Title: Quantum Theory - Lecture 220906

Speakers: Dan Wohns

Collection: Quantum Theory (2022-2023)

Date: September 06, 2022 - 10:45 AM

URL: https://pirsa.org/22090032

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Welcome to the Quantum Theory course

6-20 September 2022

Instructor's introduction

Name: Bindiya Arora

Affiliation: PSI fellow (currently on sabbatical from Guru Nanak Dev University, India)

Educational Background: PhD. in Atomic Physics, University of Delaware, USA.

Research interests: High precision calculation of atomic properties and their applications in quantum computation and atomic clocks. *Machine learning for atomic calculations.*

Other activities: Teacher-in-charge of a science club, SciRox. Involved in a number of science outreach activities.

Hobbies: Playing badminton, Indian Bollywood dance, discussions on random topics.

Important information

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Important information

How to reach me: Dropping an email to fix an appointment is the best way (barora@perimeterinstitute.ca).

Note: Indian Standard Time is 9 and a half hours ahead of Waterloo time.

Office hours: 30 mins after lectures/tutorials

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Office hours: 30 mins after lectures/tutorials

Regularly check PSI portal for quizzes/feedback.

Tutorials: One device per group.

Our learning goals:

→ Kinematics: Description of the wave functions and observable (energy). Might have covered in undergrad classes: introducing perturbation to the system.

→ Statistical mixtures of quantum systems: How quantum systems distribute/ organize themselves in various allowed energy eigen states?

→ Dynamics: Description of the time evolution of states/observable or both, the Schr'odinger, the Heisenberg and interaction picture)

→ Open quantum systems: Density matrix, What happens when systems interact with environment or a bath (brief)?

Quantum Theory (6 September, 2022)

Our learning goals:

→ Brief overview of quantum mechanics.

→ Introduction to approximate methods of solving the Schrodinger equation.

→ Validity of perturbative approach to solve Schrodinger equation.

→ First & second order correction in energy.

→ First order correction in wavefunction.

→ Analyzing the results.

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$$i\hbar \frac{\partial \psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(r,t)}{\partial t} + V$$

$$\psi(r,t) = \psi(r)\, f(t)$$

$\psi(r)$ → Spatial

$f(t)$ → time dependent

BA

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Spatial

Time independent

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

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$\underline{\psi_n(r)}$ → stationary states

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$ → eigenvalue equation

$|\psi_n\rangle$ → solutions

BA

$|\psi_n\rangle \rightarrow$ solutions

eigen ket / basis ket.

$$\underbrace{|\psi\rangle}_{\text{general solution}} = \sum_n c_n |\psi_n\rangle$$

eigen states

general solution

State ket

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State ket

Properties of eigenket/ basis ket

1) orthogonal & normalized

$$\underbrace{\langle \psi_n | \psi_m \rangle}_{\text{inner product}} = \delta_{mn}$$

BA

1) orthogonal & normalized

$$\underbrace{\langle \psi_n | \psi_m \rangle}_{\text{inner product}} = \delta_{mn}$$

component of ψ_m along ψ_n

2) complete set $\rightarrow$

$|\psi\rangle =$

Inner product

component of ψ_m along ψ_n

2) complete set $\rightarrow$

$$|\psi\rangle = \sum_n c_n |\psi_n\rangle$$

$$|c_n|^2 = |\langle \psi_n | \psi \rangle|^2 \rightarrow \text{probability of finding my system in } |\psi_n\rangle$$

exactly by solving SE using standard technique

→ integrating / power series

→ ladder operator

→

Solving S.E

exactly by solving S.E using standard technique

→ integrating / power series ✓

→ ladder operator

→ Numerical technique

→ ladder operator

→ Numerical technique

$|\psi\rangle \to$ State of our system

Observables $\rightarrow$ ope...

$$Q = \begin{bmatrix} \\ \\ \\ \end{bmatrix}$$

square matrix

$$\begin{bmatrix} Q_{11} & Q_{12} & \cdots \\ & Q_{22} & \\ & & \ddots \end{bmatrix}$$

$|\psi\rangle \rightarrow$ State of our system $\begin{bmatrix} \vdots \\ c_2 \\ \vdots \end{bmatrix}$ column matrix

Observables $\rightarrow$ operators (Matrix form)

$$Q = \begin{bmatrix} Q_{11} & Q_{12} & \cdots \\ & Q_{22} & \\ & & \ddots \end{bmatrix}$$

square matrix

2-level system $\left.\begin{array}{l} E_1 \;—\; |1\rangle \\ E_0 \;—\; |0\rangle \end{array}\right\}$ $H = \begin{bmatrix} E_0 & 0 \\ 0 & E_1 \end{bmatrix}$

$$H = \begin{bmatrix} E_0 & 0 \\ 0 & E_1 \end{bmatrix}$$

$$H|\psi_n\rangle = \underline{E_n}\,|\psi_n\rangle$$

$$|H - \lambda I| = 0$$

$\lambda \rightarrow E_n$

$|\psi_n\rangle$

Characteristic equati.

$\boxed{|\psi_n\rangle}$ ✓

Characteristic equation

I unique sol.^{n} (non-degenerate) ✓

II m duplicate roots (m-fold degeneracy) ✓

$$|\psi_n^1\rangle \quad |\psi_n^2\rangle \quad - \;\; -- \quad |\psi_n^m\rangle \longrightarrow E_n$$

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$$H = \begin{bmatrix} E_0 & 0 \\ 0 & E_1 \end{bmatrix}$$

$$H|\psi_n\rangle = \underline{E}_n |\psi_n\rangle$$

$$\boxed{|H - \lambda I| = 0}$$

$\lambda \to E_n$ ✓

$\boxed{|\psi_n\rangle}$ ✓

Characteristic equation

$\underline{I}$ unique sol.^{n} (non-degenerate) ✓

BA

H Bohr $-\frac{1}{n^2}$

$n = 2$ $\rightarrow$ $|\psi_{2s}\rangle$, $|\psi_{2p}\rangle$

2-fold degeneracy.

n^2

$|\psi_{2p}\rangle$

2-fold degeneracy.

observable $\underline{Q} \rightarrow$ Hermitian (real / orthogonal)

✓ $\langle \underline{Q}\alpha | \beta \rangle = \langle \alpha | \underline{Q}\beta \rangle$

expectation value $\underline{Q}$ $\underbrace{\langle \psi | Q | \psi \rangle}_{\int}$

General formalism of the problem:

$$H = \underbrace{H^0}_{\text{exactly solvable}} + V \longrightarrow \text{tim.}$$

Now we slightly perturb the potential. For example, we raise the bottom of the infinite square well or put a little bump in between.

General formalism of the problem:

$$H = \underbrace{H_0}_{\text{exactly solvable}} + \underbrace{V}_{} \rightarrow \text{time indep. pot / perturbation}$$

unpertubed

$$\checkmark\ H_0 |\psi_n^0\rangle = E_n^0 |\psi_n^0\rangle$$

Now we slightly perturb the potential. For example, we raise the bottom of the infinite square well or put a little bump in between.

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General formalism of the problem:

$$H = \underbrace{H_0}_{\text{exactly solvable}} + \underbrace{V} \rightarrow \text{time indep. pot / perturbation}$$

unpertubed

✓ $H_0 |\psi_n^0\rangle = E_n^0 |\psi_n^0\rangle \longrightarrow$ known

$H|\psi_n\rangle = E_n |\psi_n\rangle \rightarrow$ Find out

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

Now we slightly perturb the potential. For example, we raise the bottom of the infinite square well or put a little bump in between.

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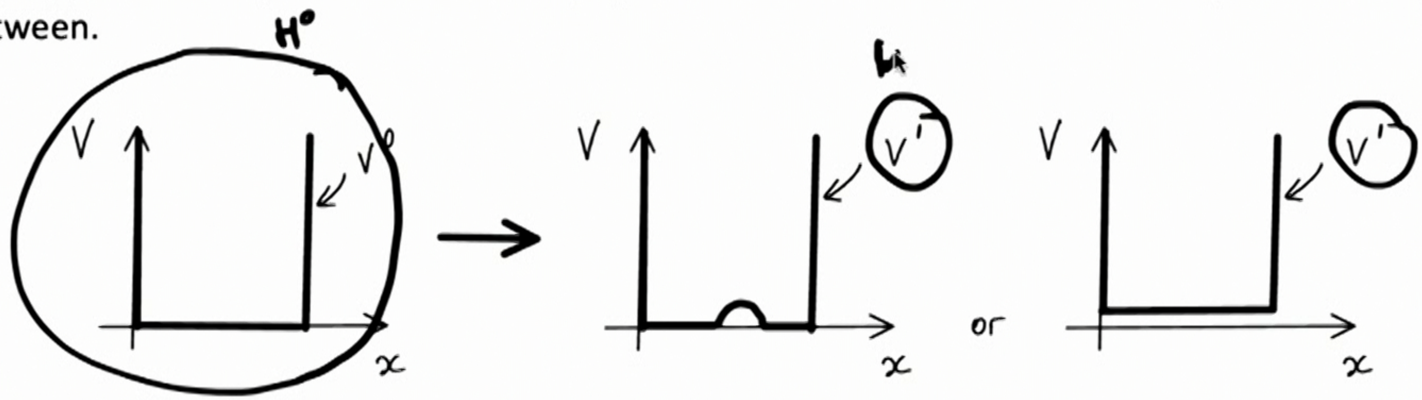
$$(H_0+V)|\psi_n\rangle = E_n|\psi_n\rangle$$

Now we slightly perturb the potential. For example, we raise the bottom of the infinite square well or put a little bump in between.



The problem is to find eigenvalues and eigenfunctions of the perturbed potential, i.e. to solve approximately the following equation:

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

λ → parameter ~~to~~ to measure the order of the perturbation

$\lambda \to 0$ to $1 \longrightarrow$ full strength.

0 → no perturbation

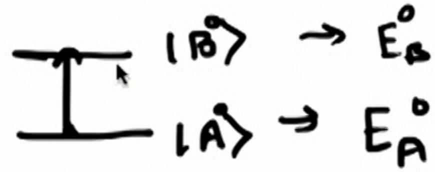
Using the known solutions of the unperturbed problem

Let us first consider a two-state problem with unperturbed states $|A^0\rangle$ and $|B^0\rangle$ and unperturbed energy eigenvalues $E_A^{\{0\}}$ and $E_B^{\{0\}}$.The unperturbed H of the system can be represented as

Now consider a potential V such that it causes transitions between states $|A^0\rangle$ and $|B^0\rangle$

Total Hamiltonian of the problem will be

Introduced λ



✓ Let us first consider a two-state problem with unperturbed states $|A^0\rangle$ and $|B^0\rangle$ and unperturbed energy eigenvalues $E_A^{\{0\}}$ and $E_B^{\{0\}}$.The unperturbed H of the system can be represented as

$$H^0 = \begin{bmatrix} E_A^0 & 0 \\ 0 & E_B^0 \end{bmatrix}$$

Now consider a potential V such that it causes transitions between states $|A^0\rangle$ and $|B^0\rangle$

Total Hamiltonian of the problem will be

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Total Hamiltonian of the problem will be

$$H^0 + \lambda V = \begin{bmatrix} E_0^A & \lambda V_{AB} \\ \lambda V_{BA} & E_B^0 \end{bmatrix} = H$$

This representation of Hamiltonian is given in density matrix form which will be introduced in coming lectures. For now you want to convince that the form of Hamiltonian we wrote is correct (try operating H on $|A^0\rangle$ and $|B^0\rangle$ you will see more familiar form).

$$(H^0 + \lambda V)|\psi_n\rangle = E_n|\psi_n\rangle$$

H may be represented by a square matrix (assuming that $V_{\{AB\}} = V_{\{BA\}}$)

$$\begin{bmatrix} E_A^0 & \lambda V_{AB} \\ \lambda V_{BA} & E_B^0 \end{bmatrix} \begin{bmatrix} \cdot \\ \end{bmatrix}$$

Our equation (1) reduced to solving the following eigen value problem

BA

$$\begin{bmatrix} \cdots & \cdots \\ \lambda V_{BA} & E_B^0 \end{bmatrix} \begin{bmatrix} \cdots \\ |B\rangle \end{bmatrix} = E \begin{bmatrix} \cdots \\ |B\rangle \end{bmatrix}$$

Our equation (1) reduced to solving the following eigen value problem

$$|H - \lambda I| = 0$$

$$\left\{ \begin{matrix} E_A \\ E_B \end{matrix} \right\}$$

Let us suppose

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BA

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$$\begin{Bmatrix} E_A \\ E_B \end{Bmatrix} = \frac{E_A^{(0)} + E_B^{(0)}}{2} \pm \sqrt{\frac{\left(E_A^{(0)} - E_B^{(0)}\right)^2}{4} + \lambda^2 |V_{AB}|^2}$$

$$\lambda |V_{AB}| \ll \left(E_A^{(0)} - E_B^{(0)}\right)$$

Let us suppose $= E_A^{(0)}$

BA

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$$\left\{\begin{matrix} E_A \\ E_B \end{matrix}\right\} = \frac{E_A^{(0)} + E_B^{(0)}}{2} \pm \sqrt{\frac{\left(E_A^{(0)} - E_B^{(0)}\right)^2}{4} + \lambda^2 |V_{AB}|^2}$$

$$\lambda |V_{AB}| \ll \left(E_A^{(0)} - E_B^{(0)}\right) \checkmark$$

Let us suppose

$$= \frac{E_A^{(0)} + E_B^{(0)}}{2} \pm \left(\frac{E_A^{(0)} - E_B^{(0)}}{2}\right) \sqrt{1 + \frac{4\lambda^2 |V_{AB}|^2}{\left(E_A^{(0)} - E_B^{(0)}\right)^2}}$$

BA

$$\lambda |V_{AB}| \ll \left(E_A^{(0)} - E_B^{(0)}\right) \checkmark$$

Let us suppose

$$= \frac{E_A^{(0)} + E_B^{(0)}}{2} \pm \left(\frac{E_A^{(0)} - E_B^{(0)}}{2}\right) \underbrace{\sqrt{1 + \frac{4\lambda^2 |V_{AB}|^2}{\left(E_A^{(0)} - E_B^{(0)}\right)^2}}}$$

$$\lambda |V_{AB}| \ll \left(E_A^{(0)} - E_B^{(0)}\right) \quad \checkmark$$

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$$\begin{Bmatrix} E_A \\ E_B \end{Bmatrix} = \frac{E_A^{(0)} + E_B^{(0)}}{2} \pm \left(\quad \right)\left[1 + \frac{2\lambda^2 |V_{BA}|^2}{\left(E_A^{(0)} - E_B^{(0)}\right)^2} + \cdots\right]$$

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$$\left.\begin{matrix} E_B \end{matrix}\right\} \qquad 2$$

validity of P.T. $\leftarrow$ $\boxed{\lambda |V_{AB}| \ll \left(E_A^{(0)} - E_B^{(0)}\right)}$ ✓

Let us suppose

$$= \frac{E_A^{(0)} + E_B^{(0)}}{2} \pm \left(\frac{E_A^{(0)} - E_B^{(0)}}{2}\right)\sqrt{1 + \frac{4\lambda^2 |V_{AB}|^2}{\left(E_A^{(0)} - E_B^{(0)}\right)^2}}$$

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— B

— A

$$\checkmark \; E_A = E_A^{(0)} + \frac{\lambda^2 |V_{AB}|^2}{\left(E_A^{(0)} - E_B^{(0)}\right)} \checkmark + \cdots \quad —$$

$$\checkmark \; E_B = E_B^{(0)} + \frac{\lambda^2 |V_{AB}|^2}{\left(E_B^{(0)} - E_A^{(0)}\right)} \checkmark + \cdots \quad —$$

The starred equations look correct because it is the presence of λ which assures the fact that when perturbation V is switched off then $E_A \to E_A^0$. In the absence of λ even if V was zero the correct limit to E would not have been found.

These expressions that we have just derived for a two level system will be formally derived for a general case.

These expressions that we have just derived for a two level system will be formally derived for a general case.

The basic strategy for development of perturbation theory is to expand the perturbed wavefunctions and energies in powers of λ. Before we formally develop the perturbation expansion lets see if this expansion of wavefunctions and energies in powers of λ is correct or not.

We aim to solve eq.(1). Let us define an energy shift Δ as the difference between the perturbed eigenvalue E_n and unperturbed value E_n^0.

The basic Schrodinger equation to be solved (approximately) is

One may be tempted to invert the operator $E_n^0 - H^0$. However, the inverse operator $\frac{1}{E_n^0 - H^0}$ will not be defined properly powers of λ. Before we formally develop the perturbation expansion lets see if this expansion of wavefunctions and energies in powers of λ is correct or not.

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The basic Schrodinger equation to be solved (approximately) is

One may be tempted to invert the operator $E_n^0 - H^0$. However, the inverse operator $\frac{1}{E_n^0 - H^0}$ will not be defined properly acts on $|\psi^0\rangle$. But inverse operator $\frac{1}{E_n^0 - H^0}$ is well defined if it acts on a complimentary projector operator of following kin

Tuesday, 6 September 2022 9:11 PM

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

$$\Delta_n = \underline{E_n} - \underline{E_n^0} \Rightarrow E_n = \Delta_n + E_n^0$$

$$\Rightarrow \boxed{(E_n^0 - H_0)|\psi_n\rangle = (\lambda V - \Delta_n)|n\rangle}$$

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$$\Delta_n = \underline{E_n} - \underline{E_n} \Rightarrow \ldots$$

$$\Rightarrow \boxed{(E_n^0 - H_0)|\psi_n\rangle = (\lambda V - \Delta_n)|n\rangle}$$

algebraic $\rightarrow a\,x = y \Rightarrow x = \dfrac{y}{a}$

$$A X = Y \Rightarrow X =$$

$$\Delta_n = \underline{E_n} - \underline{E_n} \Rightarrow$$

$$\Rightarrow \boxed{\left(E_n^{\circ} - H_0\right)|\psi_n\rangle = \left(\lambda V - \Delta_n\right)|n\rangle} \checkmark$$

algebraic $\rightarrow a \underset{\sim}{x} = y \Rightarrow x = \dfrac{y}{a}$

$$A X = Y \Rightarrow X = \underset{\sim}{A^{-1}} Y$$

a

$$AX = Y \Rightarrow X = \underbrace{A^{-1}}\,Y$$

$$|\psi_n\rangle = \underbrace{\frac{1}{E_n^0 - H_0}}\,\underbrace{(\lambda V - \Delta_n)|\psi_n\rangle}_{\Downarrow\; \underbrace{|\psi_n'\rangle}}$$

$$\frac{1}{E_n^0 - H_0}|\psi_{n0}\rangle = \frac{1}{E_n^0 - E_n^0}|\psi_{n0}\rangle$$

$$|\psi_n\rangle = \underbrace{\frac{1}{E_n^0 - H_0}}\ \underbrace{(\lambda V - \Delta_n)|\psi_n\rangle}_{\Downarrow\ \underbrace{|\psi_n'\rangle}}$$

$$\frac{1}{E_n^0 - H_0}|\psi_{n0}\rangle = \frac{1}{E_n^0 - E_n^0}|\psi_{n0}\rangle$$

if $(\lambda V - \Delta_n)|\psi_n\rangle \Rightarrow$ component along .

$$= \frac{1}{E_n^0 - E_n^0} |\psi_{n_0}\rangle$$

if $\underbrace{(\lambda V - \Delta_n)|\psi_n\rangle}$ $\Rightarrow$ component along $|\psi_{n_0}\rangle$

inner product $\langle \psi_{n_0} | \lambda V - \Delta_n | \psi_n \rangle = 0$

$E_n^0 - 1$

if $(\lambda V - \Delta_n)|\psi_n\rangle \Rightarrow$ $\overset{\circ}{\text{component}}$ along $|\psi_{n_0}\rangle$

$E_n^0 - E_n^0$

inner product $\langle \psi_{n_0} | \lambda V - \Delta_n | \psi_n \rangle = 0$

$\Rightarrow \langle \psi_{n_0} | E_n^0 - H_0 | \psi_n \rangle$

$(E_n^0 - H_0)|\psi_n\rangle$
$= (\lambda V - \Delta_n)|\psi_n\rangle$

$\langle \psi_{n_0} | E_n^0 | \psi_n \rangle - \langle \psi_{n_0} | H_0 | \psi_n \rangle = 0$

$$|\psi_n\rangle = \times\frac{1}{E_n^0 - H_0}\underbrace{\left((\lambda V - \Delta_n)|\psi_n\rangle\right)}_{|\psi_n'\rangle}$$

$$\frac{1}{E_n^0 - H_0}|\psi_{n_0}\rangle = \frac{1}{E_n^0 - E_n^0}|\psi_{n_0}\rangle$$

if $(\lambda V - \Delta_n)|\psi_n\rangle \Rightarrow$ does not have component along $|\psi_{n_0}\rangle$

inner product $\langle\psi_{n_0}|\lambda V - \Delta_n|\psi_n\rangle = 0$

$$\Rightarrow \langle\psi_{n_0}|E_n^0 - H_0|\psi_n\rangle$$

$$(E_n^0 - H_0)|\psi_n\rangle = (\lambda V - \Delta_n)|\psi_n\rangle$$

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$$\Rightarrow \langle \psi_{n_0} | E_n^0 - H_0 | \psi_n \rangle$$

$$(E_n^0 - H_0)|\psi_n\rangle = (\lambda V - \Delta_n)|\psi_n\rangle$$

$$\langle \psi_{n_0} | E_n^0 | \psi_n \rangle - \langle \psi_{n_0} | H_0 | \psi_n \rangle = 0$$

operator $\rightarrow$ complementary projection operator.

$$|\psi_0\rangle\langle\psi_0|$$

BA

operator → complementary projection

$$\phi_n = 1 - |\psi_n^0\rangle\langle\psi_n^0| = \sum_{k\neq n} |k^0\rangle\langle k^0|$$

$$\frac{1}{E_n^0 - H_0}\phi_n = \sum_{k\neq n} \frac{1}{E_n^0 - H_0} |k^0\rangle\langle k^0|$$

$$\frac{1}{E_n^0 - H_0}$$

$$\frac{1}{E_n^0 - H_0}$$

$|n_0\rangle$

$|n\rangle \quad |\psi_n\rangle$

$$(E_n^0 - H_0)|\psi_n\rangle = (\lambda V - \Delta_n)|\psi_n\rangle$$

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$|n\rangle \qquad |\psi_n\rangle$

$E_n^0 - H_0$

$$(E_n^0 - H_0)|\psi_n\rangle = \underbrace{(\lambda V - \Delta_n)|\psi_n\rangle}$$

$$(\lambda V - \Delta_n)|\psi_n\rangle = \phi_n (\lambda V - \Delta_n)|\psi_n\rangle$$

$$= \left[1 - |\psi_n^0\rangle\langle\psi_n^0|\right](\lambda V - \Delta_n)|\psi_n\rangle$$

$$=$$

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$E_n^0 - H_0$ $|n\rangle$ $|\psi_n\rangle$

$$(E_n^0 - H_0)|\psi_n\rangle = \underbrace{(\lambda V - \Delta_n)|\psi_n\rangle}$$

$$(\lambda V - \Delta_n)|\psi_n\rangle = \phi_n (\lambda V - \Delta_n)|\psi_n\rangle$$

$$= [1 - |\psi_n^0\rangle\langle\psi_n^0|](\lambda V - \Delta_n)|\psi_n\rangle$$

$$= (\lambda V - \Delta_n)|\psi_n\rangle = \phi_n(\lambda V - \Delta_n)|\psi_n\rangle$$

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$$= \left[1 - |\psi_n^0\rangle\langle\psi_n^0| \right] (\lambda V - \Delta_n)|\psi_n\rangle$$

$$= (\lambda V - \Delta_n)|\psi_n\rangle = \phi_n(\lambda V - \Delta_n)|\psi_n\rangle$$

$$|\psi_n\rangle = \frac{1}{E_n^{(0)} - H_0}\phi_n \, \underline{(\lambda V - \Delta_n)|\psi_n\rangle} \quad ?$$

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$$|\psi_n\rangle = \frac{1}{E_n^{(0)} - H_0}\,\phi_n\,(\lambda V - \Delta_n)\,|\psi_n\rangle \quad ?$$

$\lambda \to 0$ $\quad \Delta_n \to 0$

$|\psi_n\rangle \to 0 \qquad \times$

$|\psi_n\rangle \to |\psi_n^0\rangle$

$$|\psi_n\rangle = |\psi_n^0\rangle + \frac{1}{E_n^{(0)} - H_0}\,\phi_n\,(\lambda V - \Delta_n)\,|\psi_n\rangle$$

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$$|\psi_n\rangle \to |\psi_n^0\rangle$$

$$|\psi_n\rangle = |\psi_n^0\rangle + \frac{1}{E_n^{(0)} - H_0}\phi_n(\lambda V - \Delta_n)|\psi_n\rangle$$

$$= |\psi_n^0\rangle + \frac{1}{E_n^{(0)} - H_0}\phi_n(\lambda V - \Delta_n)\Big[|\psi_n^0\rangle + \frac{1}{E_n^{(0)} - H_0}\phi_n(\lambda V - \Delta$$

$$|\psi_n\rangle \to \underbrace{|\psi_n^0\rangle}$$

$$|\psi_n\rangle = \underbrace{|\psi_n^0\rangle} + \frac{1}{E_n^{(0)} - H_0}\,\phi_n\,(\lambda V - \Delta_n)\underbrace{|\psi_n\rangle}$$

$$= \underbrace{|\psi_n^0\rangle} + \frac{1}{E_n^{(0)} - H_0}\,\phi_n\,(\lambda V - \Delta_n)\left[\,|\psi_n^0\rangle + \frac{1}{E_n^{(0)} - H_0}\,\phi_n\,(\lambda V - \Delta_n)|\psi_n\rangle\right]$$

$$\lambda$$

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$$= \underbrace{|\psi_n\rangle} + \frac{1}{E_n^{(0)} - H_0} \phi_n (\lambda V - \Delta_n) \Big[|\psi_n\rangle + \frac{1}{E_n^{(0)} - H_0} \phi_n (\ldots - \Delta_n) \ldots$$

$$\lambda$$

$$|\psi_n\rangle = |\psi_n^0\rangle + \lambda |\psi^1\rangle + \lambda^2 |\psi^2\rangle + \cdots\cdots$$

BA

$E_n^{(0)} - H_0$ $\qquad\qquad$ $E_n - H_0$

λ first order correction to ψ

$$|\psi_n\rangle = |\psi_n^0\rangle + \lambda|\psi^1\rangle + \lambda^2|\psi^2\rangle + \cdots\cdots$$

second order.

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots\cdots$$

first order correction

λ first order correction to ψ

$$|\psi_n\rangle = |\psi_n^0\rangle + \lambda \underbrace{|\psi^1\rangle} + \lambda^2 |\psi^2\rangle + \cdots$$

second order.

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_{\cancel{n}}^2 + \cdots$$

first order correction

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$$(H^0 + \lambda V)|\psi_n\rangle = E_n|\psi_n\rangle$$

$$(H^0 + \lambda V)\{|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda|\psi_n^2\rangle + \cdots\} =$$

$$\{E_n^0 + E_n^1 + E_n^2 + \cdots\}[|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda|\psi_n^2\rangle + \cdots]$$

BA

$$(H^0 + \lambda V)\left[|\psi_n^0\rangle + \lambda |\psi_n^1\rangle + \lambda |\psi_n^2\rangle + \cdots \right] =$$

$$\left[E_n^0 + E_n^1 + E_n^2 + \cdots \right]\left[|\psi_n^0\rangle + \lambda |\psi_n^1\rangle + \lambda |\psi_n^2\rangle + \cdots \right]$$

$$H^0 |\psi_n^0\rangle = E_n^0 |\psi_n^0\rangle$$

$$H^0 |\psi_n^1\rangle + V |\psi_n^0\rangle =$$

$$H^0|\psi_n^0\rangle = E_n^0|\psi_n^0\rangle \quad \text{— zeroth}$$

$$H^0|\psi_n^1\rangle + V|\psi_n^0\rangle = E_n^0|\psi_n^1\rangle + E_n^1|\psi_n^0\rangle \quad \text{— first}$$

$$H^0|\psi_n^2\rangle + V|\psi_n^1\rangle = E_n^0|\psi_n^2\rangle + E_n^1|\psi_n^1\rangle + E_n^2|\psi_n^0\rangle$$

$$H|\psi_n\rangle + V|\psi_n\rangle = E_n|\psi_n\rangle + E_n|\psi_n\rangle + E_n|\psi_n\rangle$$

First order correction in energy.

$$\langle\psi_n^0|$$

$$\underbrace{\langle\psi_n^0|H^0|\psi_n^1\rangle}_{E_n^0\langle\psi_n^0|} + \langle\psi_n^0|V|\psi_n^0\rangle = \underbrace{\langle\psi_n^0|E_n^0|\psi_n^1\rangle}_{E_n^0\langle\psi_n^0|\psi_n^1\rangle} + \underbrace{\langle\psi_n^0|E_n^1|\psi_n^0\rangle}_{E_n^1}$$

$$\langle\psi_0|\psi_n\rangle = 0$$

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$\langle \psi_n^0 |$

$$\underbrace{\langle \psi_n^0 | H^0 | \psi_n^1 \rangle}_{E_n^0 \cancel{\langle \psi_n^0 | \psi_n^1 \rangle}} + \langle \psi_n^0 | V | \psi_n^0 \rangle = \underbrace{\langle \psi_n^0 | E_n^0 | \psi_n^1 \rangle}_{E_n^0 \cancel{\langle \psi_n^0 | \psi_n^1 \rangle}} + \underbrace{\langle \psi_n^0 | E_n^1 | \psi_n^0 \rangle}_{E_n^1}$$

$\langle \psi_0 | \psi_n \rangle = 0$

$$\boxed{E_n^1 = \langle \psi_n^0 | V | \psi_n^0 \rangle}$$

BA

$$H^0|\psi_n^2\rangle + V|\psi_n^1\rangle = E_n^0|\psi_n^2\rangle + E_n^1|\psi_n^1\rangle + E_n^2\underbrace{|\psi_n^0\rangle}$$

$$\langle\psi_n^0|H^0|\psi_n^2\rangle + \langle\psi_n^0|V|\psi_n^1\rangle = E_n^0\cancel{\langle\psi_n^0|\psi_n^2\rangle} + E_n^1\underbrace{\langle\psi_n^0|\psi_n^1\rangle} + E_n^2$$

$$E_n^0\cancel{\langle\psi_n^0|\psi_n^2\rangle}$$

$$H^0|\psi_n^2\rangle + V|\psi_n^1\rangle = E_n^0|\psi_n^2\rangle + E_n^1|\psi_n^1\rangle + E_n^2|\psi_n^0\rangle$$

$$\langle\psi_n^0|H^0|\psi_n^2\rangle + \langle\psi_n^0|V|\psi_n^1\rangle = E_n^0\cancel{\langle\psi_n^0|\psi_n^2\rangle} + \underbrace{E_n^1\langle\psi_n^0|\psi_n^1\rangle}_{0} + E_n^2$$

$$E_n^0\cancel{\langle\psi_n^0|\psi_n^2\rangle}$$

$$E_n^2 = \langle\psi_n^0|V|\psi_n^1\rangle$$

$$H^0|\psi_n^2\rangle + V|\psi_n^1\rangle = E_n^0|\psi_n^2\rangle + E_n^1|\psi_n^1\rangle + E_n^2|\psi_n^0\rangle$$

$$\langle\psi_n^0|H^0|\psi_n^2\rangle + \langle\psi_n^0|V|\psi_n^1\rangle = E_n^0\cancel{\langle\psi_n^0|\psi_n^2\rangle} + \underbrace{E_n^1\langle\psi_n^0|\psi_n^1\rangle}_{\Downarrow \; 0} + E_n^2$$

$$E_n^0\cancel{\langle\psi_n^0|\psi_n^2\rangle}$$

$$|\psi_n^1\rangle$$

$$E_n^2 = \langle\psi_n^0|V|\psi_n^1\rangle \qquad E_n^{(i)} = \langle\psi_n^0|V|\psi_n^{i-1}\rangle$$