morrison

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The authors of "A technique for evaluating sums by means of complex integration"[1] state in reference to their formula (12): "To our knowledge, this result has not been published previously." This formula, together with many similar ones and many applications, appears in Lindelöf's classic monograph of 1905[2] as formula (9) [together with formula (2)] of Chap. III. The same material also appears in more recent books.[3]

[1] R. P. Leavitt and C. A. Morrison, Am. J. Phys. **50**, 1112 (1982).

[2] E. Lindelöf, *Le Calcul des Résidus et ses Applications a la Théorie des Fonctions* (Gauthier-Villars, Paris, 1905; reprinted by Chelsea, New York, 1947).

[3] E.g., F. W. J. Olver, *Asymptotics and Special Functions* (Academic, New York, 1974), Chap. 8.

Response to letter by Yanowitch

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One of the main results in our recent paper in this journal[1] was derived for the first time many years ago in Lindelöf's book; we were, naturally, quite unaware of this when preparing our manuscript. This fact was pointed out to us by Professor Yanowitch and also in a personal communication from Professor R. P. Boas of the Mathematics Department at Northwestern University. We thank Professors Yanowitch and Boas for bringing this matter to our (and the reader's) attention. Nevertheless, one can still regard our article as bringing the subject of summation and approximation of sums by contour integrals to the physics community, in which the techniques are not well known. It is worth concluding by quoting from Professor Boas' letter: "Every generation must make its own discoveries."

[1] R. P. Leavitt and C. A. Morrison, Am. J. Phys. **50**, 1112 (1982).