Lecture 19. Approximate Methods

Time-Independent Perturbation Theory

* Time-independent perturbation theory

  $\Rightarrow$ Zeroth-, first- & second-order corrections

  $\Rightarrow$ Implications & limitations

Time-Independent Perturbation Theory

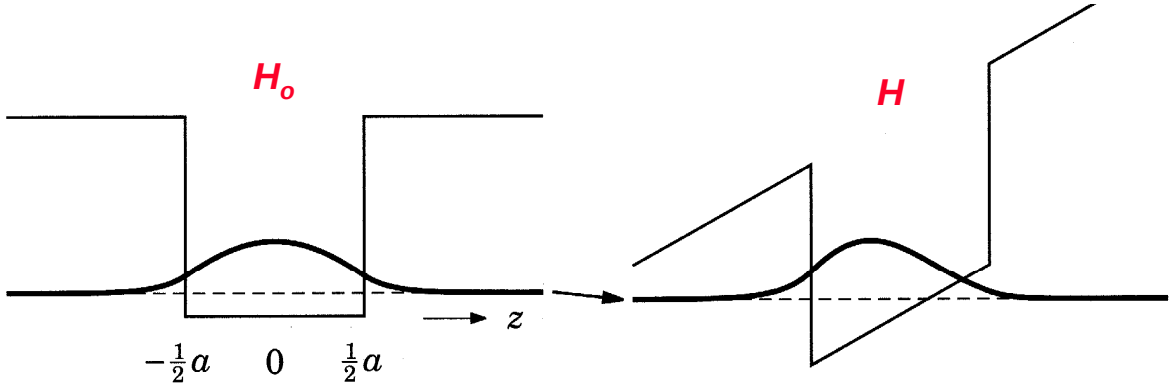
• **Previously we introduced the concept of PERTURBATION THEORY which is used to obtain the eigenvalues and eigenfunctions for a system whose Hamiltonian may be written as**

$$H = H_o + V \qquad (18.16)$$

*** Here *H* is the Hamiltonian of the PERTURBED system while H_o is that for a system that may be solved EXACTLY**

⇒ The additional term *V* on the RHS of Eq. 18.16 represents the PERTURBATION to the exact system and should be SMALL

⇒ In the example we considered previously the exact system was a SQUARE well while the perturbed system was a TILTED potential well



Time-Independent Perturbation Theory

• **The starting point in our development of perturbation theory is the eigenvalue equation for the EXACT system**

$$H_o \varphi_n = \varepsilon_n \varphi_n \qquad (19.1)$$

*** While the solutions to this problem are known we wish to find the eigenvalues (E_n) and eigenfunctions (ψ_n) of the perturbed system**

$$H\psi_n = E_n \psi_n \qquad (19.2)$$

*** The basic idea of perturbation theory is to EXPAND the energy and wavefunctions of the perturbed system in powers of the small potential *V***

$\Rightarrow$ For this purpose we rewrite Eq. 19.16 as

$$H = H_o + \lambda V \qquad (19.3)$$

LATER ON WE WILL SET $\lambda = 1$

Time-Independent Perturbation Theory

• **Next we write the eigenvalues and eigenfunctions of the PERTURBED system as**

n^{th} EIGENVALUE OF H

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots \qquad (19.4)$$

n^{th} EIGENFUNCTION OF H

$$\psi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \ldots \qquad (19.5)$$

ZEROTH ORDER TERM

FIRST ORDER CORRECTION

SECOND ORDER CORRECTION

*** The idea is to now calculate the MINIMUM number of terms in this expansion that are necessary to achieve satisfactory approximations for E_n and ψ_n**

Time-Independent Perturbation Theory

- **Substituting Eqs. 19.4 & 19.5 into Eq. 19.3 yields**

$$(H_o + \lambda V)(\psi_n^{(0)} + \lambda\psi_n^{(1)} + \ldots) = (E_n^{(0)} + \lambda E_n^{(1)} + \ldots)(\psi_n^{(0)} + \lambda\psi_n^{(1)} + \ldots) \qquad (19.6)$$

*** In order for this equation to hold the coefficients of common powers on both sides of the equation MUST be EQUAL to each other**

$\Rightarrow$ The reason for introducing the constant λ now becomes clear since it helps us to identify the common powers in Eq. 19.6

*** For the first three powers of λ this approach leads to the following relations**

$$H_o\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)} \qquad (19.7)$$

$$V\psi_n^{(0)} + H_o\psi_n^{(1)} = E_n^{(1)}\psi_n^{(0)} + E_n^{(0)}\psi_n^{(1)} \qquad (19.8)$$

$$V\psi_n^{(1)} + H_o\psi_n^{(2)} = E_n^{(2)}\psi_n^{(0)} + E_n^{(1)}\psi_n^{(1)} + E_n^{(0)}\psi_n^{(2)} \qquad (19.9)$$

Time-Independent Perturbation Theory

• **Eq. 19.7 shows that to ZEROTH order the eigenvalues and eigenfunctions of the perturbed system are just those of the UNPERTURBED system**

$$H_o\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)} \qquad (19.7)$$

$$\psi_n = \varphi_n \qquad (19.10) \qquad\qquad E_n = \varepsilon_n \qquad (19.11)$$

*** To obtain the NEXT order approximation we substitute Eqs. 19.10 & 19.11 into Eq. 19.8**

$$(H_o - \varepsilon_n)\psi_n^{(1)} = (E_n^{(1)} - V)\varphi_n \qquad (19.12)$$

*** Next we write the 1st-order correction to the *n*th eigenfunction as the LINEAR SUM**

$$\psi_n^{(1)} = \sum_k a_{nk}^{(1)}\varphi_k \qquad (19.13)$$

Time-Independent Perturbation Theory

- **With Eq. 19.13 we may rewrite Eq 19.12 as**

$$\sum_k (H_o - \varepsilon_n) a_{nk}^{(1)} \varphi_k = (E_n^{(1)} - V)\varphi_n \qquad (19.14)$$

*** Eq. 19.1 allows us to rewrite this last equation in the following form however**

$$\sum_k a_{nk}^{(1)} (\varepsilon_k - \varepsilon_n)\varphi_k = (E_n^{(1)} - V)\varphi_n \qquad (19.15)$$

*** The next step is to use the ORTHONORMALITY of the eigenfunctions φ_n and multiply Eq. 19.15 by φ_n^* then integrate**

$\Rightarrow$ The LHS of this equation then VANISHES to yield the important result

$$E_n^{(1)} = \int \varphi_n^* V \varphi_n \equiv V_{nn} \qquad (19.16)$$

THE FIRST-ORDER CORRECTION TO THE ENERGY IS JUST THE EXPECTATION VALUE OF THE PERTURBATION … MAKES SENSE!

Time-Independent Perturbation Theory

• **To determine the first-order correction to the wavefunction we multiply Eq. 19.15 by φ_m^* ($m \neq n$) then integrate to obtain**

$$a_{nm}^{(1)}(\varepsilon_m - \varepsilon_n) = -\int \varphi_m^* V \varphi_n \equiv -V_{mn} \qquad (19.17)$$

*** In this way we can write the first-order correction to the wavefunction as**

$$\psi_n^{(1)} = a_{nn}^{(1)}\varphi_n + \sum_{k,k\neq n} \frac{V_{nk}}{\varepsilon_n - \varepsilon_k}\varphi_k \qquad (19.18)$$

⇒ **Note here that the coefficient $a_{nn}^{(1)}$ only affects the normalization and so can be taken as ZERO**

*** Next we can proceed to obtain the SECOND-ORDER corrections to the eigenvalues and eigenfunctions by introducing our results into Eq. 19.9**

$$V\psi_n^{(1)} + H_o\psi_n^{(2)} = E_n^{(2)}\psi_n^{(0)} + E_n^{(1)}\psi_n^{(1)} + E_n^{(0)}\psi_n^{(2)} \qquad (19.9)$$

Time-Independent Perturbation Theory

• **Using the results we have developed thus far for zeroth- and first-order terms Eq. 19.9 may be rewritten as**

$$(H_o - \varepsilon_n)\psi_n^{(2)} = (V_{nn} - V)\sum_k a_{nk}^{(1)}\varphi_k + E_n^{(2)}\varphi_n \qquad (19.19)$$

*** Similar to our discussion of the first-order corrections we EXPAND the second-order eigenfunction correction as**

$$\psi_n^{(2)} = \sum_k a_{nk}^{(2)}\varphi_k \qquad (19.20)$$

*** Introducing this form into Eq. 19.19 then gives**

$$\sum_k a_{nk}^{(2)}(\varepsilon_k - \varepsilon_n)\varphi_k = (V_{nn} - V)\sum_k a_{nk}^{(1)}\varphi_k + E_n^{(2)}\varphi_n \qquad (19.21)$$

Time-Independent Perturbation Theory

• **To obtain the second-order energy correction we next multiply Eq. 19.21 by φ_n^* and then integrate which yields (after some rearrangement)**

$$E_n^{(2)} = \sum_{k,k\neq n} a_{nk}^{(1)} V_{nk} = \sum_{k,k\neq n} \frac{V_{kn}V_{nk}}{\varepsilon_n - \varepsilon_k} = \sum_{k,k\neq n} \frac{V_{nk}^* V_{nk}}{\varepsilon_n - \varepsilon_k} \qquad (19.22)$$

*** In the last step we have exploited the fact that since *V* is HERMITIAN $V_{nk}^* = V_{kn}$**

*** We can now SUMMARIZE our results for the expansion of the energy to second order and the expansion of the wavefunction to first order**

$$E_n = \varepsilon_n + V_{nn} + \sum_{k,k\neq n} \frac{V_{nk}^* V_{nk}}{\varepsilon_n - \varepsilon_k} + \ldots \qquad (19.23)$$

$$\psi_n = \varphi_n + \sum_{k,k\neq n} \frac{V_{nk}^*}{\varepsilon_n - \varepsilon_k} \varphi_k + \ldots \qquad (19.24)$$

NOTE HOW THE SOLUTIONS OF THE PERTURBED SYSTEM ARE MIXTURES OF THOSE OF THE EXACT SYSTEM!

Time-Independent Perturbation Theory

• **Before discussing the applications of perturbation theory in following classes we briefly consider some of the IMPLICATIONS of our analysis**

$$E_n = \varepsilon_n + V_{nn} + \sum_{k,k\neq n} \frac{V_{nk}^* V_{nk}}{\varepsilon_n - \varepsilon_k} + \ldots \qquad (19.23)$$

$$\psi_n = \varphi_n + \sum_{k,k\neq n} \frac{V_{nk}^*}{\varepsilon_n - \varepsilon_k} \varphi_k + \ldots \qquad (19.24)$$

*** Previously we mentioned that perturbation *V* to the exact Hamiltonian should be a SMALL quantity**

⇒ We now see that this requires the matrix elements V_{nk} to be much smaller than the energy denominator ($V_{nk} << \varepsilon_n - \varepsilon_k$)

⇒ In other words the COUPLING between the states induced by the perturbation should be much SMALLER than the separation between the original energy levels

Time-Independent Perturbation Theory

• **A problem clearly arises with the forgoing discussion if the energy levels of the unperturbed system are DEGENERATE since the denominator in Eq. 19.23 then VANISHES**

$$E_n = \varepsilon_n + V_{nn} + \sum_{k,k\neq n} \frac{V_{nk}^* V_{nk}}{\varepsilon_n - \varepsilon_k} + \ldots \qquad (19.23)$$

*** The approach we have taken here is referred to as NON-DEGENERATE perturbation theory and a different approach will be developed to deal with degenerate systems**

*** The first-order energy correction V_{nn} in Eq. 19.23 may be of EITHER sign but often VANISHES due to the symmetry of the wavefunctions that appear in its integral**

$$E_n^{(1)} = \int \varphi_n^* V \varphi_n \equiv V_{nn} \qquad (19.16)$$

⇒ **The second term in Eq. 19.23 then determines the energy and in the case of the GROUND STATE level this correction is always NEGATIVE since $\varepsilon_n < \varepsilon_k$**

⇒ **This is easy to understand since Eq. 19.24 shows that the perturbation MIXES other states into the ground-state wavefunction and the system can use this freedom to LOWER its energy**

Homework

P19.1 Derive Eqs. 19.23 and 19.24