PHY 571: Quantum Physics

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Spring 2008

1-dimensional Eigenvalue Problems

Module 2, Lectures 9-14

Book, Web and Java-based resources

- Download topics and references: Eigenvalue problems *if you haven't already done so*.
- Bookmark Quantum Resources on the course website and *explore these in your own time*.
- Use the CUPS program (an old DOS program, for which there is a useful book) to explore questions on Problem sheets #2 and #3
- Use one or more of the Open-source PhET programs, either via the PhET site (University of Colorado), or our Blackboard course shell. *Read a recent paper on the use of simulations in teaching Quantum Mechanics*

Separation of Variables:
The time-independent Schrödinger Equation

- time-dependent SE: $i\hbar\partial/\partial t(\psi) = H(\psi)$
- The time-independent SE: $H(\psi) = E(\psi)$ is obtained by assuming the product solution $\psi(\mathbf{r},t) = T(t).\ u(\mathbf{r})$. We then find that this only works if
- $i\hbar\partial T(t)/\partial t = ET(t)$, where E is constant (the energy), and then $T(t) = C\exp(-iEt/\hbar)$, with $E = \hbar\omega$.
- The remainder of the equation gives $Hu(\mathbf{r}) = Eu(\mathbf{r})$. Substituting for H = K +V in the low energy regime yields $-(\hbar^2/2m)\partial^2 u(x)/\partial x^2 + V(x)\ u(x) = Eu(\mathbf{x})$, in 1D.
- Exercise: *Generalize the result to 3D, and include the time dependence to get* $\psi(\mathbf{r},t)$.

Is the total energy positive or negative #1?

- for $E > 0$ and $E < 0$, the solutions are ***quite different;*** *diagram & handouts of continuum (unbound) solutions for* $E > 0$, *and discrete (bound) solutions for* $E < 0$.
- Stick with the example of a "finite box", a "finite potential well". This example is very versatile, with two parameters: V_0 (well depth) and $\pm a$ (well width)
- We illustrate solutions for *bound states*: within the well $u(x) = A\cos(kx)$ *or* $B\sin(kx)$, with even *or* odd *parity*; outside the well $Ce^{\pm \kappa x}$, sketching solutions
- Boundary conditions 1: u(x) continuous $A\cos(ka)$ *or* $B\sin(ka) = Ce^{-\kappa a}$ 2: u'(x) ~ current j(x) continuous

Is the total energy positive or negative #2?

- for $E > 0$ the solutions are *continuum (unbound)* These are beams, which enter from the left, interact with the well, and get transmitted and reflected. But remember these are *time-independent problems*
- Stick with the example of a "finite box", a "finite potential well". This example is very versatile, with two parameters: V_0 (well depth) and $\pm a$ (well width)
- Solutions for *unbound states*: from the left $u(x) = \exp(ikx) + R\exp(-ikx)$; in the well region $u(x) = A\exp(ikx) + B\exp(-ikx)$; and the transmitted wave $u(x) = T\exp(ikx)$ *Four equations in four unknowns*

Is the total energy positive or negative #3?

Stick with the example of a "finite box", a "finite potential well". This example is very versatile, with two parameters: V_0 (well depth) and ±a (well width)

- *Orthogonal*, *Normalized*, *Orthonormal* solutions: *O*
  No! Lets do a few exercises to check these features out
- *Orthogonal:* $\int u_n^* u_m dx = 0$ *if* $n \neq m$
- *Normalized:* $\int u_n^* u_m dx = 1$ *if* $n = m$
- *Orthonormal:* $\int u_n^* u_m dx = \delta_{nm}$; *Kronecker Delta*

Example: PheT Program #1 (Bound states)

- Link to local bound state program after downloading.
- Link to bound state program on Course web site
- Points to note: Poll of points raised by students

Example: PheT Program #2 (Tunneling)

- Link to local quantum tunneling program after downloading.
- Link to bound state program on Course web site
- Points to note: Poll of points raised by students

Example: CUPS Programs

- Link to local CUPS program after downloading.
- Link to CUPS program on Course web site
- Points to note: Poll of points raised by students

Application 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 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

Application 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

Application Area #3: Band Structure

- Choose the default setting in a many wells simulation, with reasonable parameters for a simple metal (Li, Na)
- Explore the wave function overlaps, spatial probability graphs, and resulting band widths for core and valence electrons; think about where the Fermi level may lie.
- If you haven't already done so, explore the Kronig-Penney model for a 1D array of δ-function potentials, band gaps, and the similarities with realistic potentials
- Think about why this 1D, 1-electron model will need modification when we go to realistic 3D potentials and many electrons: *we will come to these points later...*