substitute in eq (8).

$$\sum_m C^{(1)}_{nm} = \frac{-V_{mn}}{(E^{(0)}_m - E^{(0)}_n)}$$

Now remove the segma notation.

$$C^{(1)}_{nm} = \frac{-V_{mn}}{(E^{(0)}_m - E^{(0)}_n)}$$

As we have applied the condition $m \neq n$

So we have

$$C^{(1)}_{nn} = 0$$

This is Ist order correction to wave function in terms of cofficient $C^{(1)}_{nm}$.

LecB

Second Order Correction in Energy

Write the 2nd order equation.

part (b)

$$H^{(0)}\psi^{(2)}_n + V\psi^{(1)}_n = E^{(0)}_n \psi^{(2)}_n + E^{(1)}_n \psi^{(1)}_n + E^{(2)}_n \psi^{(0)}_n \quad \text{--- (1)}$$

Now re-arrange the equation.

$$(H^{(0)} - E^{(0)}_n)\psi^{(2)}_n = E^{(2)}_n \psi^{(0)}_n + E^{(1)}_n \psi^{(1)}_n - V\psi^{(1)}_n \quad \text{--- (2)}$$

Now xing with $\psi^{(0)*}_n$ at both sides and integrate w.r.t all coordinates.

$$\int \psi^{(0)*}_n (H^{(0)} - E^{(0)}_n)\psi^{(2)}_n \, d\tau = \int \psi^{(0)*}_n E^{(2)}_n \psi^{(0)}_n \, d\tau +$$

$$\int \psi^{(0)*}_n E^{(2)}_n \psi^{(1)}_n + \int \psi^{(0)*}_n V \psi^{(1)}_n \, d\tau \quad \text{--- (3)}$$

Now take the Ist term of R.H.S

and solve it - "take out energy outside of integral.

$$\int \psi_n^{(0)*} E_n^{(2)} \psi_n^{(0)} d\tau = E_n^{(2)} \int \psi_n^{(0)*} \psi_n^{(0)} d\tau$$

the integral becomes equal to one due to normalization condition:

$$\therefore \int \psi_n^{(0)*} \psi_n^{(0)} d\tau = 1$$

So $$\int \psi_n^{(0)*} E_n^{(2)} \psi_n^{(0)} d\tau = E_n^{(2)} \int \psi_n^{(0)*} \psi_n^{(0)} d\tau$$

$$= E_n^{(2)}$$

Now substitute this value in eq (3)

$$\int \psi_n^{(0)*} (H^{(0)} - E_n^{(0)}) \psi_n^{(2)} d\tau = E_n^{(2)} + \int \psi_n^{(0)*} E_n^{(2)} \psi_n^{(1)} d\tau + \int \psi_n^{(0)*} V \psi_n^{(1)} d\tau \quad \text{— (3a)}$$

substitute $\psi_n^{(1)} = \sum_m C_{nm}^{(1)} \psi_m^{(0)}$ in eq (3a).

$$\int \psi_n^{(0)*} (H^{(0)} - E_n^{(0)}) \psi_n^{(2)} d\tau = E_n^{(2)} + \int \psi_n^{(0)*} E_n^{(1)} \sum_m C_{nm}^{(1)} \psi_m^{(0)} d\tau - \int \psi_n^{(0)*} V \sum_m C_{nm}^{(1)} \psi_m^{(0)} d\tau \quad \text{— (3b)}$$

Now take the 2nd term of eq (3b) and take energy term out

$$\int \psi_n^{(0)*} E_n^{(1)} \sum_m C_{nm}^{(1)} \psi_m^{(0)} d\tau = E_n^{(1)} \int \psi_n^{(0)*} \sum_m C_{nm}^{(1)} \psi_m^{(0)} d\tau$$

$$= E_n^{(1)} \sum_m C_{nm}^{(1)} \int \psi_n^{(0)*} \psi_m^{(0)} d\tau$$

~~take~~ replace integral by Chronomical delta.

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$$= E_n^{(1)} \sum_m C_{nm}^{(1)} \delta_{nm}$$

Now apply the condition of orthogonality and take $n \neq m$. So we have $\delta_{nm} = 0$

$$= E_n^{(1)} \sum_m C_{nm}^{(1)} (0)$$

$$= 0$$

So the whole term is now zero. Now substitute this in eq (3b).

$$\int \psi_n^{(0)*} (H^{(0)} - E_n^{(0)}) \psi_n^{(2)} d\tau = E_n^{(2)} + \int \psi_n^{(0)*} E_n^{(1)} \sum_{nm} C_{nm}^{(1)} \psi_m^{(0)} d\tau$$

$$- \int \psi_n^{(0)*} V \sum_m C_{nm}^{(1)} \psi_m^{(0)} d\tau$$

$$= E_n^{(2)} + \int 0 - \int \psi_n^{(0)*} V \sum_m C_{nm}^{(1)} \psi_m^{(0)} d\tau \quad \text{—(3c)}$$

Now take the last term of (3c) and substitute potential in the form of symbol.

$$\int \psi_n^{(0)*} V \sum_m C_{nm}^{(1)} \psi_m^{(0)} d\tau = \sum_m C_{nm}^{(1)} \int \psi_m^{(0)*} V \psi_m^{(0)} d\tau$$

$$= \sum_m C_{nm}^{(1)} V_{nm}$$

Now substitute in eq (3c)

$$\int \psi_n^{(0)*} (H^{(0)} - E_n^{(0)}) \psi_n^{(2)} d\tau = E_n^{(2)} - \sum_m C_{nm}^{(1)} V_{nm} \quad \text{—(4)}$$

Now to solve the L.H.S of the equation (4)

$$\int \psi_n^{(0)*} (H^{(0)} - E_n^{(0)}) \psi_n^{(2)} d\tau$$

As $H^{(0)}$ operator can not operate on $\psi_n^{(2)}$ it can only operat on $\psi_n^{(0)*}$, So we take only the 1st term- because $H^{(0)}$ is Hermition operator so we can change the order-

$$\psi_n^{(0)*} H^{(0)} = H^{(0)} \psi_n^{(0)*} = E_n^{(0)*} \psi_n^{(0)*}$$

so

$$E_n^{(0)*} \psi_n^{(0)*} = E_n^{(0)} \psi_n^{(0)*} \quad \because E_n^{(0)*} = E_n^{(0)}$$

Now substitute this value in the integral.

$$= \int \psi_n^{(0)*} (E_n^{(0)} - E_n^{(0)}) \psi_n^{(2)} d\tau$$

$$= 0$$

So the L.H.S of eq 4 also forms zero-

$$0 = E_n^{(2)} - \sum_m C_{nm}^{(1)} V_{nm}$$

$$E_n^{(2)} = \sum_m C_{nm}^{(1)} V_{nm}$$

by putting value of calculated $C_{nm}^{(1)} = \dfrac{-V_{mn}}{(E_m^{(0)} - E_n^{(0)})}$

substitute in eq.

$$E_n^{(2)} = \sum_m \frac{-V_{mn}}{(E_m^{(0)} - E_n^{(0)})} V_{nm} \quad \text{—} \; 5$$

we take V_{nm} as given below.

$$V_{nm} = \int \psi_n^{(0)*} V \psi_m^{(0)} d\tau$$