12.2 easier solutions?

If we had only chosen ψ_+ and ψ_- as our original wavefunctions then we would have had a much simpler equation to solve - its diagonal, so we could just read off the solutions

$$\begin{pmatrix} W_{++} & 0 \\ 0 & W_{--} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

i.e.

$$\begin{pmatrix} W_{++} - E^1 & 0 \\ 0 & W_{--} - E^1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$$

so this has solutions $(W_{++} - E^1)\alpha = 0$ i.e. $E^1_+ = W_{++} =< \psi_+|H'\psi_+ >$ and $(W_{--} - E^1)\alpha = 0$ i.e. $E^1_- = W_{++} =< \psi_-|H'\psi_- >$

if we feed each of these into the matrix then we get for $E^1 = W_{++}$

$$\begin{pmatrix} 0 & 0 \\ 0 & W_{--} - W_{++} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$$

so the first line is zero by construction, and the second line is $(W_{--} - W_{++})\beta = 0$ so $\beta = 0$ and the wavefunction is ψ_+

while for $E^1 = W_{--}$ we get $(W_{++} - W_{--})\alpha = 0$ so $\alpha = 0$ and the wavefunction is ψ_-

so these are the wavefunctions which diagonalise the perturbation. and our solutions are simply the equations we'd have picked if we hadn't bothered thinking at all about the levels being degenerate!!

12.3 link to non-degenerate perturbation theory

but how do we get there in advance ? how do we be clever, not just lucky! we know we want the off axis terms to be zero, so we are just solving

$$\begin{pmatrix} W_{aa} - E^1 & 0 \\ 0 & W_{bb} - E^1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

i.e. $< \psi_a^0 | H' \psi_b^0 >= 0$. The obvious way this is true is if ψ_b^0 is also an eigenfunction of H' as then $H'\psi_b^0 = b\psi_b^0$ and then $< \psi_a^0 | H' \psi_b^0 >= b < \psi_a^0 | \psi_b^0 >= 0$

what we do is find some Hermitian operator A which shares common eigenfunctions with H^0 i.e. $[A, H^0] = 0$. Thus ψ_a^0 and ψ_b^0 are also eigenfunctions of A - but where the eigenvalues are distinct unlike the case for H^0 where they are degenerate i.e $A\psi_a = \mu\psi_a$ and $A\psi_b = \nu\psi_b$ for $\mu \neq \nu$. If this operator also commutes with the perturbation i.e. $[A, H'] = 0$ then ψ_a and ψ_b are the states where the non-diagonal terms in the matrix $W_{ab} =< \psi_a^0 | H' \psi_b^0 >= 0$ and so we can use non-degenerate perturbation theory to work it out

Lets show this explicitally:

$$< \psi_a | [A, H'] \psi_b >= 0$$
$$< \psi_a | AH' \psi_b > - < \psi_a | H' A \psi_b >= 0$$
$$< A\psi_a | H' \psi_b > - < \psi_a | H' \nu \psi_b >= 0$$
$$\mu < \psi_a | H' \psi_b > - \nu < \psi_a | H' \psi_b >= 0$$
$$(\mu - \nu) W_{ab} = 0$$

12.4 higher order degeneracy

This generalises very easily for n-fold degeneracy. We form the matrix elements $W_{ij} = \int \psi_i^{0*} H' \psi_j^0 dx$ where i, j go from $1, 2...n$. then we get an nxn matrix, with n separate roots (some of which may be zero if the matrix is very sparse)

12.5 3D square well example

$V(x, y, z) = 0$ for $0 < x < a$ and $0 < y < a$ and $0 < z < a$, otherwise its ∞ this had wavefunctions

$$\psi^0_{n_x,n_y,n_x} = \left(\frac{2}{a}\right)^{3/2} \sin n_x \pi x/a \sin n_y \pi y/a \sin n_z \pi z/a$$

$$E^0_{nx,ny,nz} = \frac{\pi^2 \hbar^2}{2\mu a^2}(n_x^2 + n_y^2 + n_z^2)$$

the ground state in non-degenerate but the first excited state is tripally degenerate as we can have $\psi_{211}, \psi_{121}, \psi_{112}$ all with the same energy.

introduce the perturbation of V_0 for $0 < x < a/2$ and $0 < y < a/2$. - but this extends over all z.

now lets do the first excited state which is 3 fold degenerate let $\psi_1 = \psi_{211}$, $\psi_2 = \psi_{121}$ and $\psi_3 = \psi_{112}$ we can calculate each matrix element

$$W_{11} = \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} \sin^2 2\pi x/a dx \int_0^{a/2} \sin^2 \pi y/a dy \int_0^a \sin^2 \pi z/a dz$$

look up the integral

$$\int_0^{a/2} \sin^2 \pi x/a dx = [\frac{x}{2} - \frac{\sin(2\pi x/a)}{4\pi/a}]_0^{a/2} = \frac{a}{4}$$

so we get

$$= \left(\frac{2}{a}\right)^3 \int_0^{a/2} \sin^2 2\pi x/a dx \int_0^{a/2} \sin^2 \pi y/a dy \int_0^a \sin^2 \pi z/a dz = \frac{V_0}{4}$$

similarly $W_{22} = W_{33} = V_0/4$. but the off diagonal get a bit trickier

$$W_{12} = \Big(\frac{2}{a}\Big)^3 V_0 \int_0^{a/2} \sin 2\pi x/a \sin \pi x/a dx \int_0^{a/2} \sin 2\pi y/a \sin \pi y/a dy \int_0^a \sin^2 \pi z/a dz$$

but

$$\int_0^{a/2} \sin(2\pi x/a)\sin(\pi x/a)dx = [\frac{a\sin(\pi x/a}{2\pi} - \frac{a\sin(3\pi x/a}{6\pi}]_0^{a/2}$$

$$= \frac{a}{2\pi} + \frac{a}{6\pi} = \frac{2a}{3\pi}$$

so the full thing is

$$W_{12} = \Big(\frac{2}{a}\Big)^3 V_0 \frac{2a}{3\pi}\frac{2a}{3\pi}\frac{a}{4} = \frac{2^3 V_0 2^3}{2^2 3^2} = \frac{16}{9\pi^2} V_0 = \kappa V_0/4$$

where $\kappa = 16.4/(9\pi^2)$ as it just makes life easier

$$W_{13} = \Big(\frac{2}{a}\Big)^3 V_0 \int_0^{a/2} \sin 2\pi x/a \sin \pi x/a dx \int_0^{a/2} \sin^2 \pi y/a dy \int_0^a \sin 2\pi z/a \sin \pi z/a dz = 0$$

since $W_{ij} = W_{ji}^*$ then we now know $W_{31} = 0$ and $W_{21} = \kappa V_0/4$

$$W_{23} = \Big(\frac{2}{a}\Big)^3 V_0 \int_0^{a/2} \sin 2\pi x/a \sin \pi x/a dx \int_0^{a/2} \sin^2 \pi y/a dy \int_0^a \sin 2\pi z/a \sin \pi z/a dz = 0$$

so the full matrix is

$$\begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = E_2^1 \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

so

$$\frac{V_0}{4}\begin{pmatrix} 1 & \kappa & 0 \\ \kappa & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = E_2^1\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

$$\begin{pmatrix} 1 & \kappa & 0 \\ \kappa & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \frac{4E_2^1}{V_0}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

so let $w = 4E_2^1/V_0$ and subtract and get

$$\begin{pmatrix} 1-w & \kappa & 0 \\ \kappa & 1-w & 0 \\ 0 & 0 & 1-w \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

so the non-trivial solution (i.e. $\alpha, \beta, \gamma \neq 0$) is when the determinant of the matrix is zero