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Further Quantum Mechanics HT 2014
Problems 1 (HT weeks 6 – 8)

1.1 A harmonic oscillator with mass m and angular frequency ω is perturbed by $\delta H = \epsilon x^2$. (a) What is the exact change in the ground-state energy? Expand this change in powers of ϵ up to order ϵ^2. (b) Show that the change given by first-order perturbation theory agrees with the exact result to $\mathrm{O}(\epsilon)$ (c) Show that the first-order change in the ground state is $|b\rangle = -(\epsilon\ell^2/\sqrt{2}\hbar\omega)|E_2\rangle$. (d) Show that second-order perturbation theory yields an energy change $E_c = -\epsilon^2\hbar/4m^2\omega^3$ in agreement with the exact result.

1.2 The harmonic oscillator of Problem 1.1 is perturbed by $\delta H = \epsilon x$. Show that the perturbed Hamiltonian can be written

$$H = \frac{1}{2m}\left(p^2 + m^2\omega^2 X^2 - \frac{\epsilon^2}{\omega^2}\right),$$

where $X = x + \epsilon/m\omega^2$ and hence deduce the exact change in the ground-state energy. Interpret these results physically.

What value does first-order perturbation theory give? From perturbation theory determine the coefficient b_1 of the unperturbed first-excited state in the perturbed ground state. Discuss your result in relation to the exact ground state of the perturbed oscillator.

1.3 The harmonic oscillator of Problem 1.1 is perturbed by $\delta H = \epsilon x^4$. Show that the first-order change in the energy of the n^{th} excited state is

$$\delta E = 3(2n^2 + 2n + 1)\epsilon\left(\frac{\hbar}{2m\omega}\right)^2. \tag{1.1}$$

Hint: express x in terms of $A + A^\dagger$.

1.4 The infinite square-well potential $V(x) = 0$ for $|x| < a$ and ∞ for $|x| > a$ is perturbed by the potential $\delta V = \epsilon x/a$. Show that to first order in ϵ the energy levels of a particle of mass m are unchanged. Show that even to this order the ground-state wavefunction *is* changed to

$$\psi_1(x) = \frac{1}{\sqrt{a}}\cos(\pi x/2a) + \frac{16\epsilon}{\pi^2 E_1\sqrt{a}}\sum_{n=2,4,}(-1)^{n/2}\frac{n}{(n^2-1)^3}\sin(n\pi x/2a),$$

where E_1 is the ground-state energy. Explain physically why this wavefunction does not have well-defined parity but predicts that the particle is more likely to be found on one side of the origin than the other. State with reasons but without further calculation whether the second-order change in the ground-state energy will be positive or negative.

1.5 An atomic nucleus has a finite size, and inside it the electrostatic potential $\Phi(r)$ deviates from $Ze/(4\pi\epsilon r)$. Take the proton's radius to be $a_\mathrm{p} \simeq 10^{-15}$ m and its charge density to be uniform. Then treating the difference between Φ and $Ze/(4\pi\epsilon_0 r)$ to be a perturbation on the Hamiltonian of hydrogen, calculate the first-order change in the ground-state energy of hydrogen. Why is the change in the energy of any P state extremely small? Comment on how the magnitude of this energy shift varies with Z in hydrogenic ions of charge Z. Hint: exploit the large difference between a_p and a_0 to approximate the integral you formally require.

Degenerate perturbation theory

1.6 A particle of mass m moves in the potential $V(x,y) = \frac{1}{2}m\omega^2(x^2+y^2)$, where ω is a constant. Show that the Hamiltonian can be written as the sum $H_x + H_y$ of the Hamiltonians of two identical one-dimensional harmonic oscillators. Write down the particle's energy spectrum. Write down kets for two stationary states in the first-excited level in terms of the stationary states $|n_x\rangle$ of H_x and $|n_y\rangle$ of H_y. Show that the n^{th} excited level is $n+1$ fold degenerate.

The oscillator is disturbed by a small potential $H_1 = \lambda xy$. Show that this perturbation lifts the degeneracy of the first excited level, producing states with energies $2\hbar\omega \pm \lambda\hbar/2m\omega$. Give expressions for the corresponding kets.

The mirror operator M is defined such that $\langle x,y|M|\psi\rangle = \langle y,x|\psi\rangle$ for any state $|\psi\rangle$. Explain physically the relationship between the states $|\psi\rangle$ and $M|\psi\rangle$. Show that $[M, H_1] = 0$. Show that $MH_x = H_yM$ and thus that $[M, H] = 0$. What do you infer from these commutation relations?

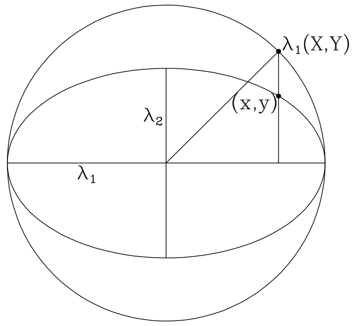

Figure 1.0 The relation of input and output vectors of a 2×2 Hermitian matrix with positive eigenvalues $\lambda_1 > \lambda_2$. An input vector (X, Y) on the unit circle produces the output vector (x, y) that lies on the ellipse that has the eigenvalues as semi-axes.

1.7* The Hamiltonian of a two-state system can be written

$$H = \begin{pmatrix} A_1 + B_1\epsilon & B_2\epsilon \\ B_2\epsilon & A_2 \end{pmatrix}, \tag{1.2}$$

where all quantities are real and ϵ is a small parameter. To first order in ϵ, what are the allowed energies in the cases (a) $A_1 \neq A_2$, and (b) $A_1 = A_2$?

Obtain the exact eigenvalues and recover the results of perturbation theory by expanding in powers of ϵ.

Variational Principle

1.8 State Rayleigh's theorem. The 2×2 Hermitian matrix $\mathbf{H}$ has positive eigenvalues $\lambda_1 > \lambda_2$. The vectors (X, Y) and (x, y) are related by

$$\mathbf{H} \cdot \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix}.$$

Show that the points $(\lambda_1 X, \lambda_1 Y)$ and (x, y) are related as shown in Figure 1.0. How does this result generalise to 3×3 matrices? Explain the relation of Rayleigh's theorem to this result.

1.9 We find an upper limit on the ground-state energy of the harmonic oscillator from the trial wavefunction $\psi(x) = (a^2 + x^2)^{-\alpha}$. Using the substitution $x = a \tan\theta$, or otherwise, show that when $\alpha = 1$

$$\int_0^\infty \mathrm{d}x\, |\psi|^2 = \tfrac{1}{4}\pi a^{-3} \quad \int_0^\infty \mathrm{d}x\, x^2 |\psi|^2 = \tfrac{1}{4}\pi a^{-1} \quad \int_0^\infty \mathrm{d}x\, |p\psi|^2 = \tfrac{1}{8}\pi\hbar^2 a^{-5}. \tag{1.3}$$

Hence show that $\langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle$ is minimised by setting $a = 2^{l/4}\ell$, where ℓ is the characteristic length of the oscillator. Show that our upper limit on E_0 is $\hbar\omega/\sqrt{2}$. Plot the final trial wavefunction and the actual ground-state wavefunction and infer how α should be changed to obtain a better trial wavefunction.

1.10* Show that with the trial wavefunction $\psi(x) = (a^2 + x^2)^{-2}$ the variational principle yields an upper limit $E_0 < (\sqrt{7}/5)\hbar\omega \simeq 0.529\,\hbar\omega$ on the ground-state energy of the harmonic oscillator.

1.11 Show that for the unnormalised spherically symmetric wavefunction $\psi(r)$ the expectation value of the gross-structure Hamiltonian of hydrogen is

$$\langle H\rangle = \left(\frac{\hbar^2}{2m_\mathrm{e}} \int \mathrm{d}r\, r^2 \left|\frac{\mathrm{d}\psi}{\mathrm{d}r}\right|^2 - \frac{e^2}{4\pi\epsilon_0} \int \mathrm{d}r\, r|\psi|^2\right) \Bigg/ \int \mathrm{d}r\, r^2|\psi|^2. \tag{1.4}$$

For the trial wavefunction $\psi_b = \mathrm{e}^{-br}$ show that

$$\langle H\rangle = \frac{\hbar^2 b^2}{2m_\mathrm{e}} - \frac{e^2 b}{4\pi\epsilon_0},$$

and hence recover the definitions of the Bohr radius and the Rydberg constant.

1.12* Using the result proved in Problem 1.11, show that the trial wavefunction $\psi_b = \mathrm{e}^{-b^2r^2/2}$ yields $-8/(3\pi)\mathcal{R}$ as an estimate of hydrogen's ground-state energy, where $\mathcal{R}$ is the Rydberg constant.

1.13 Show that the stationary point of $\langle\psi|H|\psi\rangle$ associated with an excited state of H is a saddle point. Hint: consider the state $|\psi\rangle = \cos\theta|k\rangle + \sin\theta|l\rangle$, where θ is a parameter.

Time-dependent perturbation theory

1.14 At early times ($t \sim -\infty$) a harmonic oscillator of mass m and natural angular frequency ω is in its ground state. A perturbation $\delta H = \mathcal{E}x\mathrm{e}^{-t^2/\tau^2}$ is then applied, where $\mathcal{E}$ and τ are constants.

a. What is the probability according to first-order theory that by late times the oscillator transitions to its second excited state, $|2\rangle$?

b. Show that to first order in δH the probability that the oscillator transitions to the first excited state, $|1\rangle$, is

$$P = \frac{\pi\mathcal{E}^2\tau^2}{2m\hbar\omega}\mathrm{e}^{-\omega^2\tau^2/2}, \tag{1.5}$$

c. Plot P as a function of τ and comment on its behaviour as $\omega\tau \to 0$ and $\omega\tau \to \infty$.

1.15 A particle of mass m executes simple harmonic motion at angular frequency ω. Initially it is in its ground state but from $t = 0$ its motion is disturbed by a steady force F. Show that at time $t > 0$ and to first order in F the state is

$$|\psi, t\rangle = \mathrm{e}^{-\mathrm{i}E_0 t/\hbar}|0\rangle + a_1\mathrm{e}^{-\mathrm{i}E_1 t/\hbar}|1\rangle$$

where

$$a_1 = \frac{\mathrm{i}}{\sqrt{2m\hbar\omega}}\int_0^t \mathrm{d}t'\, F(t')\mathrm{e}^{\mathrm{i}\omega t'}.$$

Calculate $\langle x\rangle(t)$ and show that your expression coincides with the classical solution

$$x(t) = \int_0^t \mathrm{d}t'\, F(t')G(t-t'),$$

where the Green's function is $G(t-t') = \sin[\omega(t-t')]/m\omega$. Show that a suitable displacement of the point to which the oscillator's spring is anchored could give rise to the perturbation.

1.16* A particle of mass m is initially trapped by the well with potential $V(x) = -V_\delta\delta(x)$, where $V_\delta > 0$. From $t = 0$ it is disturbed by the time-dependent potential $v(x,t) = -Fx\mathrm{e}^{-\mathrm{i}\omega t}$. Its subsequent wavefunction can be written

$$|\psi\rangle = a(t)\mathrm{e}^{-\mathrm{i}E_0 t/\hbar}|0\rangle + \int \mathrm{d}k\ \{b_k(t)|k,\mathrm{e}\rangle + c_k(t)|k,\mathrm{o}\rangle\}\,\mathrm{e}^{-\mathrm{i}E_k t/\hbar}, \tag{1.6}$$

where E_0 is the energy of the bound state $|0\rangle$ and $E_k \equiv \hbar^2k^2/2m$ and $|k,\mathrm{e}\rangle$ and $|k,\mathrm{o}\rangle$ are, respectively the even- and odd-parity states of energy E_k (see Problem 5.17). Obtain the equations of motion

$$\begin{aligned}\mathrm{i}\hbar&\left\{\dot a|0\rangle\mathrm{e}^{-\mathrm{i}E_0 t/\hbar} + \int \mathrm{d}k\ \left(\dot b_k|k,\mathrm{e}\rangle + \dot c_k|k,\mathrm{o}\rangle\right)\mathrm{e}^{-\mathrm{i}E_k t/\hbar}\right\}\\ &= v\left\{a|0\rangle\mathrm{e}^{-\mathrm{i}E_0 t/\hbar} + \int \mathrm{d}k\ \left(b_k|k,\mathrm{e}\rangle + c_k|k,\mathrm{o}\rangle\right)\mathrm{e}^{-\mathrm{i}E_k t/\hbar}\right\}.\end{aligned} \tag{1.7}$$

Given that the free states are normalised such that $\langle k',\mathrm{o}|k,\mathrm{o}\rangle = \delta(k-k')$, show that to first order in v, $b_k = 0$ for all t, and that

$$c_k(t) = \frac{\mathrm{i}F}{\hbar}\langle k,\mathrm{o}|x|0\rangle\,\mathrm{e}^{\mathrm{i}\Omega_k t/2}\,\frac{\sin(\Omega_k t/2)}{\Omega_k/2}, \quad \text{where} \quad \Omega_k \equiv \frac{E_k - E_0}{\hbar} - \omega. \tag{1.8}$$

Hence show that at late times the probability that the particle has become free is

$$P_{\mathrm{fr}}(t) = \frac{2\pi m F^2 t}{\hbar^3}\left.\frac{|\langle k,\mathrm{o}|x|0\rangle|^2}{k}\right|_{\Omega_k=0}. \tag{1.9}$$

Given that from Problem 5.17 we have

$$\langle x|0\rangle = \sqrt{K}\mathrm{e}^{-K|x|} \quad \text{where} \quad K = \frac{mV_\delta}{\hbar^2} \quad \text{and} \quad \langle x|k,\mathrm{o}\rangle = \frac{1}{\sqrt{\pi}}\sin(kx), \tag{1.10}$$

show that

$$\langle k,\mathrm{o}|x|0\rangle = \sqrt{\frac{K}{\pi}}\frac{4kK}{(k^2+K^2)^2}. \tag{1.11}$$

Hence show that the probability of becoming free is

$$P_{\mathrm{fr}}(t) = \frac{8\hbar F^2 t}{mE_0^2}\frac{\sqrt{E_{\mathrm{f}}/|E_0|}}{(1+E_{\mathrm{f}}/|E_0|)^4}, \tag{1.12}$$

where $E_{\mathrm{f}} > 0$ is the final energy. Check that this expression for P_{fr} is dimensionless and give a physical explanation of the general form of the energy-dependence of $P_{\mathrm{fr}}(t)$

1.17* A particle travelling with momentum $p = \hbar k > 0$ from $-\infty$ encounters the steep-sided potential well $V(x) = -V_0 < 0$ for $|x| < a$. Use the Fermi golden rule to show that the probability that a particle will be reflected by the well is

$$P_{\mathrm{reflect}} \simeq \frac{V_0^2}{4E^2}\sin^2(2ka),$$

where $E = p^2/2m$. Show that in the limit $E \gg V_0$ this result is consistent with the exact reflection probability derived in Problem 5.10. Hint: adopt periodic boundary conditions so the wavefunctions of the in and out states can be normalised.

1.18* Show that the number of states $g(E)\,\mathrm{d}E\,\mathrm{d}^2\Omega$ with energy in $(E, E+\mathrm{d}E)$ and momentum in the solid angle $\mathrm{d}^2\Omega$ around $\mathbf{p} = \hbar\mathbf{k}$ of a particle of mass m that moves freely subject to periodic boundary conditions on the walls of a cubical box of side length L is

$$g(E)\,\mathrm{d}E\,\mathrm{d}^2\Omega = \left(\frac{L}{2\pi}\right)^3\frac{m^{3/2}}{\hbar^3}\sqrt{2E}\,\mathrm{d}E\,\mathrm{d}\Omega^2. \tag{1.13}$$

Hence show from Fermi's golden rule that the cross-section for elastic scattering of such particles by a weak potential $V(\mathbf{x})$ from momentum $\hbar\mathbf{k}$ into the solid angle $\mathrm{d}^2\Omega$ around momentum $\hbar\mathbf{k}'$ is

$$\mathrm{d}\sigma = \frac{m^2}{(2\pi)^2\hbar^4}\,\mathrm{d}^2\Omega\left|\int \mathrm{d}^3\mathbf{x}\,\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}V(\mathbf{x})\right|^2. \tag{1.14}$$

Explain in what sense the potential has to be 'weak' for this **Born approximation** to the scattering cross-section to be valid.