III. Central Potential Problem

3.1 The 2-body Problem and the C-M Frame

Up to now we have been considering the quantum mechanics of a single particle moving in a potential. The wave mechanics framework readily generalizes to describe a system comprised of N (distinguishable) particles of unequal masses $m_1, m_2, \ldots, m_N$. All information about the system is contained in the multi-particle wavefunction

$$\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; t).$$ 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 $\vec{r}_1$, and particle 2 with mass m_2 is found in volume d^3r_2 about $\vec{r}_2$ and so on. The time evolution of the multiparticle state is given by the Schrödinger equation

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

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

Of particular interest is ~~the~~ two particle system with the particles interacting through a central potential, that is a force that only depends upon the distance between the particles $V(\vec{r}_1, \vec{r}_2; t) = V(|\vec{r}_1 - \vec{r}_2|)$. The Schrödinger equation for the 2-body wavefunction's time development becomes

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

with the Hamiltonian H given as

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

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

As usual we introduce center of mass coordinates

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

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

These can be inverted to yield

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

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

Further we can use the chain rule to relate the $\vec{R}$ and $\vec{r}$ derivatives to the $\vec{r}_1$ and $\vec{r}_2$ derivatives

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

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

i.e.

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

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

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

Again inverting the derivatives we have

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

Recalling that the momentum operators are given by these derivatives

$$\vec{P} \equiv -i\hbar\vec{\nabla}_R \quad ; \quad \vec{p} \equiv -i\hbar\vec{\nabla}_r$$
$$\vec{p}_1 = -i\hbar\vec{\nabla}_{r_1} \quad , \quad \vec{p}_2 = -i\hbar\vec{\nabla}_{r_2}$$

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

The Hamiltonian will take a simpler form in the CM system. Note that

$$\vec{p}_1\cdot\vec{p}_1 = \vec{p}\cdot\vec{p} + \frac{m_1^2}{(m_1+m_2)^2}\vec{P}\cdot\vec{P} + \frac{2m_1}{m_1+m_2}\vec{p}\cdot\vec{P}$$
$$\vec{p}_2\cdot\vec{p}_2 = \vec{p}\cdot\vec{p} + \frac{m_2^2}{(m_1+m_2)^2}\vec{P}\cdot\vec{P} - \frac{2m_2}{m_1+m_2}\vec{p}\cdot\vec{P}$$

so that the kinetic energy of the 2body system becomes

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

Defining the total mass of the 2-body system as $M \equiv m_1+m_2$ and the reduced mass $m \equiv \dfrac{m_1 m_2}{m_1+m_2}$, that is

$$\frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2} \, ,$$ this becomes

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

Since $V = V(|\vec{r}_1 - \vec{r}_2|) = V(|\vec{r}|)$, the Hamiltonian in the CM coordinates becomes

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

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

The Schrödinger equation for the 2-particle system in the CM coordinates is

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

Since the potential is independent of the time we seek a stationary state solution

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

Hence the time independent Schrödinger equation is obtained

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

Further, since the potential only depends on the relative coordinate, we solve this equation by separation of variables

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

Substituting into the Schrödinger equation and dividing by $\psi(\vec{R},\vec{r})$ we have

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

Thus we obtain

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

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

with $E_T = E_{CM} + E$, E_T is the

total energy of the 2-body system, while E_{CM} is the energy of the center of mass and E is the energy of relative motion of the two particles (for example, their binding energy).

Just as in classical mechanics, the center of mass moves as a free particle of mass M with energy E_{CM}. The center of mass wavefunction is given by

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

with $E_{CM} = \frac{\hbar^2 \vec{K}^2}{2M}$ and we have used continuum normalization for ψ_{CM}

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

Finally the Schrödinger equation for the relative motion wavefunction can be studied (denoting ∇_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 $V=V(|\vec{r}|)$.