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Avoiding a trap in degenerate perturbation theory

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The plane rotator described by the Hamiltonian

$$H_0=\frac{L_z^2}{2I} \tag{1}$$

with the perturbation

$$H'=p\epsilon\cos(\phi) \tag{2}$$

often is used as an example of perturbation theory[1–3] in an undergraduate quantum mechanics course. In Eq. (2), p is the electric dipole moment of the rotator and ϵ is the applied electric field. Except for the ground state, all other states are twofold degenerate. It was pointed out many years ago that non-degenerate perturbation theory gives the second-order energy correction as[4]

$$E_n^{(2)}=\sum_{k\neq n}\frac{|\langle n|H'|k\rangle|^2}{E_n^{(0)}-E_k^0}=\frac{I}{\hbar^2}\frac{p^2\epsilon^2}{(4n^2-1)} \tag{3}$$

for all n, $n=0,\pm1,\pm2,\ldots$. The answer given in Eq. (3) happens to be correct for $n\neq1$. Although the second-order perturbation matrix is already diagonal (and the two diagonal elements are equal) for the higher excited states, the perturbation matrix for the first excited states $n=\pm1$ is not diagonal. The correct solution for the case of $n=\pm1$ was given in Ref. 5 as

$$E^{(2)}=\frac{5Ip^2\epsilon^2}{6\hbar^2},\quad -\frac{Ip^2\epsilon^2}{6\hbar^2}. \tag{4}$$

Nevertheless, the incorrect treatment appears to have persisted.[6,7]

For the plane rotator, the first-order correction vanishes. Therefore, the matrix element of interest arises in second-order degenerate perturbation theory. In many undergraduate quantum mechanics courses, there is no time to discuss second-order degenerate perturbation theory thoroughly. In this note we propose a simple example in which the above-mentioned subtlety emerges in first order. This example will help clarify the concept of degenerate perturbation theory for students in beginning quantum mechanics courses.

Consider the Hamiltonian

$$H=H_0+H', \tag{5}$$

$$H_0=aL^2+bL_z^2, \tag{6}$$

$$H'=cL_y^2, \tag{7}$$

with $c\ll a$, b. The unperturbed energy levels are

$$E_{lm}^{(0)}=al(l+1)\hbar^2+bm^2\hbar^2, \tag{8}$$

where the quantum numbers $l=0,1,2,\ldots$ and $m=0,\pm1,\pm2,\ldots,\pm l$. The unperturbed wave functions are the spherical harmonics $Y_{lm}(\theta,\phi)=\langle\hat{r}|l,m\rangle$. Except for the states $|l,0\rangle$, all other states are twofold degenerate. For the states $|l,0\rangle$, first-order non-degenerate perturbation theory gives

$$E_{l0}^{(1)}=\langle l,0|cL_y^2|l,0\rangle=\frac{c}{2}l(l+1)\hbar^2. \tag{9}$$

Equation (9) can be readily obtained by using the identity

$$L_y^2=\tfrac{1}{4}(2L^2-2L_z^2-L_+^2-L_-^2), \tag{10}$$

where L_+ and L_- are the usual raising and lowering operators.[8]

For each degenerate pair of states $|l,m\rangle$ and $|l,-m\rangle$, we should construct the 2×2 matrix with elements $\langle l,m'|cL_y^2|l,m''\rangle$ and diagonalize the matrix to obtain the first-order correction to the energy levels. These matrix elements can be easily calculated with the aid of Eq. (10) to give the diagonal elements

$$\langle l,m'|cL_y^2|l,m'\rangle=\frac{c}{2}[l(l+1)-m'^2]\hbar^2, \tag{11}$$

and the off-diagonal elements

$$\langle l,m'|cL_y^2|l,m''\rangle=0 \tag{12}$$

unless

$$m''=m'\pm2. \tag{13}$$

Because $m''=-m'$ in a given degenerate subspace, the condition in Eq. (13) is satisfied only for $m'=\pm1$. Thus, if this point is ignored, we may again be tempted to say that the first-order energy correction for all states is given by Eq. (11), which has the look of non-degenerate perturbation theory. However, for $m=\pm1$, the non-vanishing off-diagonal matrix elements are

$$\langle l,1|cL_y^2|l,-1\rangle=\langle l,-1|cL_y^2|l,1\rangle=-\frac{c}{4}l(l+1)\hbar^2 \tag{14}$$

and together with the diagonal elements given by Eq. (11) with $m'=\pm1$, a diagonalization of the matrix yields the first-order energy correction to the states $|l,\pm1\rangle$ as

$$\frac{c}{4}[3l(l+1)-2]\hbar^2, \tag{15}$$

and

$$\frac{c}{4}[l(l+1)-2]\hbar^2. \tag{16}$$

That is, the $|l,\pm 1\rangle$ states split in first order. For comparison, for the plane rotator, the $m=\pm 1$ states split in second order.

In Ref. 4, group theory was used to show that in fact all degenerate levels of the plane rotator split when the perturbation is applied. The same splitting also occurs here, and can be seen in an elementary way. In second-order degenerate perturbation theory, the off-diagonal element involves the factor $\langle l,m'|L_y^2|l,k\rangle\langle l,k|L_y^2|l,m''\rangle$, where k is an intermediate state outside the given degenerate subspace. Thus, for the second excited states specified by m', $m''=\pm 2$, the intermediate state $k=0$ will give a non-zero contribution, and therefore splitting will occur in this order. Similarly, the $m=\pm 3$ pair will split in third order when a product of three matrix elements is involved; the state $m=+3$ can be connected to the state $m=-3$ via three steps, each involving a change of two units in this quantum number. This line of reasoning can be used to see that the degeneracy will be split for all m.

We hope our simple example will be of value for students when they first encounter degenerate perturbation theory and be helpful as a reminder of a common trap.

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[4]D. Kiang, "Pedagogical aspects of a plane rotator," Am. J. Phys. **46**, 1188–1189 (1978).

[5]J. A. Cronin, D. F. Greenberg, and V. L. Telegdi, *University of Chicago Graduate Problems in Physics with Solutions* (Addison–Wesley, Reading, MA, 1967), p. 162. The problem considered in this text actually refers to a single, charged particle confined to move on a circle. This is equivalent to our plane rotator if we set $I=mR^2$ and $p=qR$.

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Heisenberg indeterminacy and the fine structure constant

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Two elementary connections are drawn between the Heisenberg relations for photons and for electrons and the maximum number of protons in a nucleus that will permit a stable electron orbital.

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I. INTRODUCTION

The fine structure constant α, which in its role as coupling constant determines the amplitude for an electron to emit or absorb a photon is, according to R. P. Feynman, "a magic number that comes to us with no understanding by man .... We know what kind of a dance to do experimentally to measure this number very accurately, but we don't know what kind of dance to do on the computer to make this number come out, without putting it in secretly!"[1]

It is remarkable, Feynman notwithstanding, that the inverse of this constant, $Z=1/\alpha\approx 137$, which sets an upper limit to the number of protons in the nuclei of stable atoms, can be arrived at in two different, but very simple, "dances" with Heisenberg, as we shall show in Secs. III and IV.

II. BACKGROUND

It is well but apparently not widely known[2] that the largest possible nucleus that can have a single electron bound state has $Z=137$. This limitation on Z follows directly from the exact energy level solution to the Dirac equation with a Coulomb potential:[3]

$$E=\mu c^2\left(1+\frac{Z^2\alpha^2}{\{n'+\sqrt{k^2-Z^2\alpha^2}\}^2}\right)^{-1/2}, \tag{1}$$

where Ze is the charge on the nucleus, α is the fine structure constant ($\alpha=e^2/4\pi\epsilon_0\hbar c$), μ is the electron/nucleus reduced mass, and n', k are integers, with $n'\geqslant 0$ and $k\geqslant 1$. For the minimum value of k, $Z\leqslant 1/\alpha=137.035\,97$ for the square root in Eq. (1) to be real.

It is of historical interest that Sommerfeld first introduced the fine structure constant in his relativistic treatment of elliptical Bohr orbits in 1916 and obtained a correct approximation[3] to Eq. (1),

$$E=\mu c^2\left(1+\frac{Z^2\alpha^2}{2n^2}\left(1+\frac{Z^2\alpha^2}{n^2}\left[\frac{n}{k}-3/4\right]+\cdots\right)\right), \tag{2}$$

where $n=n'+k$. This expansion will converge only if $Z\leqslant 1/\alpha$.

There is no obvious connection between this constraint on atomic structure and the Heisenberg uncertainty relations. However, consider the following two elementary treatments of the interaction of an electron with a nucleus containing Z protons.

III. HEISENBERG AND PHOTONS

If the electron and the nucleus are separated by a distance r, then the Heisenberg energy/time uncertainty relation allows for an exchange of virtual photons between them. The maximum allowed virtual photon energy is

$$E=\hbar/t=\hbar c/r, \tag{3}$$

because $t=r/c$ is the time of flight. Equation (3) reflects the fact that there is an indeterminacy associated with the vacuum state. Energy conservation can be "violated" for a short time t so long as the "violation" E is not greater than $\hbar/t$. Whether we imagine this energy to take the form of one photon of energy E and momentum $p=E/c=\hbar/r$, or n photons each of energy E/n and momentum $p=\hbar/nr$, the momentum transfer per second and hence the force between the electron and the nucleus is

$$F=p/t=\hbar c/r^2. \tag{4}$$

Alternatively, $F=|dE/dr|$ gives the same result.[4] This force represents the maximum that can be mediated by virtual photons, corresponding to the Coulomb force

$$F=(1/4\pi\epsilon_0)Ze^2/r^2. \tag{5}$$

If we equate Eqs. (4) and (5), we obtain

$$Z=4\pi\epsilon_0\hbar c/e^2, \tag{6}$$

the reciprocal of the fine structure constant. Thus, the largest number of protons allowed for a nucleus to admit a stable electron orbit is 137.

IV. HEISENBERG AND ELECTRONS

Alternatively, consider an electron with relativistic mass m, in a circular orbit around a nucleus of charge Ze. We have, for the centripetal force,

$$m\frac{v^2}{r}=\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r^2}. \tag{7}$$

The Heisenberg momentum/position uncertainty of such an electron is just $mvr=\hbar$, because the momentum uncertainty is $\approx mv$ and the position uncertainty is $\approx r$. The relativistic limiting value for v is c, and so the limiting value for Z from Eq. (7) is 137, as before.

Part of the beauty of physics is that we often can obtain the same result in what appear to be entirely different ways. The maximum value of Z follows directly, if roughly, from the Heisenberg relations and rigorously from the Dirac equation, giving new insight into the meaning of the fine structure constant.

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Comment on "Apparatus to measure relativistic mass increase," by John W. Luetzelschwab [Am. J. Phys. 71 (9), 878–884 (2003)]

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For a high energy physicist, it is disappointing to see the term "relativistic mass increase" in a journal article.[1] The mass (in the standard model) is a fundamental descriptor of a particle. As we have described,[2] the problem arises because of a lingering desire on the part of some physicists to preserve the low-speed (low-energy) limit of the momentum, $\mathbf{p}=m\mathbf{v}$, as the definition of momentum instead of using the correct relation at all speeds, $\mathbf{p}=\gamma m\mathbf{v}$, where $\gamma=[1-\beta^2]^{-1/2}$ and $\beta=v/c$. When β is small, $\mathbf{p}\approx m\mathbf{v}$.

The four-dimensional invariant describing a particle is (essentially) its mass: $p^\mu p_\mu=m^2c^4$. This relation is frame-independent. The use of the term "relativistic mass increase" implies that mass is a frame-dependent quantity, and acceptance of this proposition involves leaving behind the great tradition of generations of physicists since the pioneering work of Emmy Noether—exploiting the connection between universal symmetries and conservation laws.[3] The connection between invariants such as mass and spin angular momentum and fundamental physics is reflected in the frame independence of the various physical quantities.

In addition, the Eötvös experiment and its successors identify gravitational mass with inertial mass. The latter is the mass m, the same mass that determines the mass-energy of a particle.

Some might argue that the correct expression for Newton's law of universal gravitation contains the relativistic mass E/c^2, not m as is usually written. However, the gravitational field in general relativity arises through a particle's energy-momentum tensor, not a scalar mass, and the gravitational force for β near 1 does not point entirely in the radial direction, as Okun has noted.[4]

In addition, I believe the author's use of the antique unit, the curie, hides fundamental physics from the reader. I can understand the description 370 000 disintegrations per second (370 000 Bq) for the sample activity much better than the 10 μCi quoted in Ref. 1. Although one can still purchase samples in the United States designated in curies, I suggest

that the becquerel is much better for communicating among physicists (especially because it is unusual for those of us who are not nuclear or health physicists to be able to identify the amount of activity in the curie, that is, the activity in one gram of radium). I suggest future use of statements such as "a 370 000 Bq (equivalent to 10 μCi) source" to minimize reader confusion.

Reference 1 describes a nice experiment to determine that the relativistic relations $\mathbf{p}=\gamma m\mathbf{v}$ and $E=\gamma mc^2$ correctly characterize particles with large β. I wish it had been labeled that way.

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The longitudinal momentum of transverse traveling waves on a string

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Several years ago in this journal, Rowland and Pask[1] took note of a confusion in the literature regarding the longitudinal momentum carried by transverse traveling waves on a string. Through a combined numerical and analytical approach, they reached (what I take to be) a convincing resolution of the matter. Rowland and Pask accurately diagnosed the source of error by several authors in an unfounded assumption that the instantaneous velocity of an infinitesimal segment of string is always perpendicular to the segment. This is not the source of error, however, in the influential text by Elmore and Heald,[2] which is invariably cited by papers on the subject and contains a frequently quoted incorrect expression for momentum density. The purpose of this note is to identify the mistake, which is found in Chapter 1, Section 11, pages 46–47 of the book, as well as to demonstrate that by correcting this mistake we arrive at the result of Rowland and Pask.

In the notation of Elmore and Heald, the wave equation is

$$\frac{\partial^2\eta}{\partial t^2}=c^2\frac{\partial^2\eta}{\partial x^2}, \tag{1}$$

where $\eta(x,t)$ is the transverse displacement and $c=(\tau_0/\lambda_0)^{1/2}$ is the propagation velocity, with τ_0 the tension and λ_0 the linear mass density. Their treatment of longitudinal momentum starts with an expression for the longitudinal component of force density due to string curvature:

$$-\tau_0\frac{\partial^2\eta}{\partial x^2}\frac{\partial\eta}{\partial x}=\lambda_0\frac{\partial^2\xi}{\partial t^2} \tag{2}$$

with $\xi(x,t)$ the longitudinal displacement of the string resulting from the transverse wave.[3] Then, in their own words, "we integrate with respect to time from t_0, a time when no wave is present on the string, to an arbitrary later time t and with respect to x over a finite string segment lying between x_1 and x_2. The result should be the momentum G_x acquired by the string segment as the result of transverse wave motion." These integrations lead to the following:

$$G_x=-\lambda_0\int_{x_1}^{x_2}\frac{\partial\eta}{\partial x}\frac{\partial\eta}{\partial t}dx+\int_{t_0}^{t}[K_1(x_2,t)-K_1(x_1,t)]dt, \tag{3}$$

where $K_1=dK/dx=\frac{1}{2}\lambda_0(d\eta/dt)^2$ is the kinetic energy density due to transverse motion of the string.

According to Elmore and Heald, "[Eq. (3)] for the momentum G_x has the following interpretation: the second integral on the right clearly represents momentum delivered to the string segment by impulses at the two boundaries at x_1 and x_2. If these boundaries are very remote, so that a wave disturbance initiated on the string segment has not yet had time to reach them, this integral vanishes. We are thus left with the first integral, whose form suggests that the quantity

$$g_x(x,t)\equiv-\lambda_0\frac{\partial\eta}{\partial t}\frac{\partial\eta}{\partial x} \tag{4}$$

may be interpreted as a localized momentum density in the x direction associated with a transverse wave."

Here is the problem: the initiation of wave motion on a previously quiescent segment of string requires either that a wave propagates onto that segment from elsewhere on the string, or that external forces—other than the forces associated with wave propagation itself—are imposed from outside the system. The first alternative directly violates the authors' assumption that both ends of the string remain undisturbed during the integration time. The second alternative admits forces not described by the expression being integrated.

Let us adopt the first alternative, allowing for the wave to propagate onto the string segment at x_1. Then we have

$$\begin{aligned}\int_{t_0}^{t}K_1(x_1,t)dt&=\frac{1}{2}\lambda_0\int_{t_0}^{t}\left(\frac{\partial\eta}{\partial t}\right)^2dt\\&=\frac{1}{2}\lambda_0\int_{t_0}^{t}\frac{\partial\eta}{\partial t}\frac{\partial\eta}{\partial t}dt\\&=-\frac{1}{2}\lambda_0\int_{x_1}^{x_2}\frac{\partial\eta}{\partial t}\frac{\partial\eta}{\partial x}dx,\end{aligned} \tag{5}$$

the last equality holding by virtue of $(\partial y/\partial t)dt = -(\partial y/\partial x)dx$ for the traveling wave, which permits us to convert the time integral to an integral over x at time t (whereas the time integrals were carried out at $x = x_1$). This integral, inserted into Eq. (3), just cancels half the first integral on the right-hand side of the equation, leaving the result

$$G_x = -\frac{1}{2}\lambda_0 \int_{x_1}^{x_2} \frac{\partial \eta}{\partial t}\frac{\partial \eta}{\partial x}dx, \tag{6}$$

which leads to identification of

$$g_x = -\frac{1}{2}\lambda_0 \frac{\partial \eta}{\partial t}\frac{\partial \eta}{\partial x} \tag{7}$$

as the momentum density. This is the result obtained by Rowland and Pask, under the usual conditions pertaining to transverse waves on a string.

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[3]We are speaking here of small longitudinal motions associated with a transverse wave. The wave equation itself is derived under the approximation of purely transverse motion and uniform tension. Due to curvature of the string, the tension forces at opposite ends of an infinitesimal segment do not cancel. The longitudinal component of the resulting net force is much smaller than the transverse component if we have $|\partial\eta/\partial x| \ll 1$. The longitudinal motions may then be treated as a perturbation on the dominant transverse motions. Longitudinal motions are also produced by the variations in string tension associated with *longitudinal* waves; indeed, the physical impetus which establishes a transverse wave is likely to generate a longitudinal wave too, and longitudinal waves are essential to the conservation of momentum when a transverse wave encounters a density discontinuity. Interested readers should consult Rowland and Pask.

Impedance between adjacent nodes of infinite uniform *D*-dimensional resistive lattices

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Infinite resistive network problems have served as excellent vehicles for helping electrical engineering and physics students recognize and appreciate the power of superposition and symmetry in the analysis of electrical networks. These problems have been studied extensively using superposition and symmetry.[1–10] A special case of this class of problems involves the calculation of the effective resistance between two adjacent nodes of an infinite uniform two-dimensional (2D) resistive lattice (periodic in both dimensions with a zero-potential boundary condition at infinity) comprised of identical resistors each of value R. In particular, the effective resistance between two adjacent nodes of the 2D Liebman resistive mesh (the infinite 2D square resistive lattice) was calculated by Aitchison[1] and found to be $(1/2)R$. Bartis[2] calculated the resistance between adjacent nodes for three other infinite 2D resistive lattices, the triangular, Honeycomb, and Kagomé lattices, and found the effective resistances to be $(1/3)R$, $(2/3)R$, and $(1/2)R$, respectively.

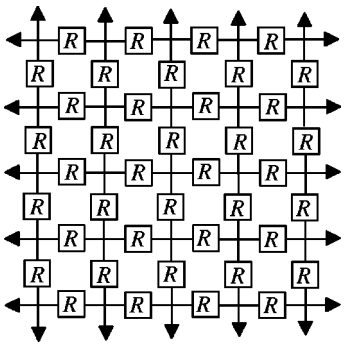

Fig. 1. Infinite 2D square resistive lattice.

The goal of this paper is to extend the results of Refs. 1 and 2 to the general problem of finding the total effective resistance R_{eff} between two adjacent nodes of any infinite D-dimensional resistive lattice, where $D = 1, 2, 3,...$ and the lattice is periodic and infinite in all D dimensions with a zero-potential boundary condition at infinity. Our general solution for R_{eff} is of pedagogical interest because it generalizes the previous results of Refs. 1 and 2 to a simple and elegant equation that covers all adjacent-node infinite D-dimensional resistive networks and because it reinforces the power of the superposition principle and symmetry in electrical circuit analysis.

For the purpose of illustration, consider the infinite 2D square resistive lattice shown in Fig. 1. The number of resistors connected to each node is denoted by M ($M = 4$ in Fig. 1). As in Refs. 1 and 2, we use superposition and symmetry along with two test current sources each of value I to calculate the effective resistance R_{eff} between two adjacent nodes by injecting a test current I into any single node on the D-dimensional resistive lattice from the zero-potential boundary at infinity and then extracting another identical test current I from an adjacent node connected to a current sink kept at zero potential. By using Kirchhoff's current law and symmetry, we find that each of the M resistors connected to the original node will receive I/M of the injected current. Similarly, we find that each of the M resistors connected to the adjacent node will receive $-I/M$ of the extracted current in the opposite direction. Therefore, by superposition, the total resulting current flowing in the resistor R connecting the two adjacent nodes will be $2I/M$, which leads to a voltage drop across the resistor R of $V = (2I/M)R$. Thus the effective resistance is

$$R_{\text{eff}} = V/I = 2R/M. \tag{1}$$

Equation (1) is a new and remarkably simple, elegant, and powerful result that applies to any infinite D-dimensional resistive lattice.

As an aside, we note that using symmetry, superposition, and a Laplacian analysis, the corresponding effective impedances for an infinite D-dimensional purely inductive or capacitive lattice can be determined in a similar way as $L_{\text{eff}} = 2L/M$ and $C_{\text{eff}} = MC/2$, respectively. These results are new and equally simple, elegant, and interesting (especially C_{eff} due to its different and nonintuitive dependence on M).

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