FY2045 Quantum Mechanics I

Fall 2023

Henning Goa Hugdal

Week 11

Degenerate perturbation theory

Non-degenerate perturbation theory

The solution to the eigenvalue problem

$$(H_0 + V)|\psi_n\rangle = E_n|\psi_n\rangle$$

is

$$|\psi_n\rangle = |n\rangle + \sum_{m \neq n} \frac{\langle m|V|n\rangle}{E_n^0 - E_m^0}|m\rangle + \dots,$$

$$E_n = E_n^0 + \langle n|V|n\rangle + \sum_{m \neq n} \frac{|\langle m|V|n\rangle|^2}{E_n^0 - E_m^0} + \dots$$

Ø15.4, H7.2, G7.2

With degenerate unperturbed states, we risk having $E_n^0 - E_m^0 = 0$, giving divergent expressions. Possible way out: $\langle m|V|n\rangle = 0$.
We therefore need a more careful treatment.

Degenerate perturbation theory

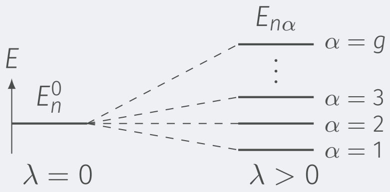
Consider a system where the unperturbed level n is degenerate

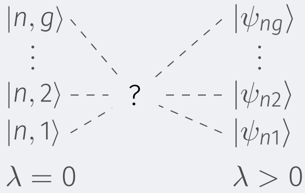
$$H_0|n,r\rangle = E_n^0|n,r\rangle, \quad (r = 1,\dots,g_n),$$

with degree of degeneracy g_n for level n, and we assume orthonormalized states, $\langle n,s|n,r\rangle = \delta_{sr}$. For notational simplicity we drop the subscript n and write $g = g_n$.

Write exact energies and state vectors as power series in λ, with $\alpha = 1,\dots,g$:

$$E_{n\alpha} = E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \qquad |\psi_{n\alpha}\rangle = |\psi_{n\alpha}^{(0)}\rangle + \lambda|\psi_{n\alpha}^{(1)}\rangle + \lambda^2|\psi_{n\alpha}^{(2)}\rangle + \dots$$





Degenerate perturbation theory

Inserting the expansions into the eigenvalue equation

$$H|\psi_{n\alpha}\rangle = (H_0 + \lambda V)|\psi_{n\alpha}\rangle = E_{n\alpha}|\psi_{n\alpha}\rangle,$$

and collecting like orders of λ, we get

$$\begin{aligned}
\lambda^0 : &\quad H_0|\psi_{n\alpha}^{(0)}\rangle = E_n^0|\psi_{n\alpha}^{(0)}\rangle, \\
\lambda^1 : &\quad (H_0 - E_n^0)|\psi_{n\alpha}^{(1)}\rangle + (V - E_{n\alpha}^{(1)})|\psi_{n\alpha}^{(0)}\rangle = 0,
\end{aligned}$$

etc. From the first, we see that

$$|\psi_{n\alpha}^{(0)}\rangle = \sum_{r=1}^{g} U_{r\alpha}|n,r\rangle, \quad (\alpha = 1, \ldots, g),$$

the “limit states” $|\psi_{n\alpha}^{(0)}\rangle$ are in general linear combinations of the unperturbed states $|n,r\rangle$.

Multiplying the λ^1 equation by $|n, s\rangle$ from the left, we get

$$\langle n, s|[V - E^{(1)}_{n\alpha}] \sum_r U_{ra}|n, r\rangle = \sum_r [V_{sr} - E^{(1)}_{n\alpha}\delta_{sr}]U_{r\alpha} = 0,$$

with matrix elements for known states,

$$V_{sr} \equiv \langle n, s|V|n, r\rangle.$$

Considering all values $s = 1, \dots, g$, we get the matrix equation

$$\begin{pmatrix} V_{11} - E^{(1)}_{n\alpha} & V_{12} & \dots & V_{1g} \\ V_{21} & V_{22} - E^{(1)}_{n\alpha} & & \\ \vdots & & \ddots & \vdots \\ V_{g1} & \dots & & V_{gg} - E^{(1)}_{n\alpha} \end{pmatrix} \begin{pmatrix} U_{1\alpha} \\ U_{2\alpha} \\ \vdots \\ U_{g\alpha} \end{pmatrix} = 0.$$

Degenerate perturbation theory

Non-trivial solutions are obtained when

$$\det \begin{pmatrix} V_{11} - E_{n\alpha}^{(1)} & \cdots \\ \vdots & \ddots \end{pmatrix} = 0,$$

resulting in an equation of degree g, with solutions $E_{n\alpha}^{(1)}$, $\alpha = 1, \ldots, g$.

We can calculate the coefficients $U_{r\alpha}$ and the "limit" states $|\psi_{n\alpha}^{(0)}\rangle$ by inserting the solutions $E_{n\alpha}^{(1)}$ into the matrix equation.

Special case

In some cases the off-diagonal matrix elements are all zero, $V_{rs} = 0$ for $s \neq r$. We then get

$$E_{nr}^{(1)} = \langle n, r|V|n, r\rangle, \ (r = 1, 2, \ldots, g),$$

just as in the non-degenerate case. The perturbation V does not connect the unperturbed states, and we have $|\psi_{nr}^{(0)}\rangle = |n, r\rangle$.

Finding the "good" or "limit" states

Theorem: Let $\{F_i\}$, $i = 1, 2, \ldots$ be a set of Hermitian operators that commute with H_0 and V. If we choose a set of states $|n, r\rangle$ which are degenerate eigenfunctions of H_0,

$$H_0|n, r\rangle = E_n^0|n, r\rangle, \ (r = 1, \ldots, g_n),$$

and eigenfunctions of F_i with distinct eigenvalues, that is

$$F_i|n, r\rangle = f_{ir}|n, r\rangle,$$

with $f_{ir} \neq f_{is}$ if $r \neq s$, then the states $|n, r\rangle$ are the "good" or "limit" states — the states the exact solutions $|\psi_{n\alpha}\rangle$ approach when $\lambda \to 0$.

In some cases we can use this theorem to find the "good" states before performing the calculation.

Example — 2D Perturbed Harmonic Oscillator

The system is described by $H = H_0 + V$, with

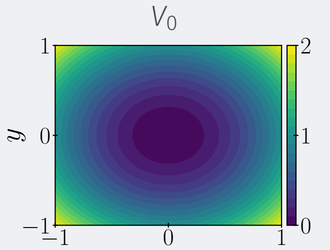
$$H_0 = \frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_y^2\right) + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2),$$
$$V = \epsilon m\omega^2\hat{x}\hat{y},$$

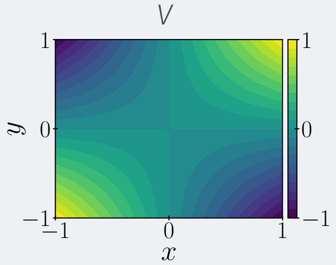
where ϵ is a dimensionless number.

Eigenstates and eigenvalues of H_0:

$$E^0_{n_x n_y} = \hbar\omega[n_x + n_y + 1], \text{ and } |n_x n_y\rangle \equiv |n_x\rangle|n_y\rangle.$$

What are the first-order corrections to the doubly degenerate first excited state, with energy $E^0_1 = 2\hbar\omega$?



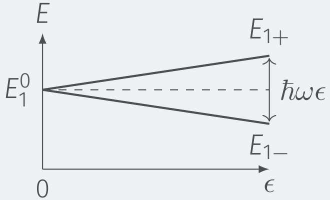


Example — 2D Perturbed Harmonic Oscillator

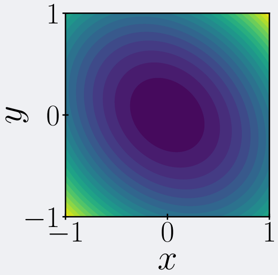
Using degenerate perturbation theory, we find the first order corrections

$$E_{1\pm}^{(1)} = \pm\frac{\hbar\omega\epsilon}{2}$$

The perturbation lifts the degeneracy of the first excited state:



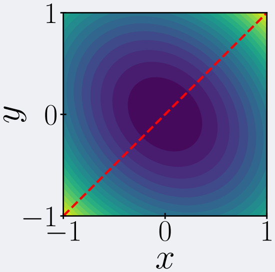
The degeneracy in this case was due to rotational symmetry. This symmetry is removed by the perturbation, as seen from the total potential:



Here $\epsilon = 0.5$.

Example — 2D Perturbed Harmonic Oscillator

We still have a symmetry — the interchange of x and y, a reflection about the red line below.



The "good" states correspond to oscillations either along the red or white line, which have different effective spring constants.