III.) Three Dimensions - Central Potentials

Wave Mechanics for N-distinguishable particles of unequal masses $m_1, m_2, \ldots, m_N$. All information about the system is contained in the multi-particle wave function (state of system)

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; t).$$

In Particular

$$dP(t) = |\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; t)|^2 d^3r_1 \cdots d^3r_N$$

is the probability that the particle 1 with mass m_1 is found in volume d^3r_1 about $\vec{r}_1$, <u>and</u> particle 2 with mass m_2 is found in volume d^3r_2 about $\vec{r}_2$, <u>and</u> so on.

The time evolution of the multiparticle state is given by the Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; t)$$
$$= \left[\sum_{i=1}^{N} \frac{-\hbar^2}{2m_i} \nabla_i^2 + V(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; t) \right] \Psi(\vec{r}_1, \ldots, \vec{r}_N; t).$$

III.) In particular, consider the 2-body system with the particles interacting through a central potential, that is a "force" that only depends on the distance between them:

$$\boxed{V(\vec{r}_1, \vec{r}_2; t) \equiv V(|\vec{r}_1 - \vec{r}_2|)}$$

The Schrödinger equation for the 2-body wavefunction

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}_1, \vec{r}_2; t) = H \psi(\vec{r}_1, \vec{r}_2; t)$$

with the Hamiltonian given by

$$H = \frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} + V(|\vec{r}_1 - \vec{r}_2|)$$

$$= -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(|\vec{r}_1 - \vec{r}_2|).$$

As in classical mechanics introduce the center of mass coordinates

$$\vec{R} \equiv \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2} = \text{position of center of mass}$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2 = \text{relative coordinate}$$

III.) As usual we can invert this

$$\vec{r}_1 = \vec{R} + \frac{m_2}{m_1+m_2}\vec{r}$$

$$\vec{r}_2 = \vec{R} - \frac{m_1}{m_1+m_2}\vec{r}.$$

Also use the chain rule to relate $\vec{R}, \vec{r}$ derivatives to $\vec{r}_1, \vec{r}_2$ derivatives

$$\vec{\nabla}_{r_1} = \vec{\nabla}_r + \frac{m_1}{m_1+m_2}\vec{\nabla}_R$$

$$\vec{\nabla}_{r_2} = -\vec{\nabla}_r + \frac{m_2}{m_1+m_2}\vec{\nabla}_R$$

ex.

$$\vec{\nabla}_{r_1} = \left\{\begin{array}{l} \dfrac{\partial}{\partial x_1} = \dfrac{\partial x}{\partial x_1}\dfrac{\partial}{\partial x} + \dfrac{\partial X}{\partial x_1}\dfrac{\partial}{\partial X} \\ \dfrac{\partial}{\partial y_1} = \dfrac{\partial y}{\partial y_1}\dfrac{\partial}{\partial y} + \dfrac{\partial Y}{\partial y_1}\dfrac{\partial}{\partial Y} \\ \dfrac{\partial}{\partial z_1} = \dfrac{\partial z}{\partial z_1}\dfrac{\partial}{\partial z} + \dfrac{\partial Z}{\partial z_1}\dfrac{\partial}{\partial Z} \end{array}\right\} = \vec{\nabla}_r + \frac{m_1}{m_1+m_2}\vec{\nabla}_R$$

where we used

$$\vec{r}_1 = x_1\hat{i} + y_1\hat{j} + z_1\hat{k}$$
$$\vec{r}_2 = x_2\hat{i} + y_2\hat{j} + z_2\hat{k}$$

and

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$$
$$\vec{R} = X\hat{i} + Y\hat{j} + Z\hat{k}.$$

- III.) Again we can invert the derivative expressions to obtain

$$\vec{\nabla}_R = \vec{\nabla}_{r_1} + \vec{\nabla}_{r_2}$$

$$\vec{\nabla}_r = \frac{m_2}{m_1+m_2}\vec{\nabla}_{r_1} - \frac{m_1}{m_1+m_2}\vec{\nabla}_{r_2} .$$

Now the momentum operators are just given by these derivatives

$$\vec{p}_1 = \frac{\hbar}{i}\vec{\nabla}_{r_1} \quad ; \quad \vec{p}_2 = \frac{\hbar}{i}\vec{\nabla}_{r_2}$$

and we define

$$\vec{P} \equiv \frac{\hbar}{i}\vec{\nabla}_R \quad ; \quad \vec{p} \equiv \frac{\hbar}{i}\vec{\nabla}_r$$

we see that the chain rule results in the usual center of momentum formulae

$$\vec{p}_1 = \vec{p} + \frac{m_1}{m_1+m_2}\vec{P}$$

$$\vec{p}_2 = -\vec{p} + \frac{m_2}{m_1+m_2}\vec{P}$$

and inverting $\quad \vec{P} = \vec{p}_1 + \vec{p}_2$

$$\vec{p} = \frac{m_2}{m_1+m_2}\vec{p}_1 - \frac{m_1}{m_1+m_2}\vec{p}_2 .$$

II.) So let's re-express the Hamiltonian in the CM system:

$$\vec{p}_1\cdot\vec{p}_1 = \vec{p}\cdot\vec{p} + \frac{m_1^2}{(m_1+m_2)^2}\vec{P}\cdot\vec{P} + \frac{2m_1}{m_1+m_2}\vec{p}\cdot\vec{P}$$

$$\vec{p}_2\cdot\vec{p}_2 = \vec{p}\cdot\vec{p} + \frac{m_2^2}{(m_1+m_2)^2}\vec{P}\cdot\vec{P} - \frac{2m_2}{m_1+m_2}\vec{p}\cdot\vec{P}$$

$\Rightarrow$

$$\frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} = \left(\frac{1}{m_1}+\frac{1}{m_2}\right)\frac{1}{2}\vec{p}^{\,2} + \frac{m_1+m_2}{2(m_1+m_2)^2}\vec{P}^{\,2}$$

$$+\cancel{\frac{1}{2m_1}\left(\frac{2m_1}{m_1+m_2}\right)\vec{p}\cdot\vec{P}} - \cancel{\frac{1}{2m_2}\left(\frac{2m_2}{m_1+m_2}\right)\vec{p}\cdot\vec{P}}$$

Define: Total mass $= M \equiv m_1 + m_2$

Reduced mass $= m \equiv \dfrac{m_1 m_2}{m_1+m_2}$

i.e. $\dfrac{1}{m} = \dfrac{1}{m_1} + \dfrac{1}{m_2}$

We finally obtain

$$\boxed{\frac{\vec{p}_1^{\,2}}{2m_1} + \frac{\vec{p}_2^{\,2}}{2m_2} = \frac{\vec{p}^{\,2}}{2m} + \frac{\vec{P}^{\,2}}{2M}}$$

III.) Since $V = V(|\vec{r}_1 - \vec{r}_2|) = V(|\vec{r}|)$
the Hamiltonian for the 2-body system becomes

$$H = \frac{\vec{P}^2}{2M} + \frac{\vec{p}^2}{2m} + V(|\vec{r}|)$$

$$= -\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2m}\nabla_r^2 + V(|\vec{r}|)$$

So the Schrödinger equation for the 2 particle system in the CM coordinates is

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{R},\vec{r};t) = H\psi(\vec{R},\vec{r};t)$$

where we have used $\psi(\vec{r}_1,\vec{r}_2;t) \to \psi(\vec{R},\vec{r};t)$

As in the 1 particle system, V is time independent hence we can solve the time dependent Sch. eq. by separation of the time and space parts of the wavefunction

Ansatz:

$$\psi(\vec{R},\vec{r};t) \equiv \psi(\vec{R},\vec{r})\, e^{-i\frac{E_T}{\hbar}t}$$

and the stationary state has total energy E_T, III.) and the time independent Sch. eq. for the energy eigenfunction becomes

$$H\,\psi(\vec{R},\vec{r}) = E_T\,\psi(\vec{R},\vec{r}) .$$

Further the potential only depends on the relative coordinate, so we expect the CM to move as a free particle —

Ansatz 2: Separation of CM and relative coordinate wavefunctions

$$\psi(\vec{R},\vec{r}) \equiv \psi_{CM}(\vec{R})\,\psi(\vec{r}) .$$

Plug into time indep. Sch. Eq.

$$\left(-\frac{\hbar^2}{2M}\nabla_R^{\,2}\,\psi_{CM}(\vec{R})\right)\psi(\vec{r})$$

$$+\left(-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})\right)\psi_{CM}(\vec{R}) + \left(V(|\vec{r}|)\psi(\vec{r})\right)\psi_{CM}(\vec{R})$$

$$= E_T\,\psi_{CM}(\vec{R})\,\psi(\vec{r})$$

III.) Divide eq. by $\frac{1}{\psi(\vec{R},\vec{r})} = \frac{1}{\psi_{CM}(\vec{R})}\frac{1}{\psi(\vec{r})}$

$\Rightarrow$

$$\underbrace{\frac{1}{\psi_{CM}(\vec{R})}\left[-\frac{\hbar^2}{2M}\nabla_R^2\psi_{CM}(\vec{R})\right]}_{\substack{\text{function of } R \text{ only} \\ \equiv E_{CM} \ (= \text{separation constant})}} + \underbrace{\frac{1}{\psi(\vec{r})}\left[-\frac{\hbar^2}{2m}\nabla_r^2 + V(|\vec{r}|)\right]\psi(\vec{r})}_{\substack{\text{function of } \vec{r} \text{ only} \\ \equiv E \ (= \text{Separation constant})}} = \underbrace{E_T}_{\text{constant}}$$

Thus the 2-body problem reduces to

1) $$-\frac{\hbar^2}{2M}\nabla_R^2\psi_{CM}(\vec{R}) = E_{CM}\,\psi_{CM}(\vec{R})$$

2) $$\left[-\frac{\hbar^2}{2m}\nabla_r^2 + V(|\vec{r}|)\right]\psi(\vec{r}) = E\,\psi(\vec{r})$$

3) $E_T = E_{CM} + E$, where E_T is the total energy of the 2-body system, E_{CM} is the energy of the center of mass,

-III.) and E is the energy of relative motion of the 2-particles (ex., their binding energy).

Just as in classical mechanics, the center of mass moves as a free particle of mass M, the total mass of the system, with energy E_{CM}. The center of mass wave function is given by a plane wave:

$$\psi_{CM,\vec{K}}(\vec{R}) = e^{i\vec{K}\cdot\vec{R}}$$

with

$$E_{CM} = \frac{\hbar^2 \vec{K}^2}{2M}$$ and we

use continuum normalization for ψ_{CM}

$$\int \frac{d^3R}{(2\pi)^3}\, \psi^*_{CM,\vec{K}'}(\vec{R})\, \psi_{CM,\vec{K}}(\vec{R}) = \delta^3(\vec{K}-\vec{K}').$$

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and they are complete

$$\int \frac{d^3K}{(2\pi)^3}\, \psi^*_{CM,\vec{K}}(\vec{R}')\, \psi_{CM,\vec{K}}(\vec{R}) = \delta^3(\vec{R}-\vec{R}')$$

III.) Finally, the Schrödinger equation for the relative motion wavefunction can be studied (denote ∇_r^2 by ∇^2 now)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(|\vec{r}|)\right]\psi(\vec{r}) = E\,\psi(\vec{r})$$

This is just the Schrödinger equation for a particle of mass m moving in the central potential $V = V(|\vec{r}|)$.

A.) Spherical Polar Coordinates and Separation of Variables

Since the interaction of the (relative) particle with the potential only depends of the magnitude $|\vec{r}|$ of the position coordinate we can imagine that the motion in the other directions with $|\vec{r}|$ fixed should separate from the $|\vec{r}|$ radial motion — This is readily seen by using spherical polar coordinates: