Appendix F

N-particle Systems: Quantum Mechanical Viewpoint

- $\hat{H}$: describes the N-particle system
- Generally, the N particles (in Volume V) interact. They may also be under the influence of an external potential that acts on everyone of the particles.
- Thus, in general

$$\hat{H}(\vec{x}_1,\ldots,\vec{x}_N;\vec{p}_1,\ldots,\vec{p}_N) = \hat{H}(\{x_i,p_i\})$$

$$= \underbrace{\sum_{i=1}^{N}\Big(\underbrace{\frac{\vec{p}_i^{\,2}}{2m}}_{\text{k.e. of particle } i} + \underbrace{V(\vec{x}_i)}_{\text{p.e. of particle } i}\Big)}_{\substack{\text{single-particle hamiltonian}\\ \text{(particle } i)}} + \underbrace{\sum_{\substack{\text{distinct pairs}\\ \text{of particles } i\,\&\,j}} \underbrace{U(\vec{x}_i,\vec{x}_j)}_{\substack{\text{interaction}\\ \text{between particles}\\ i\,\&\,j}}}$$

$$= \sum_{i=1}^{N} \hat{h}_i + \sum_{\text{pairs }(i,j)} U(\vec{x}_i,\vec{x}_j)$$

$\underbrace{\text{(N-particle Hamiltonian)}}_{\text{a many-body problem}}$

The question of "what are the allowed energies in the N-particle system" is answered by solving the Schrödinger Equation.

$$\boxed{\hat{H}(\{x_i,p_i\})\,\psi(\vec{x}_1,\ldots,\vec{x}_N) = E\;\psi(\vec{x}_1,\ldots,\vec{x}_N)}$$

- An eigenvalue problem
- E is in general discrete (i.e. not all E values are allowed)
- For an (allowed) eigenvalue (energy) E, there could be different states (different $\psi(\vec{x}_1,\ldots,\vec{x}_N)$) corresponding to the same E.

$$\boxed{\#\text{ different states with } E = \text{Degeneracy of eigenvalue } E}$$

Recall: $W(E,V,N)$ = # microstates (# different states) of energy E

$\therefore$ $\boxed{W(E,V,N) \text{ is the degeneracy at energy } E}$

Pictorially,

energy	states	degeneracy
⋮		
E_7		
E_6	⋮	⋮
E_5		
E_4	$\psi_{E_4}^{(1)}, \psi_{E_4}^{(2)}, \cdots, \psi_{E_4}^{(W(E_4))}$	$W_S(E_4,N,V)$
E_3	⋮	⋮
E_2		
E_1	$\psi_{E_1}^{(1)}, \psi_{E_1}^{(2)}, \cdots \psi_{E_1}^{(W(E_1))}$	$W_S(E_1,N,V)$

allowed energy LEVELS

implicit V-dependence

degenerate eigenstates (STATES)

$W_S(E_1,N,V)$ of them corresponding to E_1

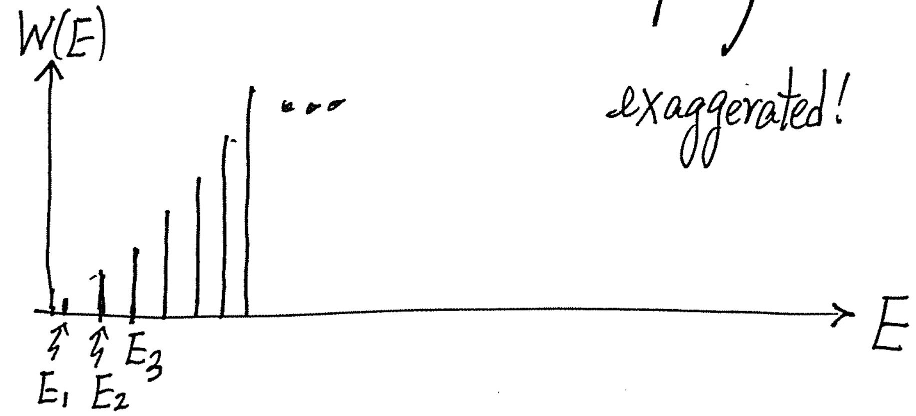
"system" (N-particle system)

degeneracy of energy E_1

For macroscopic system, $W(E_1)^{+}$ varies with E_1 rapidly!

Remarks:

- In general, $E_1, E_2, \cdots, E_6, E_7, \cdots$ take on discrete values and $W(E_i)$ increases rapidly with E_i:



But we want to take $\frac{\partial}{\partial E} \ln W(E)$!

- Don't worry, be practical!

  Macroscopic systems (not an atom or a molecule) give densely packed allowed energies (thus almost continuous)

- Still not happy?

  OK! Take an interval ΔE on energy axis and consider # different states in the interval E to $E+\Delta E$, and it gives a continuous function to work on!

- What are single-particle states?

If the particles do not interact with each other, then $U(\vec{x}_i;\vec{x}_j)=0$ [or weak enough to be ignored]

$$\hat{H}(\{x_i,p_i\}) = \sum_{i=1}^{N} \hat{h}_i = \sum_{i=1}^{N}\underbrace{\left(\frac{p_{ix}^2}{2m}+\frac{p_{iy}^2}{2m}+\frac{p_{iz}^2}{2m}+V(\vec{x}_i)\right)}_{\text{has to do with } i^{th} \text{ particle only}}$$

single-particle hamiltonian

$$\boxed{\text{The quantum problem is separable into single-particle problems!}}$$

All we need to solve is:

$\hat{h}\psi = \varepsilon\psi$ or $\left[\frac{p_x^2}{2m}+\frac{p_y^2}{2m}+\frac{p_z^2}{2m}+V(x,y,z)\right]\psi(x,y,z) = \varepsilon\,\psi(x,y,z)$

single-particle hamiltonian

or $\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x}) + V(\vec{x})\psi(\vec{x}) = \varepsilon\,\psi(\vec{x})}$

single-particle Schrödinger equation

single-particle energies

single-particle states

Thus an easier problem!

But! After solving for $\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_7, \varepsilon_8, \cdots$ and the single-particle states (degeneracies), you need to fill these states with N particles.

- The filling depends on ...
  - particles are fermions or bosons?
  - under what conditions we could ignore the fermionic/bosonic nature of particles?

To handle this problem, the occupation number representation (see Ch. III) is useful.