

Lecture 16 - Many particle systems

What's important:

- many-particle wavefunctions
- bosons and fermions
- symmetry of wavefunction

Text: Gasiorowicz, Chap. 8

So far, we have discussed the motion of a single particle in an external fixed potential; we have not considered how the potential arises or that it might be associated with another particle. Let's now generalize our system to include the motion of several particles in interaction with each other. We won't actually implement most of the concepts presented here until much later in the course, but there are some issues that will arise in the next several lectures that are best dealt with now:

- many-particle Hamiltonians and wavefunctions
- reduced mass for two-body systems
- bosons and fermions
- symmetrization of the wavefunction.

Many-particle Hamiltonians and wavefunctions

Still working in one dimension, we consider a group of N particles having positions $x_1 \dots x_N$. The classical Hamiltonian for this system is

$$H = \sum_i (p_i^2/2m) + V(x_1 \dots x_N), \quad (1)$$

where we take the potential energy to be independent of time. The usual operator replacement can be made for the momentum of each particle, yielding

$$H = -\hbar^2 \sum_i \frac{1}{2m_i} \frac{\partial^2}{\partial x_i^2} + V(x_1, x_2, \dots, x_N) \quad (2)$$

where the particles may each have a different mass according to m_i . Because the coordinates of each particle are independent, the position-momentum commutator has the general form

$$[p_i, x_j] = -i \hbar \delta_{ij}. \quad (3)$$

The total momentum of the system has the same formal expression as in classical mechanics,

$$P_{\text{total}} = \sum_i p_i$$

and is conserved, as established in Gasiorowicz.

The system of particles is described by the wavefunction

$$\psi(x_1 \dots x_N; t) \quad (4)$$

The quantity $|\psi|^2$ gives the probability of finding all N particles at a set of specific locations ; if one wants the probability of finding particle 1 at location x_1 , irrespective of where the remaining particles are located, then one integrates over the positions of all remaining particles, as in

$$|\psi(x_1 \dots x_N; t)|^2 dx_2 \dots dx_N \tag{5}$$

If, for some reason, the motion of all the particles is independent, then $\psi(x_1 \dots x_N; t)$ can be written as a product of single-particle wavefunctions

$$\psi(x_1 \dots x_N; t) = \psi(x_1) \psi(x_2) \dots \psi(x_N) \quad \text{uncorrelated} \tag{6}$$

and the integration in Eq. (5) is trivial from the orthonormality of the solution set of wavefunctions.

Two-particle wavefunctions

As was described in PHYS 211, if the potential energy of a two-particle system is a function only of the separation between the particles, it may be more effective to replace the positions x_1 and x_2 by the cm and relative positions:

$$X_{cm} = (m_1 x_1 + m_2 x_2) / (m_1 + m_2) \tag{7}$$

and

$$x_{rel} = x_1 - x_2.$$

With this replacement, the arguments of the plane wave

$$k_1 x_1 + k_2 x_2 = K_{cm} X_{cm} + k_{rel} x_{rel}, \tag{8}$$

where the total and relative wavevectors are

$$K_{total} = k_1 + k_2 \quad \text{and} \quad k_{rel} = (m_2 k_1 - m_1 k_2) / (m_1 + m_2). \tag{9}$$

The total kinetic energy then becomes

$$E = (\hbar K_{total})^2 / 2M_{total} + (\hbar k_{rel})^2 / 2\mu. \tag{10}$$

Because the kinetic energy separates cleanly into two pieces, and the potential energy depends on relative separation, the wavefunction separates into a plane-wave part describing the cm, and a relative part which satisfies the Schrödinger equation with a reduced mass:

$$u(X_{cm}, x_{rel}) = \exp(iK_{cm} X_{cm}) \cdot \phi(x)$$

$$-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial x_{rel}^2} \phi(x_{rel}) + V(x_{rel})\phi(x_{rel}) = \varepsilon\phi(x_{rel}) \tag{11}$$

where the relevant energy is

$$\varepsilon = E - (\hbar K_{total})^2 / 2M_{total}. \tag{12}$$

Bosons and fermions

In Eq. (2), allowance is made for each particle to be different, having a different mass or other characteristics. But, at the microscopic level, we know that all members of a given class of particles are the same - all electrons are indistinguishable, all protons are indistinguishable *etc.* What impact does this have on the wavefunction of a many-particle system? Because particles of a given type are indistinguishable, one cannot say which particle is in what position. Thus, the wavefunction must be symmetric, or antisymmetric under exchange of particle label. That is, for particles 1 and 2, we must have

$$\psi(x_1, x_2, \dots, x_N; t) = \pm \psi(x_2, x_1, \dots, x_N; t) \quad (13)$$

The choice of \pm depends on whether the particle is a boson or fermion. For those students who did not take this in first year:

Among their other characteristics like mass and charge, elementary particles are labeled by a spin quantum number, quantized in units of $\hbar/2$, rather like angular momentum itself. (There are some important subtleties about the magnitude of the spin angular momentum to which we return in a few lectures!) For example, electrons and protons have spin $1/2$ (times \hbar) which pions have spin 0 and photons have spin 1. This applies even if the particles are otherwise structureless. Classified according to this spin label:

$$\begin{aligned} \text{spin label} = 0, 1, 2, \dots \text{ integers} &= \mathbf{bosons} \\ \text{spin label} = 1/2, 3/2, 5/2, \dots \text{ odd-integer}/2 &= \mathbf{fermions.} \end{aligned}$$

The symmetry of the wavefunction depends on the spin of the identical particles: under the exchange of particle labels:

bosons are symmetric
fermions are antisymmetric.

What this means for the labels (including the projection of the spin on an axis of quantization) is that

more than one boson can have the **same** set of labels
each fermion must have a unique label.

[If you try to assign the same label to two fermions, the antisymmetry of the wavefunction forces it to vanish *via* $\psi(x_1, x_2, \dots, x_N; t) = -\psi(x_2, x_1, \dots, x_N; t)$]. This is referred to as the Pauli Principle.

For a wavefunction with two particles, this implies

$$\begin{aligned} \psi^{\text{sym}}(1,2) &= [\psi(1,2) + \psi(2,1)] / N_{2S} \\ \psi^{\text{antisym}}(1,2) &= [\psi(1,2) - \psi(2,1)] / N_{2A}, \end{aligned} \quad (14)$$

where the (2 particle) normalization constants N_{2S} and N_{2A} must introduced in order to keep the complete wavefunction properly normalized; e.g.

$$|\psi^{sym}(1,2)|^2 dx_1 dx_2 = 1. \tag{15}$$

It's simple to antisymmetrize a two-particle wavefunction, but the form gets ever more cumbersome as the number of particles N increases. If the particles don't interact with each other, a compact expression for the antisymmetric wavefunction is provided by the **Slater determinant**:

$$u^{antisym}(1,2,\dots N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_{E_1}(x_1) & u_{E_1}(x_2) & \dots & u_{E_1}(x_N) \\ u_{E_2}(x_1) & u_{E_2}(x_2) & \dots & u_{E_2}(x_N) \\ \dots & \dots & \dots & \dots \\ u_{E_N}(x_1) & u_{E_N}(x_2) & \dots & u_{E_N}(x_N) \end{vmatrix} \tag{16}$$

where u_{E_i} are single particle wavefunctions. The completely symmetrized (bosonic) wavefunctions can be written formally like a determinant, but with all signs positive.

When is antisymmetrization important?

At what length scale is the symmetrization of the wavefunction important? In our everyday world, we don't see a correlation between the motion of an electron in a lab at UBC with one at SFU. Let's consider the behavior of the normalization constants in Eq. (14). The value of the normalization constant N_S or N_A is determined from

$$1 = \frac{1}{N_{S/A}^2} \int |\psi_a(x_1)\psi_b(x_2) \pm \psi_a(x_2)\psi_b(x_1)|^2 dx_1 dx_2$$

or

$$\begin{aligned} N_{S/A}^2 &= \int |\psi_a(x_1)\psi_b(x_2) \pm \psi_a(x_2)\psi_b(x_1)|^2 dx_1 dx_2 \\ &= 2 \int |\psi_a(x)|^2 dx \int |\psi_b(x)|^2 dx \pm 2 \left| \int \psi_a(x)\psi_b(x) dx \right|^2 \\ &= 2 \pm 2 \left| \int \psi_a(x)\psi_b(x) dx \right|^2 \end{aligned} \tag{17}$$

where each individual wavefunction is normalized to unity: $|\psi_a(x)|^2 dx = 1$. From the last line in (17), it is clear that the normalization constant will be changed from 2 only if there is significant spatial overlap of the two wavefunctions. Given the many wavefunctions decay exponentially with space (e.g., the free-particle wavepackets that we used, or the harmonic oscillator), the so-called overlap integral

$$\left| \int \psi_a(x)\psi_b(x) dx \right|^2$$

will be tiny for macroscopic separations. Gasiorowicz confirms this conclusion for one-particle probability distributions as well (p. 155).