Many Particle Systems - Non Interacting

We now wish to extend what has essentially been a one-body problem to the many-body problem. Let's return to the Lagrangian formalism for a moment.

Assume that we work with N particles with Cartesian coordinates $x_i^{(n)}$ $n=1,\dots N$, $i=1,\dots 3$. and corresponding velocities $\dot{x}_i^{(n)}$. The kinetic energy is then

$$T = \sum_{n=1}^{N} \frac{m_n}{2} \left|\dot{r}^{(n)}\right|^2 = \sum_{n=1}^{N}\sum_{i=1}^{3} \frac{1}{2} m_n \dot{x}_i^{(n)\,2} .$$

Suppose that we can decompose the potential energy as

$$V = \sum_{n=1}^{N} V_n + \frac{1}{2}\sum_{n=1}^{N}\sum_{l\neq n}^{N} V_{nl}$$

V_n: "external" force on particle n

V_{nl}: 2-particle interaction. Assume $V_{nl}=V_{ln}$

Now, we can differentiate this using Lagrange's equations to generate the appropriate equations of motion (3N equations in total):

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i^{(n)}}\right) = \frac{\partial L}{\partial x_i^{(n)}}$$

$$\Rightarrow \quad m_n \ddot{x}_i^{(n)} - \frac{\partial V_n}{\partial x_i^{(n)}} - \frac{\partial}{\partial x_i^{(n)}} \sum_{l\neq n}^{N} V_{nl} = 0$$

This is really $\frac{1}{2}\times 2$ from the second sum.

In classical mechanics, specifying $x_i^{(n)}$, $\dot{x}_i^{(n)}$ at some initial time $t=0$ implies that the time evolution of these variables can be determined from the equations of motion. Of course, this does not imply that the equations can be cleanly separated into a sum of 1-body equations (because of the coupling present in the V_{ne} term). There are certain forms for the interaction which allows the eq. of motion to be written as a separable set, after a coordinate transformation:

$V = \sum (x_{in} - x_{\ell})^2$ → separable under normal coordinate analysis.

Let's now take this over to the quantum case: Here, we need to construct the classical many-body Hamiltonian in the usual way. The only new feature is that the {commutation relations / Poisson brackets} can have indices referring to the particle #:

$$\left[\hat{x}_i^{(\ell)}, \hat{x}_j^{(n)}\right] = \left[\hat{p}_i^{(\ell)}, \hat{p}_j^{(n)}\right] = 0$$

$$\left[\hat{x}_i^{(\ell)}, \hat{p}_j^{(n)}\right] = \delta_{ij}\,\delta_{\ell n}\,\hat{1}\,i\hbar.$$

The Hamiltonian is, of course, the Hamiltonian of the whole system, so that

$$\hat{\mathcal{H}}\,|\epsilon_\alpha\rangle = \epsilon_\alpha\,|\epsilon_\alpha\rangle.$$

(ϵ_α = energy of the whole system.)

The position eigenkets can be written out as a product of single particle eigenkets since $[\hat{r}^{(k)}, \hat{r}^{(n)}] = 0$. That is, since

$$\hat{r}^{(k)} |r^{(1)} \ldots r^{(k)} \ldots r^{(N)}\rangle = r^{(k)} |r^{(1)} \ldots r^{(k)} \ldots r^{(N)}\rangle$$

$$\Rightarrow |r^{(1)} \ldots r^{(k)} \ldots r^{(N)}\rangle = |r^{(1)}\rangle |r^{(2)}\rangle \ldots |r^{(N)}\rangle.$$

Now, just as the single particle eigenket $|\beta\rangle$ was expressed in terms of a wavefunction ψ_β:

$$|\beta\rangle = \int dr \psi_\beta(r) |r\rangle \quad \text{with } \psi_\beta(r) = \langle r|\beta\rangle$$

so too:

$$|\beta\rangle_{\substack{\text{many}\\\text{body}}} = \int_N \cdots \int_1 dr^{(1)} \ldots dr^{(N)} \underbrace{\psi_\beta(r^{(1)} \ldots r^{(N)})}_{\text{many body wavefunction}} |r^{(1)} \ldots r^{(N)}\rangle$$

must integrate over all coordinates.

and

$$\psi_\beta(r^{(1)} \ldots r^{(N)}) = \langle r^{(1)} \ldots r^{(N)}|\beta\rangle.$$

Where we must begin to modify our single particle results is where we deal with identical particles. In a classical system, we can track particles from one point to another over time, and it often makes sense to ascribe a set of labels to the particles. Quantum mechanically, this procedure is more difficult since successive position measurements don't yield smooth motion.

Hence, if the particles are distinguishable (by mass, quantum number etc.) then the continuity problem does not do anything to the wavefunctions. However, for systems of identical particles, there is a problem. Suppose that we have a total wavefunction

$$\psi(1,2,\cdots l \cdots n \cdots N)$$

Then, if the particles are indistinguishable,

$$\psi(1,2\cdots n \cdots l \cdots N)$$

is just as appropriate. Which do we choose? It is worthwhile introducing a permutation operator $\hat{P}^{ln}$ such that

$$\hat{P}^{ln}\,\hat{A}(1,2\cdots l\cdots n\cdots N) = \hat{A}(1,2\cdots n\cdots l\cdots N)\hat{P}^{ln}$$

This definition is much like the parity operator's definition. By similar reasoning to $\hat{P}$, we can show that $\hat{P}^{ln}$ has eigenvalues ± 1. So:

$$\hat{P}^{ln}\,\psi^S(\cdots l\cdots n\cdots) = +\psi^S(\cdots n\cdots l\cdots)$$
$$\hat{P}^{ln}\,\psi^A(\cdots l\cdots n\cdots) = -\psi^A(\cdots n\cdots l\cdots).$$

symmetric / antisymmetric

[Note that $\hat{P}^{ln}$ does not generally commute among themselves: $\hat{P}^{12}\hat{P}^{23} \neq \hat{P}^{23}\hat{P}^{12}$.]

So, for any given N identical particle system, there are $N!$ ways of permuting the particle labels.

Hence, there are $N!$ possible wavefunctions. How do we combine these into one overall wavefunction? The rules turn out to be simple:

a) Bosons – particles with integer spin in units of $\hbar$.
– ψ is totally symmetric under $\hat{P}_{ln}$.

b) Fermions – particles with half-odd-integer spin (in $\hbar$)
– ψ is totally antisymmetric under $\hat{P}_{ln}$.

The nature of ψ for fermions leads immediately to the Pauli exclusion principle if we write out ψ in terms of position kets and set $r^{(l)} = r^{(n)} = r$:

$$\psi^A(1,2\cdots r\cdots r\cdots) = -\psi^A(1,2\cdots r\cdots r\cdots)$$
$$= 0.$$

In other words, the probability of finding any two identical [i.e. all the same quantum numbers] fermions at the same point in space is zero.

Ideal Systems

Let us now consider systems subject only to an external potential, which may be different for each particle.

i) Distinguishable particles:

$$\hat{\mathcal{H}}\psi_\alpha = \left\{\sum_{n=1}^{N} -\frac{\hbar^2}{2m^{(n)}}\nabla^2_{(n)} + V^{(n)}(r^{(n)})\right\}\psi_\alpha(r_1^{(1)}\cdots r^{(N)})$$
$$= E_\alpha \psi_\alpha$$

(potential felt by particle n.)

Since there are no cross terms through $V^{(N)}$, we expect that ψ can be written as

$$\psi_\alpha = \psi_i^{(1)}(r^{(1)}) \cdots \psi_j^{(N)}(r^{(N)})$$

so that the many body S.E. separates into

$$\left\{ -\frac{\hbar^2}{2m^{(n)}} \nabla^{(n)2} + V^{(n)} \right\} \psi_i^{(n)}(r^{(n)}) = \epsilon_i^{(n)} \psi_i^{(n)}(r^{(n)})$$

n labels particle in those states.

i labels set of single particle states, super n because each set has a different $V^{(n)}$

and

$$\epsilon_\alpha = \sum_{n=1}^{N} \epsilon_i^{(n)}$$

i.e. ϵ_i of n^{th} particle.

Example: Two distinguishable spinless particles of mass $m^{(1)}$ & $m^{(2)}$ in a 1-D well of width a.

$$\left[\left\{ -\frac{\hbar^2}{2m^{(1)}} \frac{d^2}{dx^{(1)2}} - \frac{\hbar^2}{2m^{(2)}} \frac{d^2}{dx^{(2)2}} + \left\{ V^{(1)} + V^{(2)} \right\} \right] \psi_\alpha(x^{(1)}, x^{(2)}) = \epsilon_\alpha \psi_\alpha(x^{(1)} x^{(2)})$$

$V^{(1)} = V^{(2)} = 0 \qquad 0 \le x \le a$

$V^{(1)} = V^{(2)} = \infty \qquad$ otherwise.

Writing $\psi_\alpha = \psi_\ell(x^{(1)}) \psi_{\ell'}(x^{(2)})$

the equation separates into the usual solutions

$$\psi_\ell(x) = \left(\frac{2}{a}\right)^{1/2} \sin \frac{\ell \pi}{a} x \qquad \epsilon_\ell = \frac{\hbar^2}{2m} \frac{\pi^2}{a^2} \ell^2 .$$

$$\Rightarrow \psi_\alpha = \frac{2}{a} \sin\frac{l\pi}{a}x^{(1)} \cdot \sin\frac{l'\pi}{a}x^{(2)}$$

$$E_\alpha = \frac{\hbar^2\pi^2}{2a^2}\left(\frac{l^2}{m^{(1)}} + \frac{l'^2}{m^{(2)}}\right).$$

A particular choice of n, n' is referred to as a configuration

ii) Indistinguishable particles.

Example

Suppose now that the particles are indistinguishable. Then all of the single particle S.E.'s become

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right\}\psi_i(r) = E_i\,\psi_i(r)$$

The overall wavefunction is now a product, as before, but must be symmetric or antisymmetric:

$$\psi_\alpha = \frac{1}{\sqrt{2}}\left\{\frac{2}{a}\sin\frac{l\pi}{a}x^{(1)}\sin\frac{l'\pi}{a}x^{(2)} \pm \frac{2}{a}\sin\frac{l\pi}{a}x^{(2)}\sin\frac{l'\pi}{a}x^{(1)}\right\}$$

(+ for bosons, − for fermions)

Show how cross terms go away in $\frac{1}{2}\langle \psi_1'\psi_2 \pm \psi_2'\psi_1 | \hat{k}_1 + \hat{k}_2 | \psi_1'\psi_2 \pm \psi_2'\psi_1 \rangle$ if orthogonal.

Example

Finally, let us just look at plane wave solutions with no potential:

$$\psi = e^{ikx_1}e^{ik'x_2} \pm e^{ikx_2}e^{ik'x_1} \quad \text{(ignoring normalization)}$$

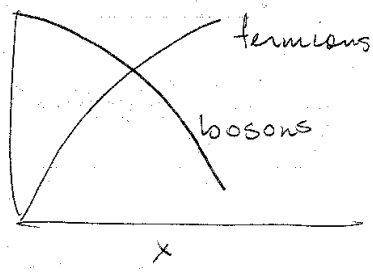
$$= e^{i(k+k')X}\left[e^{i(k-k')x/2} \pm e^{-i(k-k')\frac{x}{2}}\right]$$

where $X = \frac{1}{2}(x_1 + x_2)$ = position of cm.
$x = x_2 - x_1$ = relative coordinate.

What happens to $|\psi|^2$ at small x?

$$|\psi^S|^2 = \cos^2\left(\frac{k+k'}{2}x\right)$$

$$|\psi^A|^2 = \sin^2\left(\frac{k+k'}{2}x\right)$$



In other words, the probability of finding two fermions at small relative x is suppressed while that for bosons is enhanced.

Odds & Ends

Operators: it is often convenient to define a symmetrization operator $\hat{\mathcal{S}}$ and antisymmetrization operator $\hat{\mathcal{A}}$ for constructing states:

$$\psi^S = \frac{1}{(N!)^{1/2}}\hat{\mathcal{S}}\,\psi_i(r^{(1)})\cdots\psi_j(r^{(N)})$$

$$\psi^A = \frac{1}{(N!)^{1/2}}\hat{\mathcal{A}}\,\psi_i(r^{(1)})\cdots\psi_j(r^{(N)})$$

Slater Determinant: The form of ψ generated by $\hat{\mathcal{A}}$ is

$$\psi^A = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_i(r^{(1)}) & \cdots & \psi_j(r^{(1)}) \\ \vdots & & \\ \psi_i(r^{(N)}) & \cdots & \psi_j(r^{(N)}) \end{vmatrix}$$

← Determinant
This satisfies Pauli exclusion immediately since det. vanishes if $i=j$ or $r^{(k)} = r^{(n)}$ anywhere.