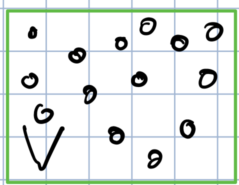
INTRO: MANY-BODY PROBLEM (IN EQUILIBRIUM)

$N \simeq 10^{23}$ particles at fixed (say) (T, V) $(N \gg 1 \rightarrow N \rightarrow \infty)$

Microscopic description $\hat{H}(\{\hat{r}_i, \hat{p}_i\}_{i=1}^{N}) \longrightarrow$ Macroscopic description

T



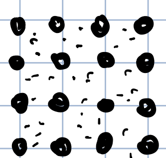
$p(T, V, N)$, $\vec{j}(T, V, N, \vec{E})$, ...

(thermodynamic and transport properties)

EXAMPLE (PROTOTYPE) MANY-BODY HAMILTONIAN

e.g. metallic material

lattice of ions + electrons



$$H_e = \sum_i \frac{\bar{p}_i^2}{2m} + \sum_{i<j} V_{ee}(\bar{r}_i - \bar{r}_j)$$

$$H_i = \sum_I \frac{\bar{P}_I^2}{2M} + \sum_{I<J} V_{ii}(\bar{R}_J - \bar{R}_I)$$

$$H_{ei} = \sum_{i,I} V_{ei}(\bar{R}_I - \bar{r}_i)$$

$$H = H_e + H_i + H_{ei}$$

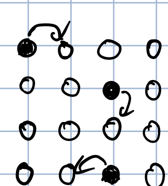
(certain elements, e.g. lattice structure put in "by hand").

- Not fully realistic (spin, impurities...)
- Valid only down to some length scale (e.g. does not resolve ions' structure)
- Valid only up to some energy scale (too high T → lattice melts...)

→ "Ab initio" approaches (take H as it is...) ⟶ numerics

→ Simplify the model to capture most essential elements related to certain phenomenology

"Reduced" hamiltonian → example (2d Hubbard model)

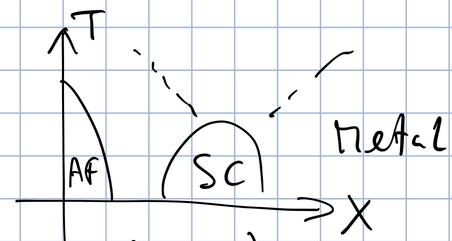


$$\hat{H} = \sum_{i,j,\sigma} t_{ij}\, c_{j\sigma}^{+} c_{i\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$ (electrons on a lattice)

- Almost exclusively approximate approaches (out of exact control)
- Many open questions
- (Supposed-to-be) effective model for Cu-based high-T_c superconductors

What do we mean by "solve the model"?

$\hat{H}$



(Phase diagram)

(among other things)

QM of many-particle systems (nonrelativistic)

States

System of N identical particles, allowed to move. For the time being forget about internal degrees of freedom (like spin).

Use position representation. For $N=1$ the system state is described by a wavefunction $\psi(\bar{r})$; $|\psi(\bar{r})|^2 d^3r \to$ probability ...

Natural generalization: $\psi(\bar{r}) \xrightarrow{N>1} \psi(\bar{r}_1, \bar{r}_2, \dots, \bar{r}_N)$ such that

$$|\psi(\bar{r}_1, \bar{r}_2 \dots \bar{r}_N)|^2 \prod_{i=1}^{N} d^3 r_i = \left(\begin{array}{l}\text{probability of finding } N \\ \text{particles in the volume} \\ \prod_i d^3 r_i \text{ around the point} \\ (\bar{r}_1 \dots \bar{r}_N) \text{ in the 3N-dimensional} \\ \text{configurational space.}\end{array}\right)$$

verified experimentally

However: indistinguishability of particles $\Longrightarrow$ constraints on $\psi(\bar{r}_1 \dots \bar{r}_N)$

e.g. $\psi(\bar{r}_1, \bar{r}_2)$ and $\psi(\bar{r}_2, \bar{r}_1)$ represent the same state.

Indistinguishability $\longmapsto$ permuting the arguments of ψ does not change the system state.

$$\psi(\bar{r}_1 \dots \bar{r}_j \dots \bar{r}_k \dots \bar{r}_N) = \lambda\, \psi(\bar{r}_1 \dots \bar{r}_k \dots \bar{r}_j \dots \bar{r}_N) = \lambda^2 \psi(\bar{r}_1 \dots \bar{r}_j \dots \bar{r}_k \dots \bar{r}_N)$$
$$(|\lambda| = 1)$$

$\Longrightarrow \lambda^2 = 1$, $\lambda = \pm 1$

$\lambda = +1$ – bosons
$\lambda = -1$ – fermions

Remark: bosons $\to s \in \mathbb{N}$, fermions $\to s \in \frac{1}{2} + \mathbb{N}$ (requires relativistic QFT)

For fermions: $\bar{r}_j = \bar{r}_k \Longrightarrow \psi = 0$ (Pauli exclusion principle)

Basis Forget indistinguishibility for a while.

$\{\psi_\nu(\bar{r})\}$ - orthonormal basis for 1-particle states $\quad (\psi_\nu(\bar{r}) = \langle \bar{r} | \nu \rangle)$

We use $\{\psi_\nu(\bar{r})\}$ to construct a basis for N-particle states

Take $\psi(\bar{r}_1 \dots \bar{r}_N)$ (N-particle state)

For a given ν_1 define $A_{\nu_1}(\bar{r}_2 \dots \bar{r}_N) = \int d^3 r_1 \, \psi^*_{\nu_1}(\bar{r}_1) \psi(\bar{r}_1 \dots \bar{r}_N)$

Knowing the set $\{A_{\nu_1}(\bar{r}_2 \dots \bar{r}_N)\}$ we may recover $\psi(\bar{r}_1 \dots \bar{r}_N)$:

$$\psi(\tilde{\bar{r}}_1, \bar{r}_2 \dots \bar{r}_N) = \sum_{\nu_1} \psi_{\nu_1}(\tilde{\bar{r}}_1) A_{\nu_1}(\bar{r}_2 \dots \bar{r}_N)$$

This is because $\sum_{\nu_1} \psi_{\nu_1}(\tilde{\bar{r}}_1) \int d^3 r_1 \, \psi^*_{\nu_1}(\bar{r}_1) \psi(\bar{r}_1 \dots \bar{r}_N) = \int d^3 r_1 \underbrace{\sum_{\nu_1} \psi^*_{\nu_1}(\bar{r}_1) \psi_{\nu_1}(\tilde{\bar{r}}_1)}_{= \delta(\bar{r}_1 - \tilde{\bar{r}}_1)} \psi(\bar{r}_1 \dots \bar{r}_N) = \psi(\tilde{\bar{r}}_1, \bar{r}_2 \dots \bar{r}_N)$

Recall the Dirac delta representation:

$$\psi(\bar{r}) = \langle \bar{r} | \psi \rangle = \langle \bar{r} | \sum_\nu |\nu\rangle \langle \nu | \psi \rangle = \sum_\nu \psi_\nu(\bar{r}) \int d^3 r' \, \psi^*_\nu(\bar{r}') \psi(\bar{r}')$$

$$\int d^3 r' |\bar{r}'\rangle \langle \bar{r}'|$$

$$\Rightarrow \psi(\bar{r}) = \int d^3 r' \underbrace{\left(\sum_\nu \psi^*_\nu(\bar{r}') \psi_\nu(\bar{r}) \right)}_{\Longrightarrow \; = \delta(\bar{r} - \bar{r}')} \psi(\bar{r}')$$

Iterate: $A_{\nu_1 \nu_2}(\bar{r}_3 \dots \bar{r}_N) = \int d^3 r_2 \, \psi^*_{\nu_2}(\bar{r}_2) A_{\nu_1}(\bar{r}_2 \dots \bar{r}_N)$

This is again invertible: $\psi(\tilde{\bar{r}}_1, \tilde{\bar{r}}_2, \bar{r}_3 \dots \bar{r}_N) = \sum_{\nu_1 \nu_2} A_{\nu_1 \nu_2}(\bar{r}_3 \dots \bar{r}_N) \psi_{\nu_1}(\tilde{\bar{r}}_1) \psi_{\nu_2}(\tilde{\bar{r}}_2)$

Repeating N times and, at the end, replacing $\{\tilde{\bar{r}}_i\} \to \{\bar{r}_i\}$ we obtain:

$$\psi(\bar{r}_1 \dots \bar{r}_N) = \sum_{\nu_1 \dots \nu_N} \underbrace{A_{\nu_1 \dots \nu_N}}_{\text{numerical coefficients}} \psi_{\nu_1}(\bar{r}_1) \psi_{\nu_2}(\bar{r}_2) \dots \psi_{\nu_N}(\bar{r}_N)$$

We expressed the N-body wavefunction as a combination of products of 1-particle wavefunctions.

We did not care about symmetry at this point - see later.

In an arbitrary representation: $\mathcal{H} \longmapsto \mathcal{H}_N = \underbrace{\mathcal{H} \otimes \mathcal{H} \otimes \dots \otimes \mathcal{H}}_{N \text{ times}}$