

1) Quantal and classical exponential atmosphere: Consider a particle of mass m moving in one spatial dimension, confined to the region $x > 0$ and subject to the linear potential $V(x) = fx$, where f is a positive constant. If, e.g., the potential were gravitational then f would be mg and the particle would be an atmospheric particle.

- a) Sketch the potential.
- b) The energy eigenproblem reads

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + fx\right) \psi(x) = \epsilon \psi(x).$$

By introducing the shifted dimensionless length $Y \equiv (x/\lambda) - (\epsilon/f\lambda)$, where λ is the characteristic length $(\hbar^2/2mf)^{1/3}$, show that the eigenproblem reduces to the dimensionless form $\Psi''(Y) - Y\Psi(Y) = 0$, i.e., to Airy's equation.

- c) By imposing appropriate boundary conditions, establish that the energy eigenvalues ϵ_n obey the quantisation condition $\text{Ai}(-\epsilon_n/f\lambda) = 0$ and that the (un-normalised) eigenfunctions are given by translations of the scaled Airy function:

$$\psi_n(x) = \text{Ai}\left(\frac{x}{\lambda} - \frac{\epsilon_n}{f\lambda}\right).$$

Give the first three eigenvalues and sketch the first three eigenfunctions.

Note: You may wish to consult a standard reference, such as *Abramowitz and Stegun*.

- d) Now apply the Bohr-Sommerfeld quantisation scheme to motion in the potential $V(x)$. Compute the lowest three eigenvalues it gives, and compare them with their exact values. Compare the Bohr-Sommerfeld eigenvalue spectrum at large n with the result you obtain for the spectrum using the asymptotic properties of the Airy function.

Recall the problem of classical statistical mechanics in which we consider a system of non-interacting particles that constitute an isothermal atmosphere. In that setting, we ask the question: What is the probability density $p(x)$ for finding a particle to be at height x , given the gravitational potential $V(x) = mgx$? We find the exponential atmosphere result: $p(x) = (mg/k_B T) \exp(-mgx/k_B T)$. Let us see how we can recover this result, starting with quantal rather than classical motion—a problem posed by my colleague Prof. Paul Debevec.

According to the canonical ensemble of quantum statistical mechanics,

$$p(x) = \frac{1}{\lambda} \mathcal{P}(X, B) \equiv \frac{1}{\lambda \sum_{n=1}^{\infty} e^{-BE_n}} \sum_{n=1}^{\infty} e^{-BE_n} \frac{\text{Ai}(X - E_n)^2}{\int_0^{\infty} dX' \text{Ai}(X' - E_n)^2},$$

where $X \equiv x/\lambda$, $B \equiv f\lambda/k_B T$ and $E_n \equiv \epsilon_n/f\lambda$,

e) Explain the elements of this formula.

Now let us try to understand the classical limit of this formula. The essential idea is to neglect tunnelling into the classically forbidden region. This means that, for a given value of x , states n only contribute to $p(x)$ if $\epsilon_n > fx$. States lower in energy come with quantal probability densities that involve Airy functions evaluated at positive arguments, and these are small, only being nonzero by virtue of tunnelling. Thus we have

$$\mathcal{P}(X, B) \approx \frac{1}{\sum_{n=1}^{\infty} e^{-BE_n}} \sum_{n > \nu(X)}^{\infty} e^{-BE_n} \frac{\text{Ai}(X - E_n)^2}{\int_0^{E_n} dX' \text{Ai}(X' - E_n)^2},$$

where $E_\nu(X) \approx X$. Generally, for larger values of x fewer states contribute.

To evaluate \mathcal{P} we approximate the sum over states (i.e. over n) by an integral over n (characteristically, as discreteness/quantisation is an essentially quantal effect). To do the resulting integral we exchange continuous n for continuous $E = (3\pi/2)^{2/3} n^{2/3}$, suggested by the asymptotic spectrum at large n .

f) Show that this leads to

$$\mathcal{P}(X, B) \approx \frac{1}{\int_0^{\infty} dE \sqrt{E} e^{-BE}} \int_X^{\infty} dE \sqrt{E} e^{-BE} \frac{\text{Ai}(X - E)^2}{\int_0^E dX' \text{Ai}(X' - E)^2}.$$

g) The asymptotic form of the Airy function at large negative argument reads

$$\text{Ai}(-z) \approx \frac{1}{\sqrt{\pi} z^{1/4}} \sin\left(\zeta + \frac{\pi}{4}\right),$$

where $\zeta \equiv (2/3)z^{3/2}$. Show that averaging over a few periods gives for the quantal probability factor

$$\text{Ai}(X - E)^2 \approx \frac{1}{2\pi} \frac{1}{\sqrt{E - X}}$$

and for its normalisation integral

$$\int_0^E dX \text{Ai}(X - E)^2 \approx \frac{\sqrt{E}}{\pi}.$$

h) Put the pieces together to obtain the classical result

$$\mathcal{P}(X, B) \approx \frac{\int_X^{\infty} dE \frac{1}{\sqrt{E - X}} e^{-BE}}{2 \int_0^{\infty} dE \sqrt{E} e^{-BE}} = B e^{-BX}.$$

Hence, we find the exponential atmosphere formula: $p(x) = (f/k_B T) \exp(-fx/k_B T)$.

2) Spin-1/2 particle in a magnetic field (after Shankar, 17.2.2) – optional: Consider a spin-half particle with gyromagnetic ratio γ in a magnetic field $\mathbf{B} = B_1\mathbf{e}_x + B_0\mathbf{e}_z$. Treating B_1 as a perturbation, calculate the first- and second-order shifts in energy and first-order shift in state vector for the ground state. Compare your answers with the exact answers expanded to the corresponding orders.

You may quote the relevant operators for the spin degrees of freedom from *Shankar*, Sec. 14.3.

3) Degenerate perturbation theory for a spin-1 particle (after Shankar, 17.3.2) – optional: Consider a spin-1 particle with no orbital degrees of freedom. Let the hamiltonian be

$$H = AS_z^2 + B(S_x^2 - S_y^2),$$

where $\{S_x, S_y, S_z\}$ are 3×3 spin matrices and $A \gg B$. Treating the B term as a perturbation, find the eigenstates of $H_0 = AS_z^2$ that are stable under the perturbation. Calculate the energy shifts to first order in B . State how these are related to the exact answers.

You have studied the relevant operators for the spin degrees of freedom for a prior homework.

4) Anharmonic oscillator – optional: *Shankar*, 17.2.1.

Note that you have obtained several relevant results for an earlier homework.

5) Hydrogen atom – optional: *Shankar*, 17.2.3.

6) Thomas-Reiche-Kuhn sum rule – optional: *Shankar*, 17.2.4.

7) Nearly degenerate perturbation theory (after Davydov, sec. 49) – optional:

The aim of this question is to work out how to handle eigenproblems perturbatively in settings in which a small collection of unperturbed eigenvalues are close in energy. By close in energy we mean that typical matrix elements of the perturbation are larger than typical differences between close unperturbed eigenvalues. The resulting “small” energy denominators preclude the use of ordinary perturbation theory for computing corrections to eigenvectors and eigenvalues. What is the remedy?

Let H_0 be an unperturbed hamiltonian having eigenvectors $\{|a\rangle\}$ and nondegenerate eigenvalues $\{E_a\}$, i.e., $H_0|a\rangle = E_a|a\rangle$. Let H_1 be a perturbation, so that the full hamiltonian is $H \equiv H_0 + H_1$. For the sake of simplicity, let us suppose that only two eigenvalues are close, and let them be E_1 and E_2 . (Extension to the more general case is straightforward.)

The remedy is to treat the subspace spanned by the vectors $|1\rangle$ and $|2\rangle$ more accurately, before applying perturbation theory. To do this, we modify the separation into unperturbed hamiltonian and perturbation as follows:

$$\begin{aligned} H_0 &\rightarrow \tilde{H}_0 \equiv H_0 + \sum_{a,b=1}^2 |a\rangle \langle a|H_1|b\rangle \langle b|, \\ H_1 &\rightarrow \tilde{H}_1 \equiv H_1 - \sum_{a,b=1}^2 |a\rangle \langle a|H_1|b\rangle \langle b|. \end{aligned}$$

Said equivalently, we move the diagonal block associated with the close eigenvalues from the perturbation to the unperturbed Hamiltonian; the latter is now not quite diagonal.

Next, we find the eigenvectors of the new unperturbed Hamiltonian \tilde{H}_0 . For $a \neq 1, 2$ the unperturbed eigenvectors and eigenvalues are unchanged.

- a) Determine the new eigenvalues associated with the $a = 1, 2$ subspace.
- b) Usual (i.e., nondegenerate) perturbation theory would hold if $|E_1 - E_2| \gg |\langle 1|H_1|2\rangle|$. Show that under this condition the new unperturbed energies are those determined by usual perturbation theory, taken to second order, at least as far as the coupling between states in the $a = 1, 2$ subspace is concerned.
- c) Suppose instead that $|E_1 - E_2| \ll |\langle 1|H_1|2\rangle|$. Determine, to leading order, the new unperturbed eigenvalues. Sketch them as a function of the parameter

$$\delta \equiv (E_1 + \langle 1|H_1|1\rangle) - (E_2 + \langle 2|H_1|2\rangle)$$

for fixed $\langle 1|H_1|2\rangle$. Observe that the coupling $\langle 1|H_1|2\rangle$ between the levels always increases their separation; this is the phenomenon of *level repulsion*.

Conclusion: The effects of the new perturbation \tilde{H}_1 can now be taken into account via usual perturbation theory. Difficulties associated with “small” energy denominators no longer arise because the corresponding numerators, the relevant matrix elements of \tilde{H}_1 from the $a = 1, 2$ subspace, vanish.

8) Rayleigh-Schrödinger and Brillouin-Wigner perturbation schemes (after Taylor and Heinonen, sec. 2.5) – optional: Let $|\psi\rangle$ be an eigenvector of a full hamiltonian $H_0 + H_1$ with eigenvalue E , and let $|\psi_0\rangle$ be the corresponding eigenvector of the unperturbed hamiltonian H_0 with eigenvalue E_0 . Thus: $(H_0 + H_1)|\psi\rangle = E|\psi\rangle$ and $H_0|\psi_0\rangle = E_0|\psi_0\rangle$.

- a) Show that if $|\psi\rangle$ is normalized such that $\langle\psi_0|\psi\rangle = 1$ then $\langle\psi_0|H_1|\psi\rangle = (E - E_0)$.
- b) By rearranging the full eigenproblem and using the result of part (a), or otherwise, show that $|\psi\rangle$ obeys the equation

$$|\psi\rangle = |\psi_0\rangle + (E_0 - H_0)^{-1} (1 - |\psi\rangle\langle\psi_0|) H_1|\psi\rangle.$$

Observe that the sole unknown quantity on the right hand side of this inhomogeneous equation is the sought eigenstate $|\psi\rangle$. Thus, by iteration one can develop a perturbative solution for $|\psi\rangle$, the *Rayleigh-Schrödinger* perturbation series. Note that the unknown quantity $|\psi\rangle$ occurs in more than one place on the right hand side. As a result, there is some intricacy to the resulting perturbation expansion.

- c) By making an alternative rearrangement of the full eigenproblem and using the result of part (a), or otherwise, show that $|\psi\rangle$ also obeys the equation

$$|\psi\rangle = |\psi_0\rangle + (E - H_0)^{-1} (1 - |\psi_0\rangle\langle\psi_0|) H_1|\psi\rangle.$$

Observe that there are now two unknown quantities on the right hand side of this inhomogeneous equation: the sought eigenstate $|\psi\rangle$ and the corresponding eigenvalue E . Iterating this equation yields the *Brillouin-Wigner* perturbation series for $|\psi\rangle$, which depends on the unknown quantity E ; however, the unknown quantity $|\psi\rangle$ no longer occurs in more than one place on the right hand side. The price of this simplification of the resulting perturbation expansion is its dependence on the unknown quantity E , which must be determined self-consistently, *a posteriori*, e.g., via the expectation value of the full hamiltonian.