TD3 : Density of states

3.1) 2-level systems

1) $\uparrow$ — $+\varepsilon_0$, — $-\varepsilon_0$ Microstate $\{|+\rangle, |-\rangle\}$

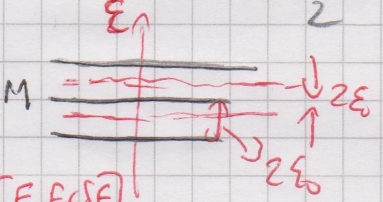
$\varepsilon_\pm = \pm\varepsilon_0 \Rightarrow N$ spins $\Rightarrow$ microstates: $\underbrace{|\sigma_1\rangle \otimes \cdots \otimes |\sigma_N\rangle}_{2^N \text{ microstate}}$

$$E = +\varepsilon_0 \sum_{i=1}^{N} \sigma_i = M\varepsilon_0$$

$$M \in [-N, \ldots, N]$$

2) E fixed $\rightarrow$ M fixed

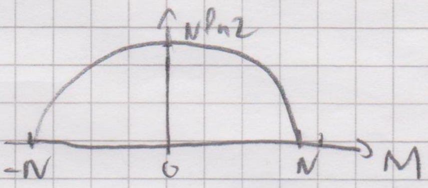
$$\begin{cases} N = N_+ + N_- \\ M = N_+ - N_- \end{cases} \Rightarrow N_\pm = \frac{N \pm M}{2} \Rightarrow g_M = \frac{N!}{N_+!\, N_-!}$$



$$\boxed{\rho(E_M) \simeq \frac{g_M}{2\varepsilon_0}} \rightarrow \text{level spacing between 2 consecutive state}$$

RQ: $\rho(E)\delta E = \#$ states in $[E, E+\delta E]$
or in $[E-\frac{\delta E}{2}, E+\frac{\delta E}{2}]$

3) $\ln g_M = \ln N! - \ln N_+! - \ln N_-!$
$\simeq N\ln N - N_+\ln N_+ - N_-\ln N_-$



we assume $M \ll N$

$$\ln g_M \simeq N\ln N - \frac{N-M}{2}\ln\frac{N-M}{2} - \frac{N+M}{2}\ln\frac{N+M}{2}$$

$$= N\ln 2 \underbrace{- \frac{N-M}{2}\ln\left(1-\frac{M}{N}\right) - \frac{N+M}{2}\ln\left(1+\frac{M}{N}\right)}$$

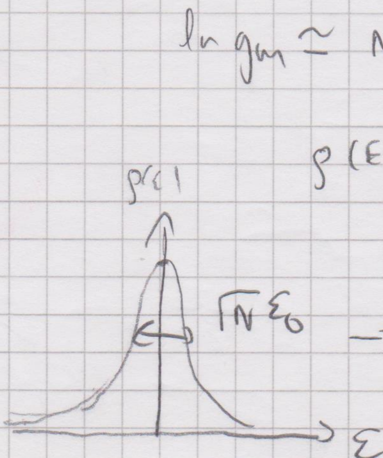
$$-\frac{N}{2}\left[\left(1-\frac{M}{N}\right)\ln\left(1-\frac{M}{N}\right) + \left(1+\frac{M}{N}\right)\ln\left(1+\frac{M}{N}\right)\right]$$

$$\sim -\frac{N}{2}\left(\frac{M}{N}\right)^2$$

$$\ln g_M \simeq N\ln 2 - \frac{M^2}{2N} = N\ln 2 - \frac{E^2}{2\varepsilon_0^2 N}$$

$$\rho(E) \simeq \frac{g_M}{2\varepsilon_0} = \frac{1}{2\varepsilon_0}\exp \ln g_M = \frac{1}{2\varepsilon_0}\exp\left(N\ln 2 - \frac{E^2}{2N\varepsilon_0^2}\right)$$

$$= \underbrace{\frac{2^N}{2\varepsilon_0}}_{\propto \rho(0)} e^{-\frac{E^2}{2N\varepsilon_0^2}}$$



Normalizat° $\rightarrow \int \rho(\varepsilon)\,d\varepsilon = 2^N$

$$\hookrightarrow \boxed{\rho(0) = \frac{2^N}{\sqrt{2\pi N}\,\varepsilon_0}}$$

3.2) Volume of the hypersphere

$$\int_{\mathbb{R}^d} d\vec{x}\, e^{-\vec{x}^{\,2}} = \left(\int dx\, e^{-x^2}\right)^d = \pi^{d/2}$$

where we use $\vec{x} = (x_1, x_2, \dots, x_d)$

We can also compute the integral in spherical coordinate

$$\int d\vec{x}\, e^{-\vec{x}^{\,2}} = \int_0^{+\infty} dR\; S_d(R)\, e^{-R^2} = \int_0^{+\infty} dR\; S_d(1)\, R^{d-1} e^{-R^2}$$

Here $S_d(1)$ = surface of hypersphere of dimension d for $R=1$

$$\int d\vec{x}\, e^{-\vec{x}^{\,2}} = S_d(1)\int_0^{+\infty} dR\, R^{d-1} e^{-R^2} = \frac{S_d(1)}{2}\int_0^{+\infty} du\, u^{\frac{d}{2}-1} e^{-u} = \frac{S_d(1)}{2}\Gamma\left(\frac{d}{2}\right)$$

$$\Rightarrow \boxed{S_d(1) = \frac{2\pi^{d/2}}{\Gamma\left(\frac{d}{2}\right)}}$$

$d=1 \to S_1(1) = 2$

$d=2 \to S_2(1) = 2\pi$

We used $\left(\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}\right) \Rightarrow \Gamma\left(\frac{3}{2}\right) = \Gamma\left(1+\frac{1}{2}\right) = \frac{\Gamma(1/2)}{2}$ $\quad d=3 \to S_3(1) = \frac{2\pi\sqrt{\pi}}{\Gamma\left(\frac{3}{2}\right)} = 4\pi$

... etc

Using $S_d(R) = V_d'(R)$

we find $S_d(1) = d\, V_d(1) \Rightarrow \boxed{V_d(1) = \frac{\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)}}$

These two results are useful for what follows

3.3) Density of states for free particles

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} \quad \text{and } V = L^3$$

1) We assume distinguishable atoms

Our starting point is the semi-classical rule (see p 14)

We have N particles. Each particle is defined by $(\vec{q}_i, \vec{p}_i)$

where $\begin{cases} \vec{q}_i = (q_{ix}, q_{iy}, q_{iz}) \\ \vec{p}_i = (p_{ix}, p_{iy}, p_{iz}) \end{cases}$

We have thus $3N$ degrees of freedom.

Our space has dimension $6N$

$$\phi_{dis}(E) = \frac{1}{h^{3N}} \int \prod_{i=1}^{N} d^3\vec{q}_i\, d^3\vec{p}_i \quad \Theta_H\left(E - \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m}\right)$$

$$= \frac{L^{3N}}{h^{3N}} \int \prod_{i=1}^{N} d^3\vec{p}_i \quad \Theta_H\left(E - \frac{1}{2m}\sum_{i=1}^{N} \vec{p}_i^{\,2}\right) = \frac{L^{3N}}{h^{3N}} \int \prod_{j=1}^{3N} dp_j \; \Theta\left(E - \sum_{j=1}^{3N} \frac{p_j^2}{2m}\right)$$

The last product of integrals represents the constraint $\sum_{j=1}^{3N} \frac{p_j^2}{2m} \leq E \Leftrightarrow \sum_{j=1}^{3N} p_j^2 \leq 2mE$

This is the volume of an hypersphere of radius $\sqrt{2mE}$ in dimension $3N$: $V_{3N}(\sqrt{2mE})$

Using 3.2)

$$\phi_{dis}(E) = \frac{V^N}{h^{3N}} \frac{\pi^{3N/2}}{\Gamma\left(\frac{3N}{2}+1\right)} (2mE)^{3N/2} = \frac{1}{\Gamma\left(\frac{3N}{2}+1\right)} \cdot \left(\frac{2\pi m E L^2}{h^2}\right)^{\frac{3N}{2}}$$

$$\boxed{\phi_{dis}(E) = \frac{1}{\Gamma\left(\frac{3N}{2}+1\right)} \left(\frac{E}{\varepsilon_0}\right)^{\frac{3N}{2}}}$$ where $\varepsilon_0 = \frac{2\pi \hbar^2}{mL^2}$

$\varepsilon_0 \approx$ energy level spacing of a particle

2) Consider indistinguishable particles

$\phi_{ind} = \frac{\phi_{dis}}{N!}$ Stirling formula $N! \sim N^N e^{-N} \sqrt{2\pi N}$

$N!\, \Gamma\left(\frac{3N}{2}+1\right) \sim N^N \left(\frac{3N}{2}\right)^{\frac{3N}{2}} e^{-5N/2} \pi N \sqrt{6}$

$$\phi_{ind}(E) \approx \frac{1}{\sqrt{6}\pi N} \left(\frac{V}{N}\right)^N \left(\frac{mE}{3\pi\hbar^2 N}\right)^{\frac{3N}{2}} e^{5N/2}$$

$$\boxed{\phi_{ind} \approx \frac{e^{\frac{5N}{2}}}{\pi\sqrt{6}N} \left(\frac{V}{N}\right)^N \left(\frac{m}{3\pi\hbar^2} \frac{E}{N}\right)^{\frac{3N}{2}}}$$

Notice ϕ_{ind} is a function of $\left(\frac{V}{N}\right)$ and $\left(\frac{E}{N}\right)$

<u>Numerically</u>: $m_{He} = 4 m_p \simeq 1.67\, 10^{-27}$ kg

I find $\varepsilon_0 \sim 6\, 10^{-23}$ eV (a very very small energy!)

3.4) Density of state for free particles

1) Non relativistic particles

$$\varepsilon_{\vec{k}} = \hbar^2 \vec{k}^2 / 2m = \frac{\vec{p}^2}{2m} \quad (\vec{p} = \hbar \vec{k})$$

We can thus directly use the previous result for $N=1$ (one free particle)

<u>In $d=3$</u>
$$\phi(E) = \frac{V}{h^3} \frac{\pi^{3/2}}{\Gamma[\frac{5}{2}]} (2mE)^{3/2}$$

$$\hookrightarrow \rho(E) = \phi'(E) = V \left(\frac{3}{2} \frac{\pi^{3/2}}{\Gamma[\frac{5}{2}]} (2m)^{3/2} \right) E^{1/2}$$

$$= V \left(2\pi (2m)^{3/2} \right) \sqrt{E} \quad \text{in } d=3$$

<u>In dimension d</u>
$$\rho(E) = V \mathcal{A}_d \, E^{\frac{d}{2}-1}$$
where $\mathcal{A}_d$ a dimensionful constant

2) $\varepsilon_{\vec{k}} = \hbar \|\vec{k}\| c$

$$\rho(\varepsilon) = \sum_{\vec{k}} \delta(\varepsilon - \varepsilon_k) = \sum_{\vec{k}} \delta(\varepsilon - \hbar c \|\vec{k}\|)$$

We use the approximation
$$\sum_{\vec{k}} \longrightarrow V \int \frac{d^d \vec{k}}{(2\pi)^d}$$

<u>RQ</u>: In 1D
$$\sum_{k} f(k) = \sum_{k_n = \frac{2\pi}{L} n} f(k_n) = \frac{L}{2\pi} \underbrace{\sum_n (k_n - k_{n-1}) f(k_n)}_{\text{Riemann sum}}$$

$$\xrightarrow{n \to \infty} \frac{L}{2\pi} \int dk\, f(k)$$

Therefore
$$\rho(\varepsilon) \simeq \frac{V}{(2\pi)^d} \int d^d k \; \delta(\varepsilon - \hbar c \|\vec{k}\|)$$

We use 3.2)

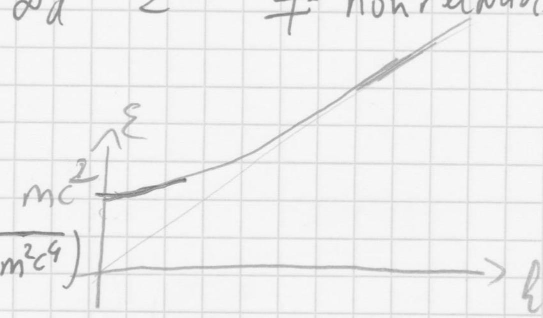
$$\rho(E) = \frac{V}{(2\pi)^d} S_d(1) \int_0^{+\infty} dk\, k^{d-1} \delta(E - \hbar c k)$$

$$= \frac{V}{(2\pi)^d} S_d(1) \frac{1}{\hbar c} \int_0^{+\infty} dk\, k^{d-1} \delta\left(k - \frac{E}{\hbar c}\right)$$

$$\Rightarrow \rho(E) = \frac{V}{(2\pi)^d} \frac{d\,\pi^{d/2}}{\Gamma(\frac{d}{2}+1)} \frac{1}{\hbar c} \left(\frac{E}{\hbar c}\right)^{d-1}$$

Notice that $\rho(E) \sim V\, \mathcal{D}_d\, \varepsilon^{d-1} \neq$ nonrelativistic case.

3) Relativistic case



$$\varepsilon_k = \sqrt{\hbar^2 k^2 c^2 + m^2 c^4}$$

$$\phi(E) = \frac{V}{h^d} \int d^d\vec{p}\; \theta\left(E - \sqrt{\hbar^2 k^2 c^2 + m^2 c^4}\right)$$

$$= \frac{V}{h^d} \hbar^d \int d^d k\; \theta\left(E - \sqrt{\hbar^2 k^2 c^2 + m^2 c^4}\right)$$

$$= \frac{V}{h^d} \hbar^d \underbrace{\int d^d k\; \theta\left(E^2 - \hbar^2 k^2 c^2 - m^2 c^4\right)}_{\text{volume of hypersphere of dimension } d \text{ of radius } \frac{\sqrt{E^2 - m^2 c^4}}{\hbar c}}$$

$$= \frac{V}{h^d} \hbar^d \frac{\pi^{d/2}}{\Gamma(\frac{d}{2}+1)} \frac{(E^2 - m^2 c^4)^{d/2}}{(\hbar c)^d} = \frac{V}{(2\pi)^d} \frac{\pi^{d/2}}{\Gamma(\frac{d}{2}+1)} \frac{(E^2 - m^2 c^4)^{d/2}}{(\hbar c)^d}$$

$$\rho(E) = \frac{V}{(2\pi)^d} \frac{d\,\pi^{d/2}}{\Gamma(\frac{d}{2}+1)} \frac{E\,(E^2 - m^2 c^4)^{d/2-1}}{(\hbar c)^d}$$

- When $\hbar k c \gg mc^2 \Rightarrow \rho(E) = \frac{V}{(2\pi)^d} \frac{d\,\pi^{d/2}}{\Gamma(\frac{d}{2}+1)} \frac{E^{d-1}}{(\hbar c)^d}$

we recover the ultrarelativistic case.

- When $E \sim mc^2$, we expand assuming $\hbar k c \ll mc^2$

$$E = mc^2\left(1 + \frac{\hbar^2 k^2 c^2}{m^2 c^4}\right)^{1/2} \simeq mc^2 + \frac{\hbar^2 k^2}{2m} + \ldots$$

$$\rho(E) = \frac{V}{(2\pi)^d} \frac{d\,\pi^{d/2}}{\Gamma(\frac{d}{2}+1)} \frac{E\,(E - mc^2)^{d/2-1} (E + mc^2)^{d/2-1}}{(\hbar c)^d}$$

$\Gamma(\frac{d}{2}+1) = \frac{d}{2}\Gamma(d)$

$$= \frac{V}{(4\pi)^{d/2}} \frac{d}{\Gamma(\frac{d}{2}+1)} \frac{(mc^2)^{d/2}\, 2^{d/2-1}}{\hbar^d c^d} \underbrace{(E - mc^2)}_{E_{cl}}{}^{d/2-1}$$

$$= \frac{V}{\Gamma(d/2)} \left(\frac{2m}{2\pi\hbar^2}\right)^{d/2} E_{cl}^{\,d/2-1} \Rightarrow \text{recover classical case}$$

3.5) Harmonic oscillators

1) $H = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 q_i^2 \right)$ in 1D

$$\phi(E) = \frac{1}{h^N} \int dq_1 \ldots dq_N \int dp_1 \ldots dp_N \; \Theta\left(E - \sum_i \frac{p_i^2}{2m} - \frac{1}{2} m\omega^2 q_i^2\right)$$

Define $P_i = \frac{p_i}{\sqrt{2m}}$; $Q_i = \omega \sqrt{\frac{m}{2}}\, q_i$

$$\phi(E) = \frac{1}{h^N} (2m)^{N/2} \left(\frac{2}{m\omega^2}\right)^{\frac{N}{2}} \int dQ_1 \ldots dQ_N \, dP_1 \ldots dP_N \; \Theta(E - \sum P_i^2 - \sum Q_i^2)$$

$$= \left(\frac{1}{\pi\hbar\omega}\right)^N V_{2N} \; E^N \;\|$$

$$\phi(E) = \frac{1}{(\pi\hbar\omega)^N} \frac{\pi^N}{\Gamma(N+1)} E^N = \frac{1}{N!} \left(\frac{E}{\hbar\omega}\right)^N \;\|$$

nothing to do with indistinguishability.

$$\rho(E) = \frac{1}{N-1!} \frac{E^{N-1}}{(\hbar\omega)^N}$$

2) Quantum $\varepsilon_n = (n+\frac{1}{2})\hbar\omega \Rightarrow$ microstate $= \{ n_1, \ldots, n_N \}$

$$E_{n_1 \ldots n_N} = \underbrace{N\frac{\hbar\omega}{2}}_{E_0} + \hbar\omega \underbrace{(n_1 + \ldots + n_N)}_{M} = N\frac{\hbar\omega}{2} + M\hbar\omega$$

degeneracy g_M ?

$$\underbrace{\circ\circ\circ\circ}_{n_1} | \underbrace{\circ \ldots \circ}_{n_2} | \ldots | \underbrace{\circ\circ\circ\circ}_{n_N}$$

$N-1$ separators

$M+N-1$ objects $\rightarrow g_M = \frac{(M+N-1)!}{M!\,(N-1)!}$

$E_M = \hbar\omega\left(M + \frac{N}{2}\right) \rightarrow E_M - E_{M-1} = \hbar\omega$

$\hookrightarrow \rho(E) = \frac{1}{\hbar\omega} g_M \;\|$

if $M \gg N$ $\quad \frac{(M+N-1)!}{M!} \approx M^{N-1} \Rightarrow \rho(E) = \frac{1}{\hbar\omega} \frac{M^{N-1}}{N-1!} \simeq \frac{1}{N-1!} \frac{E^{N-1}}{(\hbar\omega)^N} \;\|$

$\hookrightarrow M \simeq \frac{E}{\hbar\omega}$

OK