Term: Spring 2020
Meetings: Tuesday & Thursday 11:25-12:40
Location: 204 Stuart Building

Instructor: Carlo Segre
Office: 166d/172 Pritzker Science
Phone: 312.567.3498
email: segre@iit.edu


Web Site: http://phys.iit.edu/~segre/phys406/20S
Course Objectives

1. Understand the connection between symmetry and conservation laws.
Course Objectives

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2. Understand time-independent perturbation theory.
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3. Understand the variational method.
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1. Understand the connection between symmetry and conservation laws.

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4. Understand the WKB approximation and scattering theory.
Course Objectives

1. Understand the connection between symmetry and conservation laws.
2. Understand time-independent perturbation theory.
3. Understand the variational method.
4. Understand the WKB approximation and scattering theory.
5. Understand dynamical effects in quantum mechanics.
Course Objectives

1. Understand the connection between symmetry and conservation laws.

2. Understand time-independent perturbation theory.

3. Understand the variational method.

4. Understand the WKB approximation and scattering theory.

5. Understand dynamical effects in quantum mechanics.

6. Be able to solve quantum mechanics problems using the approximation method appropriate to the situation.
Course Grading

15% – Homework assignments
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   Weekly or bi-weekly
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   Due at beginning of class
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50% – Two mid-term exams
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35% – Final examination
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Grading scale
A – 88% to 100%
B – 75% to 88%
C – 62% to 75%
D – 50% to 62%
E – 0% to 50%
Topics to be Covered

1. Symmetry & conservation laws
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2. Time-independent perturbation theory
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6. Quantum dynamics
Topics to be Covered

1. Symmetry & conservation laws
2. Time-independent perturbation theory
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6. Quantum dynamics
7. Quantum paradoxes
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1. Symmetry & conservation laws
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7. Quantum paradoxes
8. Quantum Information Science
Up-to-date schedule at
http://phys.iit.edu/~segre/phys406/20S/schedule.html
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28 class sessions
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~190 pages to cover
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Focus on approximate methods for solving real problems in quantum mechanics and actual quantum mechanics research.
Today’s Outline - January 14, 2020

• Tips for success
• The big picture
• Transformations
• Translation operator
• Parity operator

Reading Assignment: Chapter 6.1-6.5

Homework Assignment #01: Chapter 6: 1,3,4,8,9,10
due Tuesday, January 21, 2020

C. Segre (IIT)
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6. Come to office hours with questions, I’ll be less lonely and it will help you too!
Why approximate methods?

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Quantum physics is the foundation of the discipline and is part of the day-to-day work of a professional physicist.
A bit more about me...

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The company . . . Influit Energy, LLC

Influit Energy R&D
NEF Gen 1 prototype development

Pilot Program
NEF battery validation on small EUV

Influit Energy R&D
NEF Gen 1 wing/motor demo

Influit Energy R&D
NEF Gen 2 demo

Influit Energy R&D
Transportable liquid battery pods

The company . . . Influit Energy, LLC

Influit Energy (IIT)
Translation operator

The translation operator, $\hat{T}(a)$, can be expressed in terms of the momentum operator by starting with the Taylor series expansion for $\psi(x - a)$ about $x$

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The translation operator, $\hat{T}(a)$, can be expressed in terms of the momentum operator by starting with the Taylor series expansion for $\psi(x - a)$ about $x$:

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$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{-ia}{\hbar} \frac{d}{i dx} \right)^n \psi(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{-ia}{\hbar} \hat{p} \right)^n \psi(x)$$

Thus, the momentum is the generator of translations and the translation operator is clearly unitary.
The translation operator, $\hat{T}(a)$, can be expressed in terms of the momentum operator by starting with the Taylor series expansion for $\psi(x - a)$ about $x$

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$$\langle \psi' | \hat{Q} | \psi' \rangle = \langle \psi | \hat{T}^\dagger \hat{Q} \hat{T} | \psi \rangle = \langle \psi | \hat{Q}' | \psi \rangle \quad \rightarrow \quad \hat{Q}' \equiv \hat{T}^\dagger \hat{Q} \hat{T}$$
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Find the operator $\hat{x}'$ obtained by applying a translation through a distance $a$ to the operator $\hat{x}$. That is, what is the action of $\hat{x}'$ on an arbitrary function $f(x)$?
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Continuous translational symmetry

We discussed the Bloch theorem previously in which there is a discrete translational symmetry. In a system with continuous translational symmetry, any choice of $a$ is possible.
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We discussed the Bloch theorem previously in which there is a discrete translational symmetry. In a system with continuous translational symmetry, any choice of $a$ is possible for an infinitesimal translation $\delta$

Thus the Hamiltonian commutes with the momentum operator

$$\hat{T}(\delta) = e^{-i\delta \hat{p}/\hbar} \approx 1 - i\delta \hbar \hat{p}$$

$$[\hat{H}, \hat{T}(\delta)] = 0$$
$$[\hat{H}, \hat{p}] = 0$$

According to Ehrenfest's Theorem, this leads to conservation of momentum

$$\frac{d}{dt} \langle p \rangle = i\hbar [\hat{H}, \hat{p}] + \langle \frac{\partial \hat{p}}{\partial t} \rangle = 0$$

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Conservation laws

If an operator $\hat{Q}$ commutes with the Hamiltonian, then by the Ehrenfest relation its expectation value $\langle Q \rangle$ is independent of time if $\partial Q / \partial t = 0$. 

Let's see where this definition leads us. The probability of getting $q_n$ when measuring $Q$ in state $|\Psi(t)\rangle$ at a time $t$ is given the time dependence of the wave function where $|\psi_m\rangle$ are the eigenfunctions of the Hamiltonian since $[H, \hat{Q}] \equiv 0$ we can find simultaneous eigenfunctions of the two: so we choose $|\psi_n\rangle = |f_n\rangle P(q_n)$
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the two definitions of conservation of $Q$ are equivalent
Parity in 1D

In one dimension, the parity operator, \( \hat{\Pi} \) inverts space.
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$$\hat{\Pi}^{-1} = \hat{\Pi} = \hat{\Pi}^\dagger$$

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Parity in 1D

In one dimension, the parity operator, $\hat{\Pi}$ inverts space

this operator is its own inverse, is Hermitian, and thus unitary

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\]

\[
\hat{\rho}' = \hat{\Pi}^\dagger\hat{\rho}\hat{\Pi} = -\hat{\rho}
\]

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$$\hat{\Pi} \hat{H} = \hat{\Pi} \hat{H}^\dagger \hat{H} \hat{\Pi} \rightarrow \hat{\Pi} \hat{H} = \hat{H} \hat{\Pi} \rightarrow [\hat{H}, \hat{\Pi}] = 0$$
Parity in 1D

For a Hamiltonian which describes a particle of mass $m$ in a one-dimensional potential $V(x)$, inversion symmetry means that $V(x) \equiv V(-x)$, an even function of position.

Because $\hat{\Pi}$ and $\hat{H}$ commute, we can find common eigenfunctions $\psi_n(x)$ such that $\hat{\Pi}\psi_n(x) = \psi_n(-x) = \pm \psi_n(x)$ since the eigenvalues of parity can only be $\pm 1$.

Thus the eigenfunctions of such a Hamiltonian are either even or odd under parity and by Ehrenfest's Theorem, we have $\frac{d}{dt} \langle \Pi \rangle = i\hbar \langle [\hat{H}, \hat{\Pi}] \rangle = 0$ which means that parity is conserved in time, that is an even function under parity will remain even for all time and an odd function under parity will remain odd for all time.
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Parity in 3D

In three dimensions, the parity operator inverts the system through the origin.
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\[ \hat{\Pi} \psi(r) = \psi'(r) = \psi(-r) \]
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In three dimensions, the parity operator inverts the system through the origin

the \( \hat{r} \) and \( \hat{p} \) operators and any arbitrary operator transform as

\[
\hat{\Pi} \psi(\vec{r}) = \psi'(\vec{r}) = \psi(-\vec{r})
\]

The Hamiltonian in three dimensions will have parity when \( V(-\vec{r}) = V(\vec{r}) \) which is true for all central potentials

The eigenstates of the hydrogen atom are in fact, also eigenstates of parity

\[
\hat{\Pi} \psi_{n\ell m}(\vec{r},\theta,\phi) = (-1)^\ell \psi_{n\ell m}(\vec{r},\theta,\phi)
\]

\[
\psi_{n\ell m}(\vec{r},\theta,\phi) = R_{n\ell}(\vec{r}) Y_{m\ell}(\theta,\phi)
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In three dimensions, the parity operator inverts the system through the origin. The \( \hat{r} \) and \( \hat{p} \) operators and any arbitrary operator transform as:

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\hat{\Pi} \psi (r) = \psi' (r) = \psi (-r) \\
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The eigenstates of the hydrogen atom are in fact, also eigenstates of parity

\[
\hat{\Pi} \psi_{nlm}(r, \theta, \phi) = (-1)^l \psi_{nlm}(r, \theta, \phi), \quad \psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y^m_l(\theta, \phi)
\]
Parity selection rules

Selection rules, which will be very important when we talk about time-dependent phenomena, indicate when a matrix element which couples two states, $\langle a | \hat{Q} | b \rangle$, is zero based on symmetry.
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A particularly important operator is the electric dipole operator, \( \hat{p}_e = q\hat{r} \) whose selection rules determine which atomic transitions are allowed and which are forbidden.
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It is evident that $\hat{p}_e$ is odd under parity because $\hat{r}$ is odd.

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Consider the matrix elements of the electric dipole operator between two atomic states $\psi_{nlm}$, and $\psi_{n'l'm'}$
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\[ \langle n'l'm' | \hat{p}_e | nlm \rangle = -\langle n'l'm' | \hat{\Pi} \hat{p}_e \hat{\Pi} | nlm \rangle \]
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$$= -\langle n'l'm' | (-1)^{l''} \hat{p}_e (-1)^l | nlm \rangle$$
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\[ = -\langle n'l'm' | (-1)^{l'} \hat{p}_e (-1)^{l} | nlm \rangle \]

\[ = (-1)^{l+l'+1} \langle n'l'm' | \hat{p}_e | nlm \rangle \]
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$$= -\langle n'l'm'|(-1)^{l'}\hat{p}_e(-1)^l|nlm\rangle$$

$$= (-1)^{l+l'+1}\langle n'l'm'|\hat{p}_e|nlm\rangle = 0 \quad \text{if } l + l' = 2n$$
Rotation about the $z$ axis

The operator $\hat{R}_z(\varphi)$ rotates the function an angle $\varphi$ about the $z$ axis.
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$$\hat{R}_z(\phi)\psi(r, \theta, \phi) = \psi'(r, \theta, \phi)$$
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just as with the translation operator we can determine the generator of rotations starting with a Taylor series (hiding the $r$ and $\theta$ variables)
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$$\hat{R}_z(\varphi)\psi(\phi) = \psi(\phi - \varphi) = \sum_{n=0}^{\infty} \frac{1}{n!} [(\phi - \varphi) - \phi]^n \frac{d^n \psi(\phi - \varphi)}{d(\phi - \varphi)^n} \bigg|_{\phi-\varphi=\phi}$$
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$$= \sum_{n=0}^{\infty} \frac{1}{n!} (-\varphi)^n \frac{d^n\psi(\phi)}{d\phi^n} \bigg|_{\phi} = \sum_{n=0}^{\infty} \frac{1}{n!} (-\varphi)^n \frac{d^n}{d\phi^n} \psi(\phi)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{-i\varphi}{\hbar} \frac{d}{i d\phi}\right)^n \psi(\phi)$$
Rotation about the $z$ axis

The operator $\hat{R}_z(\varphi)$ rotates the function an angle $\varphi$ about the $z$ axis

$$\hat{R}_z(\phi)\psi(r, \theta, \phi) = \psi'(r, \theta, \phi) = \psi(r, \theta, \phi - \varphi)$$

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$$= \sum_{n=0}^{\infty} \frac{1}{n!} (-\varphi)^n \left[\frac{d^n\psi(\phi)}{d\phi^n}\right]_{\phi} = \sum_{n=0}^{\infty} \frac{1}{n!} (-\varphi)^n \frac{d^n\psi(\phi)}{d\phi^n}$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-i\varphi \frac{\hbar}{\hbar} \frac{d}{i \ d\phi}\right)^n \psi(\phi)$$
Rotation about the z axis

The operator \( \hat{R}_z(\varphi) \) rotates the function an angle \( \varphi \) about the z axis

\[
\hat{R}_z(\phi)\psi(r, \theta, \phi) = \psi'(r, \theta, \phi) = \psi(r, \theta, \phi - \varphi)
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\]

\[
= \sum_{n=0}^{\infty} \frac{1}{n!} (-\varphi)^n \frac{d^n\psi(\phi)}{d\phi^n} \bigg|_{\phi} = \sum_{n=0}^{\infty} \frac{1}{n!} (-\varphi)^n \frac{d^n\psi(\phi)}{d\phi^n} \psi(\phi)
\]

\[
= \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{-i\varphi}{\hbar} \frac{\hat{d}}{d\phi} \right)^n \psi(\phi) = \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{-i\varphi}{\hbar} \hat{L}_z \right)^n \psi(\phi)
\]
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The operator $\hat{R}_z(\varphi)$ rotates the function an angle $\varphi$ about the $z$ axis

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$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{-i\varphi}{\hbar} \frac{d}{d\phi} \right)^n \psi(\phi) = \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{-i\varphi}{\hbar} \hat{L}_z \right)^n \psi(\phi)$$

$$= e^{-i\varphi\hat{L}_z/\hbar}\psi(\phi)$$
Rotation about the z axis

The operator $\hat{R}_z(\varphi)$ rotates the function an angle $\varphi$ about the z axis

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$$= e^{-i\varphi \hat{L}_z/\hbar} \psi(\phi) \quad \longrightarrow \quad \hat{R}_z(\varphi) = e^{-i\varphi \hat{L}_z/\hbar}$$