Non Degenerate Perturbation Theory
Second Order Correction to Energy

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1 Recall Basic Equations

In perturbation theory approach the Hamiltonian is split as

$$
\begin{aligned}
&(H_0 + \lambda H')(\psi_0 + \lambda\psi_1 + \lambda^2\psi_2 + \cdots) && (1)\\
&= (W_0 + \lambda W_1 + \lambda^2 W_2 + \cdots) && (2)\\
&\quad (\psi_0 + \lambda\psi_1 + \lambda^2\psi_2 + \cdots) && (3)
\end{aligned}
$$

Comparing powers of λ on both sides we get

$$
\begin{aligned}
H_0\psi_0 &= W_0\psi_0 && (4)\\
H_0\psi_1 + H'\psi_0 &= W_0\psi_1 + W_1\psi_0 && (5)\\
H_0\psi_2 + H'\psi_1 &= W_0\psi_2 + W_1\psi_1 + W_2\psi_0. && (6)
\end{aligned}
$$

2 Second Oder Solution

We begin with the equation

$$H_0\psi_2 + H\,'\psi_1 = W_0\psi_2 + W_1\psi^1 + W_2\psi_0. \tag{7}$$

For the n^{th} the unperturbed wave function $\psi_0(x)$ is $u_n(x)$, and W_0 is the corresponding energy E_n. Taking scalar product with u_n we get,

$$(u_n, H_0\psi_2) + (u_n, H\,'\psi_1) = (u_n, W_0\psi_2) + (u_n, W_1\psi_1) + (u_n, W_2 u_n). \tag{8}$$

$$(u_n, H_0\psi_2) + (u_n, H\,'\psi_1) = (u_n, W_0\psi_2) + (u_n, W_1\psi_1) + (u_n, W_2 u_n). \quad (9)$$

The first term on the l.h.s. cancels with the first term on the right hand side, because $W_0 = E_n$ and the hermiticity property of H_0 implies $(u_n, H_0\psi_2) = (H_0 u_n, \psi_2) = E_n(u_n, \psi_2)$. Thus we are left with

$$(u_n, H\,'\psi_1) = W_1(u_n, \psi_1) + (u_n, W_2 u_n). \quad (10)$$

The first term on the r.h.s. vanishes because ψ_1 is assumed to be orthogonal to u_n. We now substitute for ψ_1 from

$$\psi_1 = \sum_{\substack{k=1 \\ k\neq n}}^{\infty} \frac{| < k|H'|n >}{E_n - E_k} u_k \quad (11)$$

3 Final Answer

We get the desired answer for the second order correction to a non degenerate level as

$$W_2 = \sum_{\substack{k=1 \\ k\neq n}}^{\infty} \frac{< k|H'|n > |^2}{E_n - E_k}. \quad (12)$$

for the second order correction W_2 to the energy of level u_n.