



Don't Panic!

Quantum Mechanics I
Practice Problem

Nov. '98.
Handout (T. Hübsch)

1. Boxed Particle

We will consider perturbing the “particle of mass M in an $L \times L$ square box”. The system with the ‘unperturbed’ potential

$$V(x, y) = \begin{cases} 0 & \text{while } 0 \leq x, y \leq L, \\ \infty & \text{otherwise,} \end{cases}$$

is exactly known:

$$|m, n\rangle^{(0)} = \frac{2}{L} \sin(m\pi \frac{x}{L}) \sin(n\pi \frac{y}{L}) \quad (1.1a)$$

$$E_{m,n}^{(0)} = \frac{\hbar^2 \pi^2}{2ML^2} (m^2 + n^2) \quad (1.1b)$$

are the exact expressions for the ortho-normalized ‘unperturbed’ wave-functions and ‘unperturbed’ energy levels. For the record, we write the ‘unperturbed’ Hamiltonian:

$$\hat{H}^{(0)} = -\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + V(x, y). \quad (1.2)$$

The system is degenerate, and in part owing to the $x \leftrightarrow y$ symmetry, whence $E_{m,n}^{(0)} = E_{n,m}^{(0)}$ although $|m, n\rangle^{(0)} \neq |n, m\rangle^{(0)}$ unless in fact $m = n$. In addition, there is accidental degeneracy between states $|m, n\rangle^{(0)}$ and $|q, r\rangle^{(0)}$ for which $n^2 + m^2 = q^2 + r^2$. Nevertheless, we shall see that for simple enough perturbations, this degeneracy will pose no problem; we will be able to avoid the nonsensical vanishing denominators.

1. As the first perturbation, consider $\hat{H}^{(1)} = \alpha x$. The original problem, with the Hamiltonian (1.2), is separable in Cartesian coordinates as $\hat{H}^{(0)} = \hat{H}_x^{(0)} + \hat{H}_y^{(0)}$, and we find that the same is true of the perturbed Hamiltonian:

$$\hat{H} = \hat{H}_x + \hat{H}_y = [\hat{H}_x^{(0)} + \hat{H}^{(1)}] + \hat{H}_y^{(0)}. \quad (1.3)$$

Thus, the perturbed problem will also have wave-functions in the $\psi_m(x)\psi_n^{(0)}(y)$, where $\psi_n^{(0)}(y) = |n\rangle_y^{(0)} = \sqrt{\frac{2}{L}} \sin(n\pi \frac{y}{L})$ and only the $\psi_m(x)$ will differ from $\psi_m^{(0)}(x) = |m\rangle_x^{(0)} = \sqrt{\frac{2}{L}} \sin(m\pi \frac{x}{L})$.

We will need the matrix-elements of $\hat{H}^{(1)}$ are:

$${}^{(0)}\langle m, n | \hat{H}^{(1)} | m', n' \rangle^{(0)} = \alpha {}^{(0)}\langle m, n | x | m', n' \rangle^{(0)}, \quad (1.4a)$$

$$= \alpha \left[{}^{(0)}\langle m | x | m' \rangle_x \right] \left[{}^{(0)}\langle n | \mathbb{1} | n' \rangle_y \right], \quad (1.4b)$$

$$= \alpha \left[-\frac{8Lmm'}{\pi^2(m^2 - m'^2)^2} \left(\frac{1 - (-1)^{\Delta m}}{2} \right) \right] \left[\delta_{n,n'} \right], \quad (1.4c)$$

where the y -integral follows by ortho-normality, and the x -integral is the only one we needed. It was evaluated as follows (sorry for the hasty incomplete result on the hand-written note).

$${}^{(0)}\langle m | x | m' \rangle_x = \frac{2}{L} \int_0^L dx \sin(m\pi \frac{x}{L}) x \sin(m'\pi \frac{x}{L}), \quad (1.5a)$$

$$= \frac{2L}{\pi^2} \int_0^\pi d\phi \sin(m\phi) \phi \sin(m'\phi), \quad (1.5b)$$

$$= \frac{2L}{\pi^2} \int_0^\pi d\phi \frac{1}{2} \left[\cos[(m - m')\phi] - \cos[(m + m')\phi] \right] \phi, \quad (1.5c)$$

$$= \frac{L}{\pi^2} \left[\frac{\cos[(m - m')\pi]}{(m - m')^2} - \frac{1}{(m - m')^2} - \frac{\cos[(m + m')\pi]}{(m + m')^2} + \frac{1}{(m + m')^2} \right],$$

$$= \frac{L}{\pi^2} \left[\frac{(-1)^{m - m'} - 1}{(m - m')^2} - \frac{(-1)^{m + m'} - 1}{(m + m')^2} \right], \quad (1.5e)$$

$$= \frac{2L}{\pi^2} \left[\frac{(-1)^{\Delta m} - 1}{2} \right] \frac{(m + m')^2 - (m - m')^2}{(m^2 - m'^2)^2}, \quad (1.5f)$$

$$= -\frac{2L}{\pi^2} \left[\frac{1 - (-1)^{\Delta m}}{2} \right] \frac{4mm'}{(m^2 - m'^2)^2}, \quad (1.5g)$$

$$= -\frac{8Lmm'}{\pi^2(m^2 - m'^2)^2} \left[\frac{1 - (-1)^{\Delta m}}{2} \right]. \quad (1.5h)$$

We integrated by parts

$$\int_0^\pi d\phi \cos(N\phi) \phi = \left[\frac{\phi}{N} \sin(N\phi) \right]_0^\pi - \frac{1}{N} \int_0^\pi d\phi \sin(N\phi) = [0] + \frac{1}{N^2} \left[\cos(N\phi) \right]_0^\pi, \quad (1.6)$$

introduced the abbreviation $\Delta m \stackrel{\text{def}}{=} (m - m')$, used that $\cos(N\pi) = (-1)^N$, and than also that $(-1)^{m + m'} = (-1)^{m - m' + 2m'} = (-1)^{\Delta m} (-1)^{2m'} = (-1)^{\Delta m}$. Note the factor $\frac{1}{2}(1 - (-1)^{\Delta m})$: this equals 1 if Δm is odd and vanishes if Δm is even. So, in particular, the matrix element is identically zero if $m = m'$. Note also that the $\delta_{n,n'}$ factor implies that $n = n'$. To summarize,

$${}^{(0)}\langle m, n | x | m', n' \rangle^{(0)} = \begin{cases} -\frac{8\alpha Lmm'}{\pi^2(m^2 - m'^2)^2} & n=n' \text{ and } \Delta m = (m - m') \text{ odd}; \\ 0 & \text{otherwise.} \end{cases} \quad (1.7)$$

We can now address the physically interesting questions.

a. Even without any calculation, we know that the degeneracy created by the $x \leftrightarrow y$ symmetry will be lifted (lost). This is simply because the new Hamiltonian, $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$ no longer commutes with the $\mathbf{P}_{x:y}$ symmetry operator. Thus, the energies (expectation values of the new Hamiltonian) of a state $|m, n\rangle$ and its $x \leftrightarrow y$ “mirror” state, $\mathbf{P}_{x:y}|m, n\rangle$ will be different. In fact, if $|m, n\rangle$ is an eigenstate of the new Hamiltonian, $\mathbf{P}_{x:y}|m, n\rangle$ will not even be an eigenstate! To see this differently, note that the ‘unperturbed’ energy eigenvalues can be written as $E_{m,n}^{(0)} = {}^x E_m^{(0)} + {}^y E_n^{(0)}$. With the perturbation depending only on x , the exact energy eigenvalues will admit a similar separation, $E_{m,n} = {}^x E_m + {}^y E_n$. Here, however, ${}^y E_n = {}^y E_n^{(0)}$ while ${}^x E_m \neq {}^x E_m^{(0)}$ will be shifted by an amount depending on α , which is an arbitrary parameter. Therefore, for some special values of α we may find some (new) degeneracy, but all of the degeneracy of the ‘unperturbed’ case will be lost.

b. The first order shift in the energy is equal to the diagonal matrix element of $\hat{H}^{(1)}$ —which is zero: see Eq. (1.7).

c. The first order correction to the wave-function is

$$|m, n\rangle^{(1)} = - \sum_{(m', n') \neq (m, n)} \frac{\langle m', n' | \hat{H}^{(1)} | m, n \rangle^{(0)}}{E_{m', n'}^{(0)} - E_{m, n}^{(0)}} |m', n'\rangle^{(0)}, \quad (1.8a)$$

$$= \frac{16\alpha ML^3}{\hbar^2 \pi^4} \sum_{(m', n') \neq (m, n)} \frac{\frac{mm'}{(m^2 - m'^2)^2} \frac{1}{2} (1 - (-1)^{\Delta m}) \delta_{n, n'}}{m'^2 + n'^2 - m^2 - n^2} |m', n'\rangle^{(0)}, \quad (1.8b)$$

$$= \frac{16\alpha ML^3}{\hbar^2 \pi^4} \sum_{m' \neq m} \frac{mm'}{(m'^2 - m^2)^3} \frac{1 - (-1)^{\Delta m}}{2} |m', n\rangle^{(0)}, \quad (1.8c)$$

$$= \frac{16\alpha ML^3}{\hbar^2 \pi^4} \sum_{k > (1-m)/2} \frac{m(m+2k-1)}{(2k-1)^3 (2k+2m-1)^3} |m+2k-1, n\rangle^{(0)}. \quad (1.8d)$$

Note that the condition $(m', n') \neq (m, n)$ on the summation merely prevents *both* labels to be equal, *i.e.*, the sum extends over all wave-functions other than $|m, n\rangle^{(0)}$, whose correction we are calculating¹! We then used that the $\delta_{n, n'}$ factor in the matrix element enforces the y -labels (n, n') to be equal, whereupon the x -labels (m, m') must be different. In the final line we substituted $(m-m') = \Delta m = 1-2k$ since Δm must be odd for the matrix element to be non-zero. Now $m' = m+2k-1$, and since we had that $m, m' > 0$, it follows that $m+2k-1 > 0$ or $k > (1-m)/2$, as specified in the last sum.

d. The second order correction to the energy is

$$E_{m, n}^{(2)} = - \sum_{(m', n') \neq (m, n)} \frac{|\langle m', n' | \hat{H}^{(1)} | m, n \rangle^{(0)}|^2}{E_{m', n'}^{(0)} - E_{m, n}^{(0)}}, \quad (1.9a)$$

¹ A correction of $|m, n\rangle^{(0)}$ proportional to itself would be irrelevant as this would have merely produced a rescaling of the original wave-function—a multiplicative factor which would in the end be reset by normalization.

$$= -\frac{128\alpha^2 ML^4}{\hbar^2 \pi^6} \sum_{(m',n') \neq (m,n)} \frac{\frac{m^2 m'^2}{(m^2 - m'^2)^4} \left(\frac{1}{2}(1 - (-1)^{\Delta m})\right)^2 \delta_{n,n'}^2}{m'^2 + n'^2 - m^2 - n^2}, \quad (1.9b)$$

$$= -\frac{128\alpha^2 ML^4}{\hbar^2 \pi^6} \sum_{m' \neq m} \frac{m^2 m'^2}{(m'^2 - m^2)^5} \left(\frac{1 - (-1)^{\Delta m}}{2}\right)^2, \quad (1.9c)$$

$$= -\frac{128\alpha^2 ML^4}{\hbar^2 \pi^6} \sum_{k > (1-m)/2} \frac{m^2(m+2k-1)^2}{(2k-1)^5(2k+2m-1)^5}. \quad (1.9d)$$

It is not our goal here to evaluate the sums; we merely note that for any given m, n , the sums converge fairly rapidly (as $\sim k^{-5}$ for the wave-function, and as $\sim k^{-8}$ for the second order shift in the energy) to some well-defined numbers. Instead, note that the perturbative corrections all feature a factor of \hbar^{-2} . This is typical; compare with all other examples in the text (for the Hydrogen atom, recall that the Bohr radius is proportional to \hbar^2). Furthermore, note that the corrections of n^{th} order are proportional to α^n . This parameter may be thought of as the coupling or control parameter of the perturbation: in the limit $\alpha \rightarrow 0$, we recover the ‘unperturbed’ results. Indeed, the whole perturbation series of both the Energy eigenvalues and the wave-functions (and any other observable!) turns out to be a formal² power series of this α .

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2. As the second perturbation, consider $\hat{H}^{(1)} = \alpha(x + y)$. This time, $[\mathbf{P}_{x:y}, \hat{H}^{(1)}] = 0$, whence the degeneracy stemming from the $x \leftrightarrow y$ symmetry will persist. Since the perturbation is a sum of a purely x -dependent and a purely y -dependent term, we can account for them separately. Now both ${}^x E_m^{(0)}$ and ${}^y E_n^{(0)}$ are being shifted equally, by an amount proportional to α^2 , to lowest order; see (1.9)—one simply adds terms with the rôles of x, m, m' and y, n, n' swapped. α being arbitrary, the accidental degeneracy will be lifted in general, and only special choices of α will result in some (new) degeneracy.

3. The third perturbation, $\hat{H}^{(1)} = \alpha(x - y)$, does not commute with the symmetry operator $\mathbf{P}_{x:y}$, so that all degeneracy will be lifted (lost) for general α . The expressions for the shift in the energy and the change of the wave-function are obtained from those above, by subtracting terms with the rôles of x, m, m' and y, n, n' swapped.

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Most importantly of all, however, note that the vanishing of the first order perturbative correction of the energy eigenvalues certainly did not imply no correction at all. The vanishing of the diagonal matrix elements of $\hat{H}^{(1)}$ stems from a symmetry property: the energy eigenstates in a 1-dimensional box are either symmetric or antisymmetric with respect to the reflection about the mid-point, $x \mapsto (L-x)$. The diagonal matrix elements involve integration over squares of eigenfunctions which are necessarily symmetric with

² This series must be regarded as a formal one, as convergence has not been proven in general.

respect to this reflection. The perturbation being antisymmetric with respect to this reflection, the integrals vanish, as with (upon shifting the integration variable)

$$\int_{-a}^{+a} dx f(x) = 0, \quad \text{if} \quad f(-x) = -f(x). \quad (1.10)$$

2. Oscillators

Simple perturbations of the linear (and multi-dimensional) harmonic oscillator exhibit more of the hallmark of this popular paradigm: exact solubility.

Consider perturbing the standard oscillator

$$\hat{H}^{(0)} = -\frac{\hbar^2}{2M} \frac{d^2}{dx^2} + \frac{1}{2} M \omega^2 x^2, \quad (2.1)$$

by adding the perturbation

$$\hat{H}^{(1)} = \alpha x^2 + \beta x + \gamma, \quad (2.2)$$

where α, β, γ are suitable constants. Use the creation/annihilation operator formalism:

$$\begin{aligned} \hat{H}^{(1)} &= \frac{\alpha \hbar}{2M\omega} (\hat{a}^{\dagger 2} + \hat{a}^{\dagger} \hat{a} + \hat{a} \hat{a}^{\dagger} + \hat{a}^2) + \beta \sqrt{\frac{\hbar}{2M\omega}} (\hat{a}^{\dagger} + \hat{a}) + \gamma, \\ &= \frac{\alpha \hbar}{2M\omega} (\hat{a}^{\dagger 2} + 2\hat{N} + 1 + \hat{a}^2) + \beta \sqrt{\frac{\hbar}{2M\omega}} (\hat{a}^{\dagger} + \hat{a}) + \gamma. \end{aligned} \quad (2.3)$$

The matrix elements are:

$$\begin{aligned} {}^{(0)}\langle m | \hat{H}^{(1)} | n \rangle^{(0)} &= \frac{\alpha \hbar}{2M\omega} \left[\sqrt{n(n+1)} \delta_{m,n+2} + (2n+1) \delta_{m,n} + \sqrt{m(m+1)} \delta_{m+2,n} \right] \\ &\quad + \beta \sqrt{\frac{\hbar}{2M\omega}} \left[\sqrt{n} \delta_{m,n+1} + \sqrt{m} \delta_{m+1,n} \right] + \gamma \delta_{m,n}, \end{aligned} \quad (2.4a)$$

Thus, the first order shift in the energy eigenvalues are

$$E_n^{(1)} = \frac{\alpha \hbar}{2M\omega} (2n+1) + \gamma. \quad (2.5)$$

The first order correction to the wave-functions are

$$\begin{aligned} |n\rangle^{(1)} &= \frac{\alpha}{4M\omega^2} \left[\sqrt{(n-1)n} |n-2\rangle^{(0)} - \sqrt{(n+2)(n+1)} |n+2\rangle^{(0)} \right] \\ &\quad + \frac{\beta}{\sqrt{2M\hbar\omega^3}} \left[\sqrt{n} |n-1\rangle^{(0)} - \sqrt{n+1} |n+1\rangle^{(0)} \right]. \end{aligned} \quad (2.6)$$

The second order corrections to the energy eigenvalues are

$$E_n^{(2)} = -\frac{\alpha^2 \hbar^2}{4M^2 \omega^2} \left[\frac{(n+2)(n+1)}{2\hbar\omega} + \frac{n(n-1)}{-2\hbar\omega} \right] - \frac{\beta^2 \hbar}{2M\omega} \left[\frac{n+1}{\hbar\omega} + \frac{n}{-\hbar\omega} \right], \quad (2.7a)$$

$$= -\frac{\alpha^2 \hbar}{4M^2 \omega^3} [2n+1] - \frac{\beta^2 \hbar}{2M\omega} [+1], \quad (2.7a)$$

Amusingly, the perturbed linear harmonic oscillator problem

$$\hat{H} = -\frac{\hbar^2}{2M} \frac{d^2}{dx^2} + \frac{1}{2}M\omega^2 x^2 + \alpha x^2 + \beta x + \gamma, \quad (2.8)$$

can also be solved exactly. We simply shift the coordinate, the frequency and the zero-point energy:

$$\hat{H} = -\frac{\hbar^2}{2M} \frac{d^2}{dz^2} + \frac{1}{2}M\tilde{\omega}^2 z^2 + V_0, \quad (2.9)$$

where

$$z = x + \frac{\beta}{M\omega^2 + 2\alpha}, \quad V_0 = \gamma - \frac{\beta^2}{2(M\omega^2 + 2\alpha)}, \quad (2.10a)$$

$$\tilde{\omega} = \omega + \Delta\omega = \pm\sqrt{\omega^2 + \frac{2\alpha}{M}}, \quad \Delta\omega = -\omega \pm \sqrt{\omega^2 + \frac{2\alpha}{M}}, \quad (2.10b)$$

and where $\frac{d}{dz} = \frac{d}{dx}$ since the shifts are constant. However, the Hamiltonian (2.9) obviously looks the same as (2.1), except that the constant V_0 has been added. Thus, the energy eigenvalues are

$$E_n = \hbar\tilde{\omega}(n + \frac{1}{2}) + V_0. \quad (2.11)$$

In terms of the original parameters in (2.8),

$$E_n = \hbar\omega(n + \frac{1}{2})\sqrt{1 + \frac{2\alpha}{M\omega^2}} + \gamma - \frac{\beta^2}{2M\omega^2(1 + \frac{2\alpha}{M\omega^2})}. \quad (2.12)$$

Of course, this can be expanded

$$E_n = \hbar\omega(n + \frac{1}{2}) \left[1 + \frac{\alpha}{M\omega^2} - \frac{1}{8} \frac{\alpha^2}{M^2\omega^4} + \dots \right] + \gamma - \frac{\beta^2}{2M\omega^2} \left[1 - \frac{2\alpha}{M\omega^2} + \dots \right], \quad (2.13)$$

recovering the first and second order shifts in the energy eigenvalues obtained above and more. (Try expanding the wave-functions $|n\rangle \propto H_n(\zeta)e^{-\frac{1}{2}\zeta^2}$, where $\zeta = \sqrt{\frac{M\tilde{\omega}}{\hbar}}z$.)

Obviously, this latter method is not only easier but also produces the exact result (2.12). Note that this means that the perturbation series in fact converges to the neat expressions in (2.12). It should be equally obvious that this is about the only type of 1-dimensional problems so easily solved. (Try perturbing similarly various multi-dimensional oscillators.) For perturbations involving higher powers of x , it is typically fastest to use the creation/annihilation operator method used in the first part of this practice problem.

**DON'T TAKE MY WORD FOR THESE RESULTS!
CALCULATE YOURSELF!**