

## Quantum Mechanics

### Homework 6: Time-Independent Approximation Methods

015 qmult 00100 1 1 1 easy memory: time-independent perturbation

- Time-independent non-degenerate perturbation theory assumes that the stationary states and eigen-energies of a time-independent system can be expanded in convergent power series in a perturbation parameter about, respectively:
  - the stationary states and eigen-energies of another system.
  - the eigen-energies and stationary states of a time-dependent system.
  - the origin.
  - the center.
  - infinity.

**SUGGESTED ANSWER:** (a)

**Wrong Answers:**

- A time-dependent system can have eigenstates and eigen-energies only at an instant in time I think. This is a useful concept I think, but it is not a best answer.

**Redaction:** Jeffery, 2001jan01

015 qmult 00200 1 1 5 easy memory: zeroth order perturbation

- The zeroth order perturbation of a system is:
  - the most strongly perturbed system.
  - the mostest strongly perturbed system.
  - the deeply disturbed system.
  - the negatively perturbed system
  - the unperturbed system.

**SUGGESTED ANSWER:** (e)

**Wrong Answers:**

- Not grammatical, although Shakespeare got away with “most kindest” describing, I think, Julius Caesar.

**Redaction:** Jeffery, 2001jan01

015 qmult 00300 1 1 2 easy memory: 1st order energy correction

- The formula

$$E_n^{1st} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle$$

is a:

- 0th order perturbed energy.
- 1st order perturbed energy.
- 2nd order perturbed energy.
- 1st order perturbed state.
- 2nd order perturbed state.

**SUGGESTED ANSWER:** (b)

**Wrong Answers:**

- Just checking if you are awake.

**Redaction:** Jeffery, 2001jan01

015 qmult 00400 1 4 4 easy deducto-memory: 1st order eigen state correction

- The formula

$$|\psi_n^{1st}\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{\text{all } k, \text{ except } k \neq n} \frac{\langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} |\psi_k^{(0)}\rangle$$

is a:

- 0th order perturbed energy.
- 1st order perturbed energy.
- 2nd order perturbed energy.
- 1st order perturbed state.
- 2nd order perturbed state.

**SUGGESTED ANSWER:** (d)

**Wrong Answers:**

- There's only 1 power of  $\lambda$  in the expression.

**Redaction:** Jeffery, 2001jan01

015 qmult 00600 1 4 1 easy deducto-memory: degeneracy and perturbation

5. “Let’s play *Jeopardy!* For \$100, the answer is: A common cause for the failure of time-independent perturbation theory—but failure can be recovered from with diagonalization.”

What is \_\_\_\_\_, Alex?

- a) degeneracy    b) tarnation    c) subversion    d) lunacy    e) regency

**SUGGESTED ANSWER:** (a)

**Wrong answers:**

- d) Seemed likely to me too.

**Redaction:** Jeffery, 2001jan01

015 qmult 01000 1 4 5 easy deducto-memory: diagonalization

**Extra keywords:** mathematical physics

6. “Let’s play *Jeopardy!* For \$100, the answer is: A standard, non-perturbative approximate method of solving for the eigen-energies and stationary states of a system. If the system is in a finite Hilbert space (i.e., a finite function space), the method can be done for an exact solution.”

What is \_\_\_\_\_, Alex?

- a) perturbation theory    b) divagation    c) strangulation    d) triangulation  
e) diagonalization

**SUGGESTED ANSWER:** (e)

**Wrong answers:**

- a) Exactly wrong.

**Redaction:** Jeffery, 2008jan01

015 qfull 01400 2 3 0 moderate math: infinite square well Dirac delta perturbation 1

**Extra keywords:** (Gr-225:6.1) Dirac delta perturbation, 1-dimensional infinite square well

7. Say you have a 1-dimensional infinite square well with

$$V(x) = \begin{cases} 0 & \text{for the } x \text{ range } 0 \text{ to } a; \\ \infty & \text{otherwise.} \end{cases}$$

- a) Solve for the eigen-states (i.e., stationary states) and eigen-energies from the time-independent Schrödinger equation. You must properly normalize the eigen-states states to answer part (b) correctly.
- b) Say we add the Dirac delta function perturbation Hamiltonian

$$H^{(1)} = c\delta(x - a/2) .$$

What is the general expression for this perturbation for the first order perturbation energy correction for all eigen-states? Simplify the formula as much as possible.

**SUGGESTED ANSWER:**

- a) Oh you know how to do this by now. Taking an instructor’s privilege of hypocrisy, I’ll just write down the answers:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) ,$$

where  $n = 1, 2, 3, \dots$  are allowed quantum nubmers and the eigen-energies are

$$E_n = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 n^2$$

b) The first order correction formula is

$$E_n^{(1)} = \langle \psi_n | H^{(1)} | \psi_n \rangle = \frac{2c}{a} \sin^2 \left( \frac{n\pi}{2} \right) = \begin{cases} 0, & n \text{ even;} \\ 2c/a, & n \text{ odd.} \end{cases}$$

**Redaction:** Jeffery, 2001jan01

015 qfull 01404 2 3 0 moderate math: infinite square well Dirac delta perturbation 3

**Extra keywords:** (Gr-225:6.1) Dirac delta perturbation, 1-dimensional infinite square well

8. Say you have a 1-dimensional infinite square well with

$$V(x) = \begin{cases} 0 & \text{for the } x \text{ range } 0 \text{ to } a; \\ \infty & \text{otherwise.} \end{cases}$$

The stationary states are

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(k_n x) ,$$

where

$$k_n a = n\pi \quad \text{and} \quad k_n = \frac{n\pi}{a}$$

with  $n = 1, 2, 3, \dots$  as allowed quantum numbers. The eigen-energies are

$$E_n^{\{0\}} = \frac{\hbar^2}{2m} \left( \frac{\pi}{a} \right)^2 n^2 = E_1^{\{0\}} n^2 .$$

We now add the Dirac delta function perturbation Hamiltonian

$$H^{(1)} = c\delta(x - a/2) .$$

- Can we use non-degenerate perturbation theory for the infinite square well? Why or why not?
- What is the general formula for the perturbation for the 1st order perturbation energy correction for all eigen-states? Simplify the formula as much as possible.
- Now evaluate a general matrix element for the perturbation

$$\langle \psi_m | H^{(1)} | \psi_n \rangle .$$

- Simplify the general matrix element by inventing two simple functions of integer  $\ell$ . The first is zero for  $\ell$  even and 1 for  $\ell$  odd. The second is 1 for  $k$  odd and  $-1$  for  $k$  even where odd  $\ell = 2k + 1$  and  $k$  runs through all positive integers: i.e.,  $0, 1, 2, 3, \dots$ . **HINT:** If you this can't get this part, go on since the later parts don't require it.
- Write out the 1st order perturbation correction formula for a general state  $n$  in as explicit and as simplified a form as reasonably possible. Note the correction is wanted, not the full 2nd order corrected state. **HINT:** Just leave the unperturbed states in the ket form  $|\psi_n^0\rangle$ . For compactness, one doesn't want to be explicit about them.
- Write out the 2nd order perturbation correction formula for a general eigen-energy  $n$  in as explicit and as simplified a form as reasonably possible. Note the correction is wanted, not the full 2nd order corrected eigen-energy.

**SUGGESTED ANSWER:**

a) Yes we can because all the states are non-degenerate. Each state has distinct energy.

b) The first order correction formula is

$$E_n^{(1)} = \langle \psi_n | H^{(1)} | \psi_n \rangle = \frac{2c}{a} \sin^2 \left( \frac{n\pi}{2} \right) = \begin{cases} 0, & n \text{ even;} \\ 2c/a, & n \text{ odd.} \end{cases}$$

c) Behold:

$$H_{mn}^{(1)} = \langle \psi_m | H^{(1)} | \psi_n \rangle = \frac{2c}{a} \sin\left(\frac{m\pi}{2}\right) \sin\left(\frac{n\pi}{2}\right) .$$

d) Well the first function is

$$\frac{[1 - (-1)^\ell]}{2}$$

and the second is

$$(-1)^k = (-1)^{(\ell-1)/2} .$$

The marker will accept that these results are obviously right—even though the second one isn't quite obviously the simplifying function one needs.

The first function allows us to replace the absolute value of sine functions in the matrix element by 0's for even quantum numbers and 1's odd quantum numbers. The second allows us to get the alternating 1 and  $-1$  as the odd quantum number sine functions.

Anyway, with these two functions we find

$$H_{mn}^{(1)} = \frac{2c}{a} (-1)^{(m+n)/2-1} \frac{[1 - (-1)^m]}{2} \frac{[1 - (-1)^n]}{2}$$

for the simplified matrix element.

Just to satisfy paranoia, the invented functions allow us to write

$$\sin\left(\frac{\ell\pi}{2}\right) = (-1)^{(\ell-1)/2} \frac{[1 - (-1)^\ell]}{2} .$$

The zero when  $\ell$  even is obviously right. What about the second function behavior? Is it right? Well for  $\ell = 1$  and  $\ell = 3$  it clearly is. Since

$$\sin\left(\frac{\ell\pi}{2}\right)$$

is periodic over  $2\pi$  all we need to show is that the second function for  $\ell + 4$  (i.e., for four  $\pi/2$  steps) gives the same result as for  $\ell$ . Behold:

$$(-1)^{(\ell+4-1)/2} = (-1)^{(\ell-1)/2} (-1)^2 = (-1)^{(\ell-1)/2} .$$

So the second function does have the correct periodic behavior. And since it correct for  $\ell = 1$  and  $\ell = 3$ , it is correct for all odd  $\ell$ . We knew this anyway.

e) Behold:

$$\begin{aligned} |\psi_n^{(1)}\rangle &= \sum_{\text{all } m, \text{ except } m \neq n} \frac{\langle \psi_m | H^{(1)} | \psi_n \rangle}{E_n^{(0)} - E_m^{(0)}} |\psi_m^{(0)}\rangle \\ &= \frac{2c/a}{E_1^{(0)}} \sum_{\text{all } m, \text{ except } m \neq n} \frac{(-1)^{(m+n)/2-1} [1 - (-1)^m] [1 - (-1)^n]}{n^2 - m^2} \frac{[1 - (-1)^m]}{2} \frac{[1 - (-1)^n]}{2} |\psi_m^{(0)}\rangle . \end{aligned}$$

Simplicity is a bit in the eye of the beholder. I regard the last expression as simplest.

f) Behold:

$$\begin{aligned} E_n^{(2)} &= \sum_{\text{all } m, \text{ except } m \neq n} \frac{|\langle \psi_m | H^{(1)} | \psi_n \rangle|^2}{E_n^{(0)} - E_m^{(0)}} \\ &= \frac{(2c/a)^2}{E_1^{(0)}} \sum_{\text{all } m, \text{ except } m \neq n} \frac{1}{n^2 - m^2} \frac{[1 - (-1)^m]}{2} \frac{[1 - (-1)^n]}{2} . \end{aligned}$$

For me, the last expression is the simplest form.

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015 qfull 01412 3 5 0 tough thinking: 2-particle Dirac delta perturbation 2

**Extra keywords:** (Gr-226:6.3)

9. The single-particle stationary states and eigen-energies for a 1-dimensional infinite square well for region  $[0, a]$  are, respectively,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad \text{and} \quad E_n = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 n^2 .$$

- a) What is the expression for elementary 2-particle stationary states for **DISTINCT** spinless particles of the same mass? Label the particles 1 and 2 for convenience. Label the states  $n$  and  $n'$  for convenience too. What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies  $n^2 + n'^2$  up to 100? These energies can be called energy levels: the levels may correspond to more than one state. What are degeneracies of the energy levels? Remember the particles are **DISTINCT**. **HINT:** You are permitted to use a computer program to generate energy levels and degeneracies. But you can find them by hand too—a little tedious, but not hard if you go at it systematically.
- b) Now suppose we turn on a perturbation potential for the non-identical particles of the form

$$H^{(1)} = V(x_1, x_2) = aV_0\delta(x_1 - x_2) .$$

What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_1, x_2) | H^{(1)} | \psi_{nn'}(x_1, x_2) \rangle ?$$

If you expand sine functions in exponentials evaluating, the matrix element is pretty easy, but you do have to treat the cases where  $n \neq n'$  and  $n = n'$  a bit differently.

Can you do perturbation theory on all the 2-particle states?

- c) What is the expression for elementary 2-particle stationary states if we replace the distinct particles by identical spinless bosons? What is the general expression for the energy of such 2-particle states? (we have turned off the perturbation potential.) What are all the possible reduced energies  $n^2 + n'^2$  up to 100? These energies can be called energy levels: the levels may correspond to more than one state. What are degeneracies of the energy levels? **HINT:** You don't have to do part (a) all over again, just *mutatis mutandis* it.)
- d) Now suppose we turn on a perturbation potential of part (b) for the identical bosons. What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_1, x_2) | H^{(1)} | \psi_{nn'}(x_1, x_2) \rangle ?$$

If you expand sine functions exponentials evaluating, the matrix element is pretty easy, but you do have to treat the cases where  $n \neq n'$  and  $n = n'$  a bit differently. Note the perturbation correction is a bit different from the distinct particle case. Why?

Can you do perturbation theory on all the 2-particle states?

- e) What is the expression for elementary 2-particle stationary states if the 2 particles identical fermions with the same spin coordinate. Since the spin coordinates are identical, the spin part of the single-particle states are symmetrical. Don't bother writing down spinors or such. What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies  $n^2 + n'^2$  up to 100? **HINT:** You don't have to do part (a) all over again, just *mutatis mutandis* it.)
- f) Now suppose we turn on a perturbation potential of part (b) for the identical fermions. What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_a, x_b) | H^{(1)} | \psi_{nn'}(x_a, x_b) \rangle .$$

Don't whine: this is easy if you see the trick. Why do you get the simple result you get?

Can you do perturbation theory on all the 2-particle states?

g) What does the Dirac delta potential

$$V(x_a - x_b) = aV_0(x_a - x_b)$$

imply or do physically?

**SUGGESTED ANSWER:**

a) Behold:

$$\psi(x_a, x_b) = \psi_n(x_a)\psi_{n'}(x_b) \quad \text{and} \quad E_{n,n'} = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 (n^2 + n'^2).$$

I've put the table of reduced energy levels and degeneracies below all the parts of the question. Levels with different  $n$  and  $n'$  are double degenerate since two states correspond to these levels. But levels with  $n = n'$  have degeneracy 1: i.e., they are not degenerate. Note there are 3 accidental degeneracies where distinct pairs of  $n$  and  $n'$  result in the same energy. These accidental degeneracies could be combined and their degeneracies added, but it's useful to see them separated as long as we recognize what they are. There are 38 distinct energy levels not combining the accidental degeneracies. If we combined the accidental degeneracies, there are 35 distinct energy levels.

b) Behold:

$$\begin{aligned} H_{(nn')(nn')} &= \langle \psi_{nn'}(x_1, x_2) | H^{(1)} | \psi_{nn'}(x_1, x_2) \rangle \\ &= \int_0^a \int_0^a \psi_{nn'}(x_1, x_2)^* aV_0 \delta(x_1 - x_2) \psi_{nn'}(x_1, x_2) dx_1 dx_2 \\ &= aV_0 \int_0^a \psi_{nn'}(x, x)^* \psi_{nn'}(x, x) dx \\ &= aV_0 \left(\frac{2}{a}\right)^2 \int_0^a \left(\frac{e^{ikx} - e^{-ikx}}{2i}\right)^2 \left(\frac{e^{ik'x} - e^{-ik'x}}{2i}\right)^2 dx \\ &= V_0 \frac{1}{4a} \int_0^a (e^{2ikx} + e^{-2ikx} - 2) (e^{2ik'x} + e^{-2ik'x} - 2) dx \\ &= V_0 \frac{1}{4a} \begin{cases} 4a, & n \neq n' \\ (4 + 2 + 2)a, & n = n' \end{cases} \\ &= V_0 \begin{cases} 1, & n \neq n' \\ 2, & n = n' \end{cases}, \end{aligned}$$

where we got the penultimate line by pure staring at the antepenultimate line.

We can do perturbation theory. But those states that are degenerate require a diagonalization among themselves in order to obviate infinities.

c) Behold:

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2(1 + \delta_{nn'})}} [\psi_n(x_1)\psi_{n'}(x_2) + \psi_n(x_2)\psi_{n'}(x_1)]$$

and

$$E_{n,n'} = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 (n^2 + n'^2).$$

The energy levels are the same as for distinct particles. Only the degeneracies are different. All energy levels are non-degenerate, except for the 3 cases accidental degeneracy. If those levels are combined, they are all doubly degenerate. The reason for the reduction in degeneracies from the distinct particle cases is that particles 1 and 2 in single-particle states  $n$  and  $n'$  is **NOT** a different total state from particles 2 and 1 in single-particle states  $n$  and  $n'$ .

d) The diagonal matrix element is identical to that in part (b), except there is an extra factor of 2 for the case where  $n \neq n'$ . Thus

$$H_{(nn')(nn')} = 2V_0$$

for all a cases.

The extra factor of arises because for the Dirac delta function gives

$$\psi_{nn'}(x, x)^2 = \frac{4}{2(1 + \delta_{nn'})} \psi_n(x)^2 \psi_{n'}(x)^2$$

in the integrand. That extra factor of 2 cancels out for  $n = n'$ , but not for  $n \neq n'$ . The factor of 2 is a reflection of the exchange force attraction between bosons. Symmetrization makes spinless bosons closer than they would otherwise be. Since our Dirac delta function potential only gives a contribution for when the particles have the probability of being in the same place: clumping the particles together will increase the contribution.

We can do perturbation theory. But those states that are degenerate require a diagonalization among themselves in order to obviate infinities. But for bosons, we only have the accidental degeneracies to deal with

e) Behold:

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} [\psi_n(x_1)\psi_{n'}(x_2) - \psi_n(x_2)\psi_{n'}(x_1)] ,$$

where the state with  $n = n'$  is not allowed by the Pauli exclusion principle (which is a consequence of the symmetrization rule). The energies of the states are

$$E_{n,n'} = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 (n^2 + n'^2) .$$

The energy levels are the same as for distinct particles, except that there are 6 levels that ruled out by the Pauli exclusion principle. All energy levels are non-degenerate, except for the 2 cases accidental degeneracy. There are only 2 accidental degeneracy cases now since one case of the accidental degeneracies for distinct particles and bosons is eliminated by the Pauli exclusion principle. If those accidental degeneracy levels are combined, they are all doubly degenerate. The main reason for the reduction in degeneracies relative to the distinct particle case is that particles 1 and 2 in single-particle states  $n$  and  $n'$  is **NOT** a different total state from particles 2 and 1 in single-particle states  $n$  and  $n'$ .

f) The diagonal matrix element is always zero for the fermions with identical spin coordinates. The zeros arise because for the Dirac delta function gives

$$\psi(x, x) = 0$$

in the integrand. The reason is that identical fermions with the same spin have zero probability of being in the same place because of the antisymmetrization of the wave function. Spatial antisymmetry makes fermions farther than they would otherwise be. Since our Dirac delta function potential only gives a contribution for when the particles have the probability of being in the same state: forbidding the particles from being the same place kills the contribution.

In fact the Dirac delta perturbation cannot affect the system at all in this case. The off-diagonal matrix elements are all zero too. Sort of makse sense: a potential that only acts when the particles have a probability of being in one place can't have an effect on a system where the particles have zero probability of being one place. So one cannot do perturbation theory for this case, but there is no need to since effectively there is no perturbation.

g) Classically, the Dirac delta function potential only turns on when the particles are in the same place. It can be attractive (energy lowering) or repulsive (energy raising). In quantum mechanics, the Dirac delta function potential only makes a contribution for the probability density of the particles being in the same place. Now you may object that the volume of parameter space where the particles are in the same place is zero. But the Dirac delta function rises to infinity, and so even a volume zero makes a non-zero contribution. In reality there probably are no Dirac delta function potentials, but there some very sharply peaked ones. Such potentials act over a small distance and are not infinitely high: thus there is a finite volume in parameter space in which the particles can interact through the potential. They are attracted or repulsed depending on the sign of  $V_0$ .

Let's go a bit beyond the required answer.

You may ask yourself—but probably not—what is the probability that the two distinct particles are within  $dx$  of each other. Let's consider the non-identical particles for simplicity. The joint probability density for the two particles is

$$\rho(x_1, x_2) dx_1 dx_2 .$$

We have to integrate  $\rho(x_1, x_2)$  along the diagonal in the  $x_1$ - $x_2$  plane. We get

$$\sqrt{2} \begin{cases} 1/a , & n \neq n' ; \\ 2/a , & n = n' . \end{cases} .$$

This is result is just the part (b) answer divided by  $V_0 a$  to remove the potential and multiplied by  $\sqrt{2}$  which is to account for integration along the diagonal. The probability of being in a band  $dz$  in width about the diagonal neglecting the end effects and the variation in  $\rho(x_a, x_b)$  perpendicular to the diagonal is

$$dP(dz) = dz \sqrt{2} \begin{cases} 1/a , & n \neq n' ; \\ 2/a , & n = n' . \end{cases}$$

Now for a point on the edge of the band

$$dx = x_a - x_b = x\sqrt{2} + \frac{dz/2}{\sqrt{2}} - \left( x\sqrt{2} - \frac{dz/2}{\sqrt{2}} \right) = \frac{dz}{\sqrt{2}} ,$$

and thus  $dz = \sqrt{2} dx$  for any point  $x$  where the perpendicular crosses the diagonal. A diagram would help. Thus the probability of find both particles with  $dx$  of each other (neglecting the end effects and the variation in  $\rho(x_1, x_2)$  perpendicular to the diagonal) is

$$dP(dx) = dx 2 \begin{cases} 1/a , & n \neq n' ; \\ 2/a , & n = n' . \end{cases}$$

Since this probability is approximate, it can't be normalized: it is valid though for  $dx \ll a$ . (I think I did this right.)

The rest of this makes me feel wuzzy right now, and so I leave correcting *sine die*.  
Now what if you add a short-range potential

$$V(y) = V_c f(y) ,$$

where  $y = |x_a - x_b|$ ,  $V_c$  is the potential when  $y = 0$ , and  $f(y)$  is scaling rule for the potential that goes to zero as  $y \rightarrow \infty$ . Now

$$I = 2 \int_0^\infty V(y) dy = V_c C ,$$

where the 2 accounts for the  $x_a - x_b < 0$  and  $x_a - x_b > 0$  cases and  $C$  a constant with units of length. Let's assume that the  $y$  region over which  $f(y)$  is significant is so small that we can always approximate the probability density as a constant there. We can then approximate

$$V(y) = V_c f(y)$$

by

$$V(y) = V_c C \delta(y) .$$

If we use this version of the Dirac delta potential instead of the previous one we get

$$H_{(nn')(nn')} = V_c C \begin{cases} 1/a , & n \neq n' ; \\ 3/(2a) , & n = n' . \end{cases}$$

Thus we recognize that  $V_0 a = V_c C$ . Actually there seems no good reason to parameterized the potential in terms of  $a$  since that is a length scale of the infinite square well and not of the

perturbation potential itself. Now for consistency between this paragraph and the last one, what if

$$V(y) = V_c \begin{cases} 1, & y \leq s; \\ 0, & y > s, \end{cases}$$

where  $s$  is the width of the potential. In this case  $C = 2s$ , and so

$$H_{(nn')(nn')} = V_c(2s) \begin{cases} 1/a, & n \neq n'; \\ 3/(2a), & n = n'. \end{cases}$$

The  $s$  corresponds to  $dx$  in the last paragraph expression. Thus if the particles are within  $s = dx$  of each other there is an extra potential contribution with height  $V_{\text{cm}}$ . This all seems right to me: how do you all feel about it?

Table of Energy Levels

L. No.	$n$	$n'$	$E_{\text{red}}$	Non-Id. Deg.	Id. Bo. Deg.	Id. Fe. Deg.	L. No.	$n$	$n'$	$E_{\text{red}}$	Non-Id. Deg.	Id. Bo. Deg.	Id. Fe. Deg.
1	1	1	2	1	1	0	20	4	6	52	2	1	1
2	1	2	5	2	1	1	21	2	7	53	2	1	1
3	2	2	8	1	1	0	22	3	7	58	2	1	1
4	1	3	10	2	1	1	23	5	6	61	2	1	1
5	2	3	13	2	1	1	24	1	8	65	2	1	1
6	1	4	17	2	1	1	25	4	7	65	2	1	1
7	3	3	18	1	1	0	26	2	8	68	2	1	1
8	2	4	20	2	1	1	27	6	6	72	1	1	0
9	3	4	25	2	1	1	28	3	8	73	2	1	1
10	1	5	26	2	1	1	29	5	7	74	2	1	1
11	2	5	29	2	1	1	30	4	8	80	2	1	1
12	4	4	32	1	1	0	31	1	9	82	2	1	1
13	3	5	34	2	1	1	32	2	9	85	2	1	1
14	1	6	37	2	1	1	33	6	7	85	2	1	1
15	2	6	40	2	1	1	34	5	8	89	2	1	1
16	4	5	41	2	1	1	35	3	9	90	2	1	1
17	3	6	45	2	1	1	36	4	9	97	2	1	1
18	1	7	50	2	1	1	37	7	7	98	1	1	0
19	5	5	50	1	1	0	38	6	8	100	2	1	1

Note—For non-identical particles interchanging the distinct values  $n$  and  $n'$  between the particles creates a different state. We merely note that those cases exist and the energy level has a degeneracy of 2 as indicated in the table. For identical particles interchanging the values of  $n$  and  $n'$  does not create a different state. Thus for bosons the degeneracy is always 1 for each energy level. For fermions, if  $n = n'$  no state is allowed by the Pauli exclusion principle and the degeneracy is zero. There are energy levels below 100 that have one of  $n$  or  $n'$  greater than 7. I have included these for completeness. Note that there are three pairs of energy levels with each one of the pair having the same reduced energies: 50, 65, and 85. These pairs should be combined, but that is tricky to computationally and it is convenient to see them separately. These pairs are examples of accidental degeneracies: different pairs of  $n$  and  $n'$  leading to the same energy. For each accidental degeneracy we could create one combined energy level: the degeneracies of the pairs just add.

Fortran 95 Code

```
!23456789a123456789b123456789c123456789d123456789e123456789f123456789g12
!
! State determines the reduced energies and degeneracies for
! 2 non-interacting particles in an infinite square well.
!
!
```

```

program state
implicit none
```

```

!
integer, parameter :: ndble=kind(0.d0)
integer, parameter :: nprecision=ndble
integer, parameter :: nemax=100
!
integer :: i,j
integer :: ien(nemax,6)
integer :: iorder(nemax)
integer :: istate
integer :: itmp
integer :: nmax
!
nmax=ceiling(sqrt(real(nemax,nprecision)))
!
istate=0
do410: do i=1,nmax
do420: do j=i,nmax
itmp=i**2+j**2
if(itmp .gt. nemax) exit do420
istate=istate+1
ien(istate,1)=itmp
ien(istate,2)=i
ien(istate,3)=j
ien(istate,5)=1           ! identical bosons
if(i .ne. j) then
ien(istate,4)=2           ! distinct particles.
ien(istate,6)=1           ! identical fermions
else
ien(istate,4)=1           ! distinct particles.
ien(istate,6)=0           ! identical fermions.
end if
end do do420
end do do410
!
print*, 'Before order.'
call order(istate,ien(1,1),iorder)
print*, 'After order.'
!
if(mod(itmp,2) .eq. 0) then
itmp=istate/2
else
itmp=istate/2+1
ien(istate+1,1:6)=0
end if
!
print*
do430: do i=1,istate
print910,i,ien(iorder(i),2),ien(iorder(i),3),ien(iorder(i),1),      &
& ien(iorder(i),4),ien(iorder(i),5),ien(iorder(i),6)
end do do430
!
print*
write(*,910)
& (i,ien(iorder(i),2),ien(iorder(i),3),ien(iorder(i),1),          &
& ien(iorder(i),4),ien(iorder(i),5),ien(iorder(i),6),          &
& i+itmp,ien(iorder(i+itmp),2),ien(iorder(i+itmp),3),          &
& ien(iorder(i+itmp),1),                                          &
& ien(iorder(i+itmp),4),ien(iorder(i+itmp),5),                  &

```

```

&          ien(iorder(i+itmp),6),
&  i=1,itmp)
!
910 format((i3,13('&',i3)),'\cr')  ! For some reason, the
!                                  ! brackets are needed.
!
      end program state
!
!23456789a123456789b123456789c123456789d123456789e123456789f123456789g12
!
! A bubble sort.  Bubble sorts are very inefficient, but they
! are easy to code and remember.
!
      subroutine order(istate,ien,iorder)
      implicit none
      integer :: i,j
      integer :: ien(istate)
      integer :: iorder(istate)
      integer :: istate
      integer :: itmp
!
!      print*,istate
!
      do410: do i=1,istate
         iorder(i)=i
!         print*,i,ien(i)
      end do do410
!
      do420: do i=istate,2,-1
         do430: do j=2,i
            if(ien(iorder(j-1)) .gt. ien(iorder(j))) then
               itmp=iorder(j-1)
               iorder(j-1)=iorder(j)
               iorder(j)=itmp
            end if
         end do do430
      end do do420
!
!      do i=1,istate
!         write(*,*) i,ien(i),iorder(i),ien(iorder(i))
!         write(*,'(3i5)') i,ien(i),ien(iorder(i))
!      end do
!
      end subroutine order
!
!23456789a123456789b123456789c123456789d123456789e123456789f123456789g12

```

**Redaction:** Jeffery, 2001jan01

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015 qfull 03110 2 5 0 moderate thinking: 4x4 eigenproblem/perturbation

10. You are given a zeroth order Hamiltonian matrix

$$H^{(0)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

- a) Solve for the eigenvalues and normalized eigenvectors by inspection. You should label the states 1, 2, 3, and 4 for convenience. Is there any degeneracy and if so what are the degenerate states?

b) The evil wizard of physics now turns on a perturbation and the Hamiltonian becomes

$$H = \begin{pmatrix} 1 & \epsilon & 0 & 0 \\ \epsilon & 1 & 0 & 0 \\ 0 & 0 & 1 & \epsilon \\ 0 & 0 & \epsilon & -1 \end{pmatrix},$$

where  $\epsilon$  is a small quantity. Solve for the exact eigenvalues and normalized eigenvectors in this case: i.e., diagonalize the perturbed Hamiltonian matrix. Is there any degeneracy now? **HINT:** Is there any reason why the two  $2 \times 2$  blocks in the matrix cannot be treated as separate eigenvalue problems and the two-component eigenvectors extended trivially for the  $4 \times 4$  problem?

c) Do non-degenerate perturbation theory to solve for the energy to 2nd order for those initial eigenstates which are **NOT** degenerate. **HINT:** All the perturbation matrix elements can be found in the part (b) **QUESTION**.

**SUGGESTED ANSWER:**

a) By inspection, the eigenvalues and normalized eigenvectors are, respectively,  $E_1^{(0)} = 1$ ,  $E_2^{(0)} = 1$ ,  $E_3^{(0)} = 1$ ,  $E_4^{(0)} = -1$  and

$$\vec{c}_1^{(0)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \vec{c}_2^{(0)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \vec{c}_3^{(0)} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad \vec{c}_4^{(0)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

The eigenvalue 1 has a triple degeneracy: i.e., it corresponds to 3 eigenvectors or eigenstates: states 1, 2, and 3.

b) No: there is no reason why not. The states in the two blocks are completely uncoupled: there are no non-zero matrix elements that couple them. The matrix is, as we say, block diagonal.

The general eigen-equation for a  $2 \times 2$  Hamiltonian matrix (which is derive from the determinant equation  $\det|H - EI|$  where  $H$  is the Hamiltonian matrix,  $E$  is the eigen-energy, and  $I$  is the unit matrix) is

$$(H_{11} - E)(H_{22} - E) - H_{12}H_{21} = 0$$

or

$$E^2 - (H_{11} + H_{22})E + H_{11}H_{22} - H_{12}H_{21} = 0.$$

The solutions are

$$E = \frac{(H_{11} + H_{22}) \pm \sqrt{(H_{11} + H_{22})^2 - 4(H_{11}H_{22} - H_{12}H_{21})}}{2} \\ = \frac{1}{2} \left[ (H_{11} + H_{22}) \pm \sqrt{(H_{11} - H_{22})^2 + 4|H_{12}|^2} \right].$$

Using the above result for the upper block, we find

$$E = 1 \pm \epsilon.$$

The eigenvectors follow from

$$H_{11}c_1 + H_{12}c_2 = Ec_1$$

or

$$c_2 = \frac{E - H_{11}}{H_{12}}c_1 = \frac{\pm\epsilon}{\epsilon}c_1 = \pm c_1$$

Thus,

$$\vec{c}(E = 1 \pm \epsilon) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \\ 0 \\ 0 \end{pmatrix},$$

where we have extended the eigenvector to accommodate the  $4 \times 4$  problem. Neither of the two new states is in anyway a small perturbation away from the initial states. The perturbation no matter how weak has thoroughly mixed the unperturbed states. This is one of manifestations of why non-degenerate perturbation theory does not work for coupled degenerate states: no matter how small the perturbation, the states can change radically. It is not sensible to identify either of the new states with the unperturbed states 1 and 2.

Actually, the eigenvectors for the unperturbed degenerate are not unique as we should have known. There were infinitely many orthonormal choices of the form

$$\vec{c}_1^{(0)} = \begin{pmatrix} a \\ b \\ 0 \\ 0 \end{pmatrix} \quad \vec{c}_2^{(0)} = \begin{pmatrix} b^* \\ -a^* \\ 0 \\ 0 \end{pmatrix},$$

where the only constraint is

$$|a|^2 + |b|^2 = 1.$$

These are all eigenstates of the unperturbed matrix. We see that the perturbation picks out a particular choice to be the perturbed states. Which choice depends on the nature of the perturbation.

Using the formulae for the upper block, *mutatis mutandis*, for the lower block, we find

$$E = \pm\sqrt{1 + \epsilon^2}.$$

In this case,

$$c_4 = \frac{E - H_{33}}{H_{34}} c_3 = \left( \frac{\pm\sqrt{1 + \epsilon^2} - 1}{\epsilon} \right) c_3,$$

which is satisfied if

$$c_3 = \epsilon \quad \text{and} \quad c_4 = \pm\sqrt{1 + \epsilon^2} - 1.$$

Thus, the normalized eigenvectors are given by

$$\vec{c}(E = \pm\sqrt{1 + \epsilon^2}) = \frac{\pm 1}{\sqrt{\epsilon^2 + (\pm\sqrt{1 + \epsilon^2} - 1)^2}} \begin{pmatrix} 0 \\ 0 \\ \epsilon \\ \pm\sqrt{1 + \epsilon^2} - 1 \end{pmatrix},$$

where clairvoyance tells us to put the  $\pm 1$  phase factor with the overall eigenvector.

Note that if  $\epsilon \rightarrow 0$ ,

$$\vec{c}(E = \sqrt{1 + \epsilon^2}) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

and

$$\vec{c}(E = -\sqrt{1 + \epsilon^2}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

We that as  $\epsilon \rightarrow 0$ , these solutions go to the unperturbed states. The first one to state 3 and the second one, to state 4. The  $\pm 1$  phase factor gave us the right standard form for state 4, but without it we would just have gotten  $-1$  times the standard form which is an equally valid eigenvector since a global phase factor causes no physical distinction.

For the lower block, the identities of the states are not lost as the perturbation grows from 0. This is a consequence of the fact that the states are not degenerate.

The perturbation has completely broken the degeneracy: all the eigenvalues are non-degenerate: i.e., they are distinct: different: not the same: unlike: etc. But they aren't very different: the first two differ only to 1st order in  $\epsilon$  from the unperturbed energies; the second two differ only to 2nd order in  $\epsilon$  from the unperturbed energies.

c) Well only one unperturbed state is non-degenerate: state 4 with eigenvector

$$\vec{c}_4^{(0)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

The perturbation Hamiltonian is

$$H^{(1)} = \begin{pmatrix} 0 & \epsilon & 0 & 0 \\ \epsilon & 0 & 0 & 0 \\ 0 & 0 & 0 & \epsilon \\ 0 & 0 & \epsilon & 0 \end{pmatrix},$$

We see that the 1st order perturbation energy is zero since the diagonal elements are zero. The second order perturbation energy is given by

$$E_4^{(2)} = \sum_{\text{all } k, \text{ except } k \neq n} \frac{|\langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}} = -\frac{\epsilon^2}{2}.$$

Thus to 2nd order in perturbation theory

$$E_4^{2\text{nd}} = -1 - \frac{\epsilon^2}{2}.$$

The perturbation theory result agrees with the the exact result for  $E_4$  of the part (b) answer to 2nd order in small  $\epsilon$ .

One can actually do weak-coupling perturbation theory for state 3 even though it is degenerate with states 1 and 2. The reason is that state 3 is not coupled to those states: all the coupling matrix elements are zero (e.g., Gr-230). *Mutatis mutandis*, the derivation for state 4 we find:

$$E_3^{2\text{nd}} = 1 + \frac{\epsilon^2}{2}.$$

The perturbation theory result agrees with the the exact result for  $E_3$  of the part (b) answer to 2nd order in small  $\epsilon$ .

**Redaction:** Jeffery, 2001jan01

015 qfull 03300 3 5 0 tough thinking: perturbation and variation

**Extra keywords:** (Gr-235:6.9)

11. Consider quantum system of 3 dimensions with initial Hamiltonian

$$H^{(0)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

and perturbed Hamiltonian

$$H = \begin{pmatrix} 1 - \epsilon & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix}.$$

Note we assume  $\epsilon \ll 1$ . Also note that  $H^{(0)}$  and  $H$  are matrix Hamiltonians: i.e., Hamiltonians in a particular representation. The matrix elements are  $\langle \phi_i | H_{\text{op}}^{(0)} | \phi_k \rangle$ ,  $\langle \phi_i | H_{\text{op}} | \phi_k \rangle$ , respectively, where  $H_{\text{op}}^{(0)}$  and  $H_{\text{op}}$  are operator versions of the Hamiltonian and the set  $\{|\phi_i\rangle\}$  is an orthonormal basis. Usually we drop the “op” subscript and allow context to tell whether the Hamiltonian is in matrix or operator representation.

a) Solve by inspection for the eigen-energies and eigenvectors of the initial unperturbed Hamiltonian. To help with the rest of the problem label the states 1, 2, and 3 in some sensible order.

- b) Solve for the exact eigen-energies and normalized eigenvectors of the perturbed Hamiltonian: i.e., diagonalize the perturbed Hamiltonian matrix. **HINTS:** It's not so hard—if you don't make a mistake in the first step.
- c) Expand the exact eigen-energies and eigenvectors (where applicable) to 2nd order in small  $\epsilon$ . (Note I mean Taylor expansion, not perturbation series expansion although the two expansion are closely related in this case.) Simplify the eigenvectors to nice forms so that it is easy to see which perturbed vector grew out of which unperturbed vector as  $\epsilon$  grew from 0.
- d) Determine from (weak-coupling) perturbation theory the energies to 2nd order and the eigenvectors to 1st order of the perturbed Hamiltonian. How do these results compare with those of the part (c) answer? **HINT:** Perturbation theory can be applied to the degenerate states in this case because they are completely uncoupled.
- e) Now use the truncated Hamiltonian matrix method (or linear variational method if you know it) to find approximate eigen-energies and eigenvectors for the two initially degenerate eigen-energy states. To what order goodness in small  $\epsilon$  are the results? Why the are results for one perturbed state exact and for the other rather poor compared to the exact results?

**SUGGESTED ANSWER:**

- a) The eigenvalues are  $E_1^{(0)} = 1$ ,  $E_2^{(0)} = 1$ , and  $E_3^{(0)} = 2$  corresponding respectively to eigenvectors

$$\vec{c}_1^{(0)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \vec{c}_2^{(0)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad \vec{c}_3^{(0)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

- b) One can get the eigen-equation from Laplacian expansion (Ar-157):

$$[(1 - \epsilon) - E][(1 - E)(2 - E) - \epsilon^2] = 0.$$

One notes that this equation is separable in two parts immediately. In fact if we'd been smart we would have recognized that the Hamiltonian consists of two decoupled blocks that have independent solutions except for trivial zero component extensions. Smart or not, the eigen-energies are

$$E = 1 - \epsilon$$

and

$$E = \frac{3 \pm \sqrt{1 + 4\epsilon^2}}{2}.$$

We can identify the energies as

$$E_1 = 1 - \epsilon, \\ E_2 = \frac{3 - \sqrt{1 + 4\epsilon^2}}{2},$$

and

$$E_3 = \frac{3 + \sqrt{1 + 4\epsilon^2}}{2}.$$

These energies “grew” out of the unperturbed energies with the same labels. This “growth from” is demonstrated clearly in the part (c) answer where we show the 2nd order in  $\epsilon$  good perturbed eigenvectors. When the perturbation is weak, there is a one-to-one correspondence between the old states and the new states if the old states are not strongly coupled.

The eigenvector for  $E_1$  by inspection is

$$\vec{c}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

This vector clearly grew out both the original state 1 vector  $\vec{c}_1^{(0)}$  since it is, in fact, the same vector for all values of  $\epsilon$ . The eigenvectors for  $E_2$  and  $E_3$  both have  $c_1 = 0$  since they are for the 2-3 subspace which is decoupled from the 1 subspace. We find

$$c_2 + c_3\epsilon = Ec_2$$

or

$$c_3 = c_2 \frac{(E-1)}{\epsilon} .$$

Thus

$$\vec{c}_{2,3} = \frac{1}{\sqrt{\epsilon^2 + (E-1)^2}} \begin{pmatrix} 0 \\ \epsilon \\ E-1 \end{pmatrix} .$$

c) Behold to 2nd order:

$$\begin{aligned} E_1 &= 1 - \epsilon , \\ E_2 &= 1 - \epsilon^2 , \end{aligned}$$

and

$$E_3 = 2 + \epsilon^2 .$$

The eigenvectors to 2nd order are

$$\vec{c}_1^{2\text{nd}} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} , \quad \vec{c}_2^{2\text{nd}} = \frac{1}{\sqrt{1+\epsilon^2}} \begin{pmatrix} 0 \\ 1 \\ -\epsilon \end{pmatrix} , \quad \text{and} \quad \vec{c}_3^{2\text{nd}} = \frac{1}{\sqrt{\epsilon^2 + (1+\epsilon^2)^2}} \begin{pmatrix} 0 \\ \epsilon \\ 1+\epsilon^2 \end{pmatrix} .$$

As  $\epsilon \rightarrow 0$  these vectors become the zeroth order vectors. This completes our identification of which exact vector goes with which zeroth order vector.

d) Well we first note that the perturbation Hamiltonian is

$$H^{(1)} = \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & 0 & \epsilon \\ 0 & \epsilon & 0 \end{pmatrix} .$$

Recall the perturbation formula

$$E_n^{2\text{nd}} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle + \lambda^2 \sum_{\text{all } k, k \neq n} \frac{|\langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}} .$$

In this case with perturbation parameter  $\lambda = 1$ , we find

$$\begin{aligned} E_1^{2\text{nd}} &= 1 - \epsilon + 0 = 1 - \epsilon \\ E_2^{2\text{nd}} &= 1 + 0 + \frac{\epsilon^2}{1-2} = 1 - \epsilon^2 \end{aligned}$$

and

$$E_3^{2\text{nd}} = 2 + 0 + \frac{\epsilon^2}{2-1} = 2 + \epsilon^2 .$$

Now recall the perturbation formula

$$|\psi_n^{1\text{st}}\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{\text{all } k, k \neq n} \frac{\langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} |\psi_k^{(0)}\rangle .$$

In this case with perturbation parameter  $\lambda = 1$ , we find

$$\vec{c}_1^{1\text{st}} = \vec{c}_1^{(0)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} , \quad \vec{c}_2^{1\text{st}} = \vec{c}_2^{(0)} - \epsilon \vec{c}_3^{(0)} = \begin{pmatrix} 0 \\ 1 \\ -\epsilon \end{pmatrix} , \quad \text{and} \quad \vec{c}_3^{1\text{st}} = \vec{c}_3^{(0)} + \epsilon \vec{c}_2^{(0)} = \begin{pmatrix} 0 \\ \epsilon \\ 1 \end{pmatrix} .$$

The 2nd order good perturbation eigen-energies agree exactly with the 2nd order  $\epsilon$  expansion result in the part (c) answer. The 1st order good perturbation eigenvectors agree to 1st order in small  $\epsilon$  with the 2nd order  $\epsilon$  expansion result in the part (c) answer. This agreement is satisfactory since the 1st order good perturbation eigenvector is only 1st order good in a small perturbation parameter which is effectively what  $\epsilon$  is.

The perturbation results for state 1 are, in fact, exact. This is because it is uncoupled to all other states.

e) The truncated eigen-problem is

$$\begin{pmatrix} 1 - \epsilon & 0 \\ 0 & 1 \end{pmatrix} \vec{c} = E \vec{c} ,$$

By inspection, the eigen-energies from the truncated eigen-problem are

$$E_1 = 1 - \epsilon \quad \text{and} \quad E_2 = 1 ,$$

and the eigenvectors are

$$\vec{c}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \vec{c}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} ,$$

where we have extended the eigenvectors to 3 dimensions for agreement with the earlier parts of the question. The state 1 energy and eigenvector are exactly right, but the state 2 energy is only good to 1st order in small  $\epsilon$  and the  $E_2$  eigenvector is only 0th order good. The exactly right results for state 1 are because this state is entirely decoupled from the other states: there are no coupling matrix elements. Thus state 1 is exactly solvable even if you truncate the matrix just to include that state alone. The state 2 results are distinctly poorer than the exact results. The essential reason for this poorness is that state 2 is coupled through off-diagonal elements to the state 3 and in the truncated eigen-problem we neglect this coupling completely. Neglected coupling in the truncated Hamiltonian matrix method is a general problem. One just needs to make the matrix big enough that one can tolerate the errors of neglected coupling.

**Redaction:** Jeffery, 2001jan01