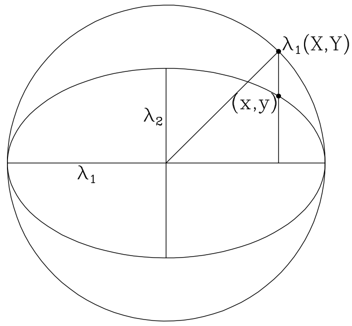

Figure 2.0 The input and output vectors of a 2×2 Hermitian matrix are related by a circle with the matrix's largest eigenvalue as radius and the ellipse that has the eigenvalues as semi-axes.

Further Quantum Mechanics TT 2013
Problems 2 (weeks 1–2)

Variational Principle

2.1 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 $(\lambda_1 X, \lambda_2 Y)$ and (x, y) are related as shown in Figure 2.0. How does this result generalise to 3×3 matrices? Explain the relation of Rayleigh's theorem to this result.

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

$$\int_0^\infty \mathrm{d}x\, |\psi|^2 = \tfrac{1}{4}\pi a^{-3} \qquad \int_0^\infty \mathrm{d}x\, x^2|\psi|^2 = \tfrac{1}{4}\pi a^{-1} \qquad \int_0^\infty \mathrm{d}x\, \psi^* p^2 \psi = \tfrac{1}{8}\pi a^{-5} \tag{2.1}$$

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 the final trial wavefunction and the actual ground-state wavefunction and (a) say whether you consider it a good fit, and (b) how it might be adapted into a better trial wavefunction.

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

$$\langle H\rangle = \left(\frac{\hbar^2}{2m_\mathrm{e}} \int \mathrm{d}r\, r^2 \left|\frac{\mathrm{d}\psi}{\mathrm{d}r}\right|^2 - \frac{e^2}{4\pi\epsilon_0} \int \mathrm{d}r\, r|\psi|^2\right) \Bigg/ \int \mathrm{d}r\, r^2|\psi|^2. \tag{2.2}$$

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.

2.4* Using the result proved in Problem 2.3, 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.

2.5 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

2.6 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 that by late times the oscillator transitions to its second excited state, $|2\rangle$?

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

$$P = \frac{\pi \mathcal{E}^2 \tau^2}{2m\hbar\omega}\mathrm{e}^{-\omega^2\tau^2/2}, \tag{2.3}$$

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

2.7 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

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

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.

2.8* 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

$$|\psi\rangle = a(t)\mathrm{e}^{-\mathrm{i}E_0 t/\hbar}|0\rangle + \int \mathrm{d}k\, \{b_k(t)|k, \mathrm{e}\rangle + c_k(t)|k, \mathrm{o}\rangle\}\, \mathrm{e}^{-\mathrm{i}E_k t/\hbar}, \tag{2.4}$$

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

$$\begin{aligned} &\mathrm{i}\hbar \left\{\dot{a}|0\rangle\mathrm{e}^{-\mathrm{i}E_0 t/\hbar} + \int \mathrm{d}k\, \left(\dot{b}_k|k, \mathrm{e}\rangle + \dot{c}_k|k, \mathrm{o}\rangle\right) \mathrm{e}^{-\mathrm{i}E_k t/\hbar}\right\} \\ &\qquad = v\left\{a|0\rangle\mathrm{e}^{-\mathrm{i}E_0 t/\hbar} + \int \mathrm{d}k\, (b_k|k, \mathrm{e}\rangle + c_k|k, \mathrm{o}\rangle)\, \mathrm{e}^{-\mathrm{i}E_k t/\hbar}\right\}. \end{aligned} \tag{2.5}$$

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

$$c_k(t) = \frac{\mathrm{i}F}{\hbar}\langle k, \mathrm{o}|x|0\rangle\, \mathrm{e}^{\mathrm{i}\Omega_k t/2}\,\frac{\sin(\Omega_k t/2)}{\Omega_k/2}, \quad \text{where} \quad \Omega_k \equiv \frac{E_k - E_0}{\hbar} - \omega. \tag{2.6}$$

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

$$P_{\mathrm{fr}}(t) = \frac{2\pi m F^2 t}{\hbar^3} \left.\frac{|\langle k, \mathrm{o}|x|0\rangle|^2}{k}\right|_{\Omega_k=0}. \tag{2.7}$$

Given that from Problem 5.17 we have

$$\langle x|0\rangle = \sqrt{K}\mathrm{e}^{-K|x|} \quad \text{where} \quad K = \frac{mV_\delta}{\hbar^2} \quad \text{and} \quad \langle x|k, \mathrm{o}\rangle = \frac{1}{\sqrt{\pi}}\sin(kx), \tag{2.8}$$

show that

$$\langle k, \mathrm{o}|x|0\rangle = \sqrt{\frac{K}{\pi}}\frac{4kK}{(k^2 + K^2)^2}. \tag{2.9}$$

Hence show that the probability of becoming free is

$$P_{\mathrm{fr}}(t) = \frac{8\hbar F^2 t}{mE_0^2}\frac{\sqrt{E_{\mathrm{f}}/|E_0|}}{(1 + E_{\mathrm{f}}/|E_0|)^4}, \tag{2.10}$$

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 $P_{\mathrm{fr}}(t)$

2.9* 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

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

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.

2.10* Show that the number states $g(E)\,{\rm d}E\,{\rm d}^2\Omega$ with energy in $(E, E+{\rm d}E)$ and momentum in the solid angle ${\rm d}^2\Omega$ 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

$$g(E)\,{\rm d}E\,{\rm d}^2\Omega = \left(\frac{L}{2\pi}\right)^3 \frac{m^{3/2}}{\hbar^3}\sqrt{2E}\,{\rm d}E\,{\rm d}\Omega^2. \qquad (2.11)$$

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 ${\rm d}^2\Omega$ around momentum $\hbar\mathbf{k}'$ is

$$d\sigma = \frac{m^2}{(2\pi)^2\hbar^4}\,{\rm d}^2\Omega\left|\int {\rm d}^3\mathbf{x}\,{\rm e}^{{\rm i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}V(\mathbf{x})\right|^2. \qquad (2.12)$$

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

2.11 Given that $a_0 = \hbar/(\alpha m_{\rm e} c)$ show that the product $a_0 k$ of the Bohr radius and the wavenumber of a photon of energy E satisfies

$$a_0 k = \frac{E}{\alpha m_{\rm e} c^2}. \qquad (2.13)$$

Hence show that the wavenumber k_α of an Hα photon satisfies $a_0 k_\alpha = \frac{5}{72}\alpha$ and determine λ_α/a_0. What is the connection between this result and our estimate that $\sim 10^7$ oscillations are required to complete a radiative decay. Does it imply anything about the way the widths of spectral lines from allowed atomic transitions varies with frequency?

2.12 Given that a system's Hamiltonian is of the form

$$H = \frac{p^2}{2m_{\rm e}} + V(\mathbf{x}) \qquad (2.14)$$

show that $[x,[H,x]] = \hbar^2/m_{\rm e}$. By taking the expectation value of this expression in the state $|k\rangle$, show that

$$\sum_{n\neq k} |\langle n|x|k\rangle|^2 (E_n - E_k) = \frac{\hbar^2}{2m_{\rm e}}, \qquad (2.15)$$

where the sum runs over all the other stationary states.

The **oscillator strength** of a radiative transition $|k\rangle \to |n\rangle$ is defined to be

$$f_{kn} \equiv \frac{2m_{\rm e}}{\hbar^2}(E_n - E_k)|\langle n|x|k\rangle|^2 \qquad (2.16)$$

Show that $\sum_n f_{kn} = 1$. What is the significance of oscillator strengths for the allowed radiative transition rates of atoms?