

# PHY 571: Quantum Physics

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*1D Eigenvalue problems summary*  
*Transition to Operator/Matrix Methods*  
Module 3, [Lectures 15,16](#) - [17,18](#)

# Summary: 1D Eigenvalue problems

- Topics and references: [Eigenvalue problems](#)
- Application areas, explore via mini-projects: [Quantum Resources](#), the [CUPS program](#) (an old DOS program, for which there is a useful book) to explore questions on [Problem sheets #2 and #3](#), and/or [Open-source PhET programs](#), either via the PhET site (University of Colorado), or our Blackboard course shell.
- Suggested applications: 1D "Molecules", Tunneling Microscopy, Band Structure, (e.g. Si, Ge eventually)
- Transition to Operator methods using SHO example

# Introduction to Operator Methods

- Revision of the **Expansion Postulate**, introduction to **Dirac notation**, bras  $\langle \psi |$  and kets  $|\psi\rangle$ . Note that the bra  $\langle \psi |$  is equivalent to  $\psi^*$  which comes before, and the ket  $|\psi\rangle$  comes after the operator.
- For the **Hamiltonian** operator  $H$ , as in the SE, we write:  $H|\psi\rangle = E|\psi\rangle$ , very compact notation
- The SE only has solutions for **eigenvectors**  $|u_n\rangle$  or simply  $|n\rangle$ , for which  $H|n\rangle = E_n|n\rangle$ ,  $E_n$  the  $n$ th **energy eigenvalue**
- Then, if  $|\psi\rangle = \sum_n A_n |n\rangle$  represents the **expansion** of the wave function in terms of the **eigenvectors**, the coefficients  $A_n$  are given by the  $A_n = \langle n|\psi\rangle$ , a scalar product, and the **expectation value** of the Hamiltonian  $\langle H \rangle = \langle \psi | H | \psi \rangle = \sum_n E_n |A_n|^2$ ; *we measure  $E_n$  with probability  $|A_n|^2 = A_n^* A_n$*

## Operator methods continued

- The form  $\langle \psi | O_p | \psi \rangle$  is the **expectation value** of *any operator*,  $O_p$ ; see if you can apply it to operators for  $\mathbf{p}$  and  $\mathbf{x}$  or  $\mathbf{r}$ , in the x- or p-representations
- An interesting special case that is usually taught this way is **Simple Harmonic Oscillator** (SHO),  $V(\mathbf{x}) = \frac{1}{2}m\omega\mathbf{x}^2$
- **Factorization of operators** in the Hamiltonian and use of commutation relation  $[p, x] = \hbar/i$  to obtain
- $H = (A^+A + \frac{1}{2})\hbar\omega$ , with  $A^+A$  as the *number* operator
- $A^+$  = the *raising* and  $A$  as the *lowering* operator; equivalently *creation*  $c^+$  and *annihilation*  $c$  operators

## SHO: zero point energy, ground state

- The term  $\frac{1}{2}\hbar\omega$  is the zero point energy, and the energy level spacing  $\hbar\omega$  is constant (see simulations)
- Acting on the ground state  $|0\rangle$  we create state  $|1\rangle$  via  $|1\rangle = A^+|0\rangle$ ; in general  $|n\rangle = (A^+)^n|0\rangle$ , with a normalization constant that turns out to be  $n^{-1/2}$ . Thus  $n^{-1/2}(A^+)^n$  is a generating function, creating state  $|n\rangle$
- Similarly  $|n-1\rangle = n^{-1/2}A|n\rangle$ , and so on to  $|0\rangle = A|1\rangle$ . Finally  $A|0\rangle = 0$ ; *you can't lower the ground state. But you can use this equation, in differential equation form, to show that the ground state wave function is  $|0\rangle = N.\exp(-m\omega x^2/\hbar)$ , Gaussian,  $N = (m\omega/\hbar\pi)^{1/4}$ .*

# Raising, Lowering and Photons

- What happens to the energy when  $|n-1\rangle = n^{-1/2}A|n\rangle$ ?  
The SHO itself has lower energy, so **energy** (and maybe **momentum** too) must have **gone somewhere...**
- If the particle considered has a charge (e.g. electron) then the energy  $\hbar\omega$  is *radiated*:
- ***A creates a photon***; similarly  $A^+$  ... *connect the dots*  
*The full theory is QED (Quantum Electro-Dynamics).*  
*1965 Nobel prize for Tomonaga, Schwinger and Feynman (1949 papers), in this course see Module 5: Time-dependent Perturbation Theory*
- Here, we consider transitions between atomic and molecular states using *Angular momentum operators*

# Introduction to Angular Momentum

- Most of these lectures were handed out in class, and gone through with frequent questions. Download the [Angular Momentum](#) reference list. There is no point in trying to write another Quantum Mechanics text book here, *is there?*
- This section concerns the SE in  $(r, \theta, \phi)$  coordinates. We start with the **Angular**  $(\theta, \phi)$  **equation** and the **two quantum numbers**  $(\ell, m)$  that go with this equation. The solutions, the angular eigenfunctions, are **Spherical Harmonics**  $Y_{\ell m}$ . These are functions of  $\theta$  and  $\phi$ :  $|\ell, m\rangle = \Theta_{\ell m}(\theta) \cdot \exp(im\phi)$
- We can see that the quantum numbers arise from the need for the wave functions to be **singled-valued**. For example, the form  $\exp(im\phi)$  arises because the angles  $\phi$  and  $(\phi + 2\pi)$  are the same, and  **$\exp(2\pi im) = 1$**  for all integers  $m$ .

# Operator Methods: $L_z$ , $L^2$ and $L_{\pm}$

- Familiarize yourself with the *shapes* of the  $Y_{\ell m}$  for  $\ell = 0, 1$  and  $2$ . These are the **s**, **p** and **d**-functions of the Periodic Table, and  $\ell$  is the **Angular momentum** quantum number.
- To prove the math behind angular momentum it is easiest to start with the operator  $L_z$ , which corresponds to rotation about the z-axis; we write:  $L_z|\phi\rangle = m\hbar|\phi\rangle$ ; you can easily deduce that the eigenvalue  $m\hbar$  arises from  $L_z \equiv (\hbar/i)d/d\phi$ ;  $m$  is known as the **magnetic quantum number**, discussed later
- The energy associated with rotation is  $L^2/2I$ , where  $I$  is the **moment of inertia**;  $L^2|Y_{\ell m}\rangle = \ell(\ell+1)\hbar^2|Y_{\ell m}\rangle$ ; *check out why*
- The mathematical details are set out in Gasiorowicz's [Web Supplements 7A and 7B](#). You have Supplement 7A: consult 7B online (*thinking green thoughts, of course, what else*)

## Raising, Lowering and Photons #2

- Here angular momentum is very similar to the SHO: the equivalent of the **raising** and **lowering** operators are  $L_+$  and  $L_-$
- The commutation relations are  $[L_x, L_y] = i\hbar L_z$  and cyclically, with  $L_+ = L_x + iL_y$ , and of course  $L_- = L_x - iL_y$
- *So now you can go to town with*  $L^2 = L_x^2 + L_y^2 + L_z^2$  and factorize  $(L_x^2 + L_y^2)$  into  $L_+ L_-$  with bits left over that don't commute, and *assuming you don't lose your nerve*, you will find the extra  $\ell\hbar^2$  in the energy that isn't obvious ( $\ell^2\hbar^2$  is obvious)
- This extra energy corresponds to the rotational zero point energy, and this is neatly visualized by the **vector model** (of the atom), and is quantified by the uncertainty principle as applied to  $L_x$  and  $L_y$ ; see [Web Supplement 5A](#), equation 5A-11
- Now start to consider how this all works; draw the vector model; show  $L_+ |Y_{\ell\ell}\rangle = 0$ ,  $L_- |Y_{\ell-\ell}\rangle = 0$ ;  $-\ell \leq m \leq \ell$ ,  $(2\ell + 1)$  m-values

# Raising, Lowering and Photons #3

- Diagram of s, p, d orbitals and the  $(2\ell + 1)$  m-values handed out; start to think about transitions between p and s-orbitals, and/or d and p, changes of angular momentum, and "dipoles" due to wave functions of the superposition form  $|\psi\rangle = A|1s\rangle + B|2p\rangle$
- "During this transition" there is an **oscillating dipole**. This **dipole** emits a photon that carries away *both energy and angular momentum*; note the lowering transition  $L_-|Y_{10}\rangle \rightarrow |Y_{00}\rangle$  emits **linearly polarized** radiation, mostly in the x-y plane;  $L_-|Y_{11}\rangle \rightarrow |Y_{00}\rangle$  and  $L_-|Y_{1,-1}\rangle \rightarrow |Y_{00}\rangle$  corresponds to (R and L) **circularly polarized** radiation, mostly along the z-axis (*which is which?*)
- Photons are **spin 1** particles; they carry away 1 unit  $\Delta L = \hbar$  of **angular momentum** as well as the **energy**  $\hbar\omega = E_{2p} - E_{1s}$  in this **electric dipole transition**. *What about d-s transitions,  $\Delta L = 2\hbar$ ?*

## Simulation Area #1: 1D "Molecules"

- Choose double well potential in **Bound State** simulation, with reasonable (chemical) parameters, e.g. hydrogen or other simple molecule/ molecular ion
- Explore the role of the **well width**, and the **width of the gap** between the wells. Note the effect on the ground state, and on the first few excited states. *Care here:* when the wells are widely separated, we have **two-fold degeneracy**, identical states in two isolated atoms. Note how many states there are, and the number of nodes in the wave-function
- Explore different **potential shapes**: square wells, hydrogen-like ( $r^{-1}$ ) and SHO ( $r^2$ ) potentials

## Simulation Area #2: Tunneling Microscopy

- Choose repulsive potential barrier in a **quantum tunneling** simulation, with reasonable parameters for a **scanning tunneling microscope** (STM)
- Explore the role of the **barrier height and width**, on the **transmission** and **reflection** coefficients and the corresponding wave functions (amplitude, phase).
- Explore the same effects when there is a **voltage drop** between the **tip** and the **sample**, with values appropriate for **STM operation**
- Think about more **realistic** potential **barrier shapes**, and the role of the **Fermi-Dirac** energy distribution