Supplement - Quick and dirty quantum mechanics for PHYS 445

What's Important:
- old quantum theory
- particle in a 1-D box
- rigid rotor
- harmonic oscillator

Old quantum theory

A very simple approach to quantization is based upon interference, where the wave in question comes from de Broglie. In systems with repetitive motion, the idea is to demand that the motion contain an appropriate number of de Broglie wavelengths to form a constructive standing wave. The de Broglie wavelength, as we recall is

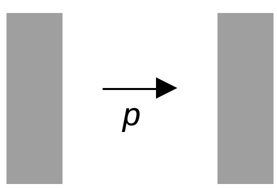
$$\lambda = h / p$$

where

λ = de Broglie wavelength
h = Planck's constant
p = particle momentum.

We reason by example.

1. Particle in a 1-dimensional box



Here, the motion is in one dimension between two perfectly reflective walls. Since there is no potential energy gradient in the region between the walls, the particle's energy and momentum must be constant. We quantize this system by demanding that the particle's de Broglie wave form a standing pattern:

L = box length

The general relation between the wavelength λ and the box size L is

$$\lambda = 2L / n \qquad n = 1, 2, 3, ...$$

where n is called the quantum number of the system. This means that the allowed values of the particle's momentum p are:

$$p = h / \lambda = h / [2L / n] = nh / 2L.$$

The corresponding kinetic energy is

$$E = p^2 / 2m = (nh / 2L)^2 / 2m$$

or

$$E_n = n^2 (h^2 / 8mL^2) \qquad n = 1, 2, 3, ...$$

The little subscript n is attached to E to specify that it is the energy of the n^{th} state. Note that E_n grows like n^2.

2. Rigid rotor

This problem involves circular motion at radius R about a fixed point. Again, we demand constructive interference so that

$$\text{circumference} = 2\pi R = n\lambda \qquad n = 1, 2, 3, ...$$

Proceeding as in example #1:

$$\lambda = 2\pi R / n$$

implies

$$p = h / \lambda = h / [2\pi R / n] = nh / 2\pi R.$$

The corresponding kinetic energy is

$$E = p^2 / 2m = (nh / 2\pi R)^2 / 2m$$

or

$$E = n^2 \frac{h^2}{8\pi^2 (mR^2)}$$

In fact, if we identify mR^2 with the moment of inertia of the particle around the axis of rotation, then we have the general result

$$E_n = n^2 \frac{h^2}{8\pi^2 I}$$

Again, note that E_n grows like n^2.

3. Harmonic oscillator

This example is not as simple as the previous ones because p is not a constant. The solution is

$$E_n = (n + 1/2)\, \omega h / 2\pi \qquad n = 0, 1, 2, 3, ...$$

where $\omega = (k/m)^{1/2}$, the same expression for angular frequency as is found in classical mechanics. The combination $\omega h / 2\pi$ or hf is familiar as the energy of a single photon.

What is surprising here is the 1/2 in the expression for E_n. Given some intuition about the energies of photons with wavelength $\lambda = c/f$, we might have guessed

$$E \sim nhf = n\omega h / 2\pi \qquad n = 1, 2, 3, ...$$

The extra factor of 1/2 means that the oscillator *always* has kinetic energy, even in its ground state. This is different from the first two examples, where E_n=0 when n = 0.

Quantum numbers in ensembles

If there are many particles present in a system, but they do not interact, then their energies add independently. We would then expect for the examples considered above:

$$E_{box} = (n_1^2 + n_2^2 + n_3^2 + ... + n_N^2)\frac{h^2}{8mL^2} \qquad n_i = 1, 2, 3, ... \text{ for all } i$$

$$E_{rotor} = (n_1^2 + n_2^2 + n_3^2 + ... + n_N^2)\frac{h^2}{8\pi^2 I} \qquad n_i = 1, 2, 3, ... \text{ for all } i$$

$$E_{oscillator} = (n_1 + n_2 + ... + n_N)\, \omega h / 2\pi \qquad n_i = 1, 2, 3, ... \text{ for all } i$$

To specify the energy of the system, we need to specify the quantum numbers n_1, n_2, ... n_N, which are the degrees of freedom of the ensemble.

What happens if the particles are **non**-interacting? Then life becomes more complicated and we have to solve for the entire system in interaction. However, if the particles are only weakly interacting, then we have approximately

$$E_{tot} \sim E_{n1} + E_{n2} + ... E_{nN}.$$

In other words, the total energy is approximately equal to the sum of the single-particle energies.