Many-Body Theory I

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I. Review of single-particle quantum mechanics + Stat. mech. of a quantum system

1. Wave function. Max Born interpretation: prob. density of finding a particle at point $\vec{r}$ is

$$P(\vec{r}, t) = |\psi(\vec{r}, t)|^2$$

2. Single-particle Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{\mathcal{H}} \psi, \qquad \hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{r})$$

in coordinate rep.: $\vec{p} = -i\hbar \vec{\nabla}$; $\quad \mathcal{H} = -\frac{\hbar^2}{2m}(\vec{\nabla})^2 + V(\vec{r})$

3. Linear superposition of waves:

If $\psi_a(\vec{r}, t)$, $\psi_b(\vec{r}, t)$ are solutions of SE, then

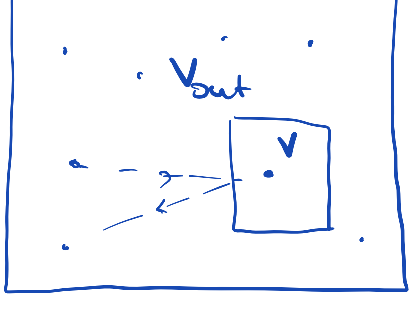
$$\psi_c = a\psi_a + b\psi_b \quad \text{is also a solution}$$

3a. Stationary states, eigenstates

$$\psi_n(\vec{r}, t) = e^{-i\varepsilon_n t/\hbar} \varphi_n(\vec{r}) \Rightarrow \hat{\mathcal{H}} \varphi_n(\vec{r}) = \varepsilon_n \varphi_n(\vec{r})$$

$$\psi(\vec{r}, t) = \sum_n \alpha_n e^{-i\varepsilon_n t/\hbar} \varphi_n(\vec{r})$$

4. Quantum Gibbs distribution



$$\psi(r_1, r_2, \ldots, r_N)$$

$$\left(\prod_{i=2}^{N} \int_V d\vec{r}_i\right) \psi^*(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)\, \psi(\vec{r}_1', \vec{r}_2, \ldots, \vec{r}_N)$$

$\equiv \rho(\vec{r}_1, \vec{r}_1')$: density matrix (coord. rep.)

$$P(\vec{r}_1) = \rho(r_1, r_1)$$

We may expand $\rho(\vec{r}, \vec{r}')$ in eigenfunctions $\psi_n(\vec{r})$ of a single-particle Hamiltonian (describing an isolated particle)

$$\rho(r, r') = \sum_{nm} w_{mn} \psi_n^*(r)\psi_m(r') \; ; \qquad \hat{\rho} = \sum_{nm} |m\rangle w_{mn} \langle n|$$

density matrix (Dirac notation)

Quantum Gibbs distribution : (equilibrium distribution)

$$\boxed{w_{mn} = \frac{1}{Z} e^{-\beta \varepsilon_n} \delta_{mn}}$$

$$\beta = \frac{1}{k_B T} \qquad \text{(we will mostly stick to } k_B \to 1 \text{)}$$

Partition function: $Z = \sum_n e^{-\beta\varepsilon_n}$ (so that $\sum_n w_{nn} = 1$)

Quantum Gibbs distribution, statistical operator

$$\hat{\rho}_G = \frac{1}{Z} \sum_n |n\rangle e^{-\beta\varepsilon_n} \langle n| = \frac{1}{Z} e^{-\beta\hat{\mathcal{H}}}$$

Partition function: $Z = \sum_n e^{-\beta\varepsilon_n} = \sum_n \langle n| e^{-\beta\hat{\mathcal{H}}} |n\rangle = Tr\, e^{-\beta\hat{\mathcal{H}}}$

The traditional point of view at microcanonical (fixed energy) and thermal (Gibbs) distributions is based on the notion of statistical ensemble, see Huang, Stat. Mech. Ch. 8 and also employs the notion of ergodicity in evolution of a classical system.

A modern point of view is based on the eigenstate thermalization hypothesis (ETH), see Mark Srednicki (Chaos and Quantum Therm.) Phys. Rev. E, 50, 888 (1994)

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5. Classical limit in Statistical mechanics:

$$Z_{cl} = \frac{1}{(2\pi\hbar)^d}\int d\vec{p}^{\,d}\int d\vec{x}^{\,d}\; e^{-\beta \mathcal{H}(p,x)} \quad \text{vs.} \quad Z = \mathrm{Tr}\, e^{-\beta\hat{\mathcal{H}}}$$

Example: 1D Harmonic oscillator $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{m\omega_0^2}{2}x^2$ (1D)

$$\varepsilon_n = \left(n+\tfrac{1}{2}\right)\hbar\omega_0$$

$$Z = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega_0(n+1/2)} = \frac{e^{-\beta\hbar\omega_0/2}}{1-e^{-\beta\hbar\omega_0}} = \frac{1}{2\sinh(\beta\hbar\omega_0/2)}$$

Classical limit: $\beta\hbar\omega_0 \ll 1 \Rightarrow Z \simeq \frac{1}{\beta\hbar\omega_0}$

$$Z_{cl} = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dp\int_{-\infty}^{\infty}dx\; e^{-\beta\left(\frac{p^2}{2m}+\frac{m\omega_0^2}{2}x^2\right)} = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dp\, e^{-\frac{\beta p^2}{2m}}\int_{-\infty}^{\infty}dx\, e^{-\frac{\beta m\omega_0^2}{2}x^2}$$

$$= \frac{1}{\beta\hbar\omega_0}$$

$\frac{1}{2\pi\hbar}$ in Z_{cl} gives the correct state counting

($\Delta p\Delta x = 2\pi\hbar$ per state)

6. Free energy

$$F = -T\ln Z$$

Classical description of harmonic oscillator:

$$F_{cl} = -T\ln Z_{cl} = -T\ln\left(\frac{T}{\hbar\omega_0}\right)$$

$S = -\frac{\partial F}{\partial T}$ (entropy, as defined in thermodynamics)

$$S_{cl} = -\frac{\partial F_{cl}}{\partial T} \underset{\text{for oscillator}}{=} 1+\ln\left(\frac{T}{\hbar\omega_0}\right)$$ problem at $T\to 0$!

full quantum result for oscillator (with $Z = \sum_n e^{-\beta\varepsilon_n}$):

$$F = \frac{1}{2}\hbar\omega_0 + T\ln\left(1 - e^{-\beta\hbar\omega_0}\right)$$

$$S = -\ln\left(1 - e^{-\hbar\omega_0/T}\right) + \frac{\hbar\omega_0/T}{e^{\frac{\hbar\omega_0}{T}} - 1}$$

$$S \propto \frac{\hbar\omega_0}{T} e^{-\hbar\omega_0/T} \quad \text{at } T \to 0$$

Entropy (the density matrix definition):

$$S = \ln[\text{number of available states}] = -\sum_n w_n \ln w_n ;$$

w_n: is the probability of state n occupation

Yields the thermodynamic def. of S for Gibbs distr. w_n

7. Expectation values

$\hat{O}$: operator of a (measurable) quantity

expectation value for a given pure state: $\langle\psi|\hat{O}|\psi\rangle$

i.e., average of $\hat{O}$ over a state $|\psi\rangle$

In the eigenstates of a Hamiltonian representation: $\psi = \sum_n \alpha_n |n\rangle$

$\psi^* = \sum_m \langle m|\alpha_n^*$

$$\langle\psi|\hat{O}|\psi\rangle = \sum_{mn} \alpha_m^* \alpha_n \underbrace{\langle m|\hat{O}|n\rangle} \equiv \sum_{mn} \alpha_m^* \alpha_n \underbrace{O_{mn}}$$

matrix element of $\hat{O}$ in the eigenstates basis

Time-averaged expectation value for a pure state:

$$\Psi = \sum_n \alpha_n |n\rangle \Rightarrow \quad \Psi(t) = \sum_n \alpha_n e^{-i\varepsilon_n t/\hbar} |n\rangle$$

$$\langle \Psi(t) | \hat{O} | \Psi(t) \rangle = \sum_{nm} \alpha_m^* \alpha_n \, e^{i \frac{\varepsilon_m - \varepsilon_n}{\hbar} t} \, O_{mn}$$

time-averaged value: $\quad \bar{A} \equiv \lim_{t_0 \to \infty} \frac{1}{t_0} \int_0^{t_0} dt \, A(t)$

$$\overline{\langle \Psi(t) | \hat{O} | \Psi(t) \rangle} = \sum_{nm} \alpha_m^* \alpha_n \, \overline{e^{i \frac{\varepsilon_m - \varepsilon_n}{\hbar} t}} \, O_{mn} = \sum_n |\alpha_n|^2 O_{nn}$$

In general, depends on the initial state (via α_n).

ETH states that for a large (infinite in the limit) system and a local quantity $\hat{O}$, $|\alpha_n|^2$ depend only on the state's energy E_n

Expectation value of $\hat{O}$ for a mixed state described by a density matrix

Return for a minute to the def. of expectation value for a one-particle system and write it out using the real-space coordinate rep.:

$$\langle \Psi | \hat{O} | \Psi \rangle = \int d\vec{r} \, \Psi^*(\vec{r}) \, \hat{O}(\vec{r}, \hat{\vec{p}}) \, \Psi(\vec{r})$$

Now suppose we have a many-particle system in a pure state, $\Psi(\bar{r}_1, \bar{r}_2, \ldots, \bar{r}_N)$, but still are interested in the expectation value of an observable associated with one specific particle, namely particle 1: $\hat{O}(\bar{r}_1, \hat{\bar{p}}_1)$

We will start now from the already introduced definition of the expectation value, $\langle\Psi|\hat{O}|\Psi\rangle$, and see how to abbreviate it using the notion of the defined earlier density matrix $\rho(\bar{r},\bar{r}')$,

$$\rho(\vec{r}_1',\vec{r}_1) \equiv \left(\prod_{i=2}^{N}\int d\vec{r}_i\right)\Psi^*(\vec{r}_1',\bar{r}_2,\ldots,\vec{r}_N)\,\Psi(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N).$$

Indeed,

$$\langle\Psi|\hat{O}|\Psi\rangle = \int dr_1 \int \prod_{i=2}^{N} dr_i \;\; \Psi^*(r_1,r_2,\ldots,r_N)\,\hat{O}(r_1,\hat{p}_1)\,\Psi(r_1,r_2,\ldots,r_N)$$

$$= \int dr_1 \int \prod_{i=2}^{N} dr_i \;\; \Psi^*(r_1,r_2,\ldots,r_N)\,\hat{O}(r_1,\hat{p}_1)\int dr_1'\,\delta(r_1-r_1')\,\Psi(r_1',r_2,\ldots,r_N)$$

$$= \int dr_1' \int dr_1 \int \prod_{i=2}^{N} dr_i \;\; \Psi^*(r_1,r_2,\ldots,r_N)\,\Psi(r_1',r_2,\ldots,r_N)\,\hat{O}(r_1,\hat{p}_1)\,\delta(r_1-r_1')$$

$$= \int dr_1' \int dr_1 \;\; \rho(r_1,r_1')\,\hat{O}(r_1,\hat{p}_1)\,\delta(r_1-r_1')$$

(vector signs omitted)

Now we can use a suitable complete basis of single-particle wave functions:

$$\rho(r,r') = \sum_{nm} w_{mn}\,\varphi_n^*(r)\,\varphi_m(r')\;; \qquad \hat{\rho} = \sum_{nm} |m\rangle w_{mn}\langle n|$$

Substitution of $\rho(r,r')$ in this form to the last line above yields

$$\langle\Psi|\hat{O}|\Psi\rangle = \int dr_1' \int dr_1 \sum_{nm} w_{mn}\,\varphi_n^*(r_1)\,\varphi_m(r')\,\hat{O}(r_1,\hat{p}_1)\,\delta(r_1-r_1')$$

Noting that $\hat{p}_1$ acts on r_1 but <u>not</u> on r_1' we may re-write

$$\langle\Psi|\hat{O}|\Psi\rangle = \int dr_1 \sum_{nm} w_{mn}\,\varphi_n^*(r_1)\,\hat{O}(r_1,\hat{p}_1)\int dr_1'\,\delta(r_1-r_1')\,\varphi_m(r_1')$$

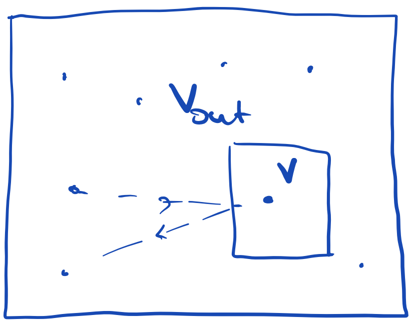
$$= \sum_{nm} w_{mn} \underbrace{\int dr_1\,\varphi_n^*(r_1)\,\hat{O}(r_1,\hat{p}_1)\,\varphi_m(r_1)}_{O_{nm}} = \sum_{nm} w_{mn}\,O_{nm}$$

$$\boxed{\langle\langle \hat{O} \rangle\rangle \equiv \sum_{nm} \omega_{mn} O_{nm} = \sum_m \sum_n \omega_{mn} O_{nm} = Tr(\hat{\rho}\hat{O})}$$

Unless the function $\psi(\bar{r}_1, \bar{r}_2, ----, \bar{r}_N)$ is factorizable, $\psi(\bar{r}_1, \bar{r}_2, ----, \bar{r}_N) = \psi(\bar{r}_1)\cdot\psi(\bar{r}_2, .., \bar{r}_N)$, the density matrix

$\hat{\rho}$ corresponds to a mixed state of particle 1. The density matrix definition of the expectation value of $\hat{O}(r_1, \hat{p}_1)$ is agnostic wrt states of other particles.

Within ETH, a thermal ensemble average of a local quantity can be obtained as an expectation value over a pure state with energy $\propto T\cdot N$ of a large system ($N \gg 1$).



We may consider a system with particle 1 confined to volume V, while other N-1 particles reside in volume V_{out}. Assuming that particle 1 interacts with other particles, but that interaction is weak compared to single-particle energies ε_m and assuming the ETH is valid, we may use

$\omega_{mn} = \frac{1}{Z} e^{-\beta\varepsilon_m}\delta_{mn}$ (Gibbs distr.) to evaluate $\langle\langle \hat{O} \rangle\rangle$:

$$\langle\langle \hat{O} \rangle\rangle = \frac{1}{Z}\sum_m e^{-\beta\varepsilon_m} O_m = \frac{1}{Z} Tr(e^{-\beta\hat{\mathcal{H}}}\hat{O})$$

In the conventional language, this is operator $\hat{O}$ averaged over the Gibbs (i.e. thermal) ensemble,

$$\hat{\rho}_G = \frac{1}{Z}\cdot\sum_m |m\rangle e^{-\beta\varepsilon_m}\langle m|$$