One particle Density Matrix

Perfect Gas

$$\rho(\vec{r},\vec{r}\,') = \langle \psi^{\dagger}(\vec{r}\,')\, \psi(\vec{r}) \rangle =$$

$$= \sum_{k,k'} u^{*}_{k'}(\vec{r}\,')\, u_{k}(\vec{r})\, \langle a^{\dagger}_{k'}\, a_{k} \rangle =$$

$$= \sum_{k} u^{*}_{k}(\vec{r}\,')\, u_{k}(\vec{r})\, n(\vec{k})$$

normalization of OBDM is

$$\int d^3\vec{r}\ \rho(\vec{r},\vec{r}) = \sum_k \int d^3\vec{r}\ |u_k(r)|^2\, n(k)$$

for large but finite volume we choose the normalization of plane wave to be

$$u_k(\vec{r}) = \frac{1}{\sqrt{V}}\, e^{i\vec{k}\cdot\vec{r}}$$

and therefore $\int d^3r\, |u(r)|^2 = 1$

Notice that normalization in ∞ volume is not possible if $\vec{p} = \hbar\vec{k}$ belongs to continuum spectrum

$$u_k(\vec{r}) = \frac{1}{(2\pi)^{d/2}}\, e^{i\vec{k}\cdot\vec{r}} \qquad \int_{V\to\infty} d^3r\, |u_k(\vec{r})|^2 = \infty$$

Boltzmann Particles

$$E(p) = \frac{p^2}{2m}$$

define $\rho^{(1)}(r) = \frac{1}{Z^{(1)}} \langle \vec{r}_1 | e^{-\beta \hat{H}^{(1)}} | \vec{r}_2 \rangle \qquad r = |\vec{r}_1 - \vec{r}_2|$

the normalization of this function is

$$\int d^3r \, \frac{1}{Z^{(1)}} \underbrace{\langle \vec{r} | e^{-\beta H^{(1)}} | \vec{r} \rangle}_{\text{indep on } r} = \frac{V}{Z^{(1)}} \langle \vec{r} | e^{-\beta H^{(1)}} | \vec{r} \rangle = 1$$

$1/\lambda^3$

see below

$$\rho^{(1)}(r) = \frac{2\pi}{Z} \frac{2\hbar}{r h^3} \int_0^\infty dp \, p \sin\frac{pr}{\hbar} \frac{1}{e^{\beta\left(\frac{p^2}{2m} - \mu\right)} \pm 1}$$

Much better doing integral in Cartesian frame

$$\rho^{(1)}(\vec{r}, \vec{r}\,') = \frac{1}{Z} \int \frac{d^3p}{h^3} e^{-\frac{i}{\hbar} \vec{p}(\vec{r} - \vec{r}\,')} e^{-\beta\left(\frac{p^2}{2m} - \mu\right)}$$

$$= \frac{1}{Z} \prod_{\alpha = x,y,z} \left(\int_{-\infty}^{+\infty} \frac{dp_\alpha}{h} e^{-\frac{i}{\hbar} p_\alpha (r_\alpha - r'_\alpha)} e^{-\beta \frac{p_\alpha^2}{2m}} \right) e^{\beta\mu}$$

$$\left(\int_{-\infty}^{+\infty} \frac{dp}{h}\, e^{-\frac{i}{\hbar} p (r-r')}\, e^{-\beta \frac{p^2}{2m}}\right) = \frac{1}{h}\sqrt{2m\pi/\beta}\; e^{-\frac{1}{2}\frac{m}{\beta}\frac{(r-r')^2}{\hbar^2}}$$

$$\rho^{(1)}(r) = \underset{\uparrow \atop V/\lambda^3}{\frac{1}{Z}} \underbrace{\left(\frac{1}{h}\sqrt{\frac{2m\pi}{\beta}}\right)^3}_{1/\lambda^3} e^{-\underbrace{\frac{m}{2\beta\hbar^2}}\, r^2}$$

$$\frac{2\, h^2}{(2\pi)^2 m\, k_B T} = \frac{2}{2\pi}\, \lambda^2$$

$$\boxed{\rho^{(1)}(r) = \frac{1}{V}\, e^{-\frac{\pi r^2}{\lambda^2}}} \longleftarrow \text{Boltzmann particles}$$

the normalization is therefore

$$\int_V d^3r\; \rho(r=0) = 1$$

Fermions & Bosons (beware of normalization)

$$\frac{1}{e^{\beta(\varepsilon_p-\mu)}\pm 1} = \frac{z}{e^{\beta\varepsilon_p}\pm z} = z e^{-\beta\varepsilon(p)} \frac{1}{1\pm z e^{-\beta\varepsilon_p}}$$

let's consider the expansion

$$\frac{1}{1\pm z e^{-\beta\varepsilon_p}} = \sum_0^\infty n\,(\mp)^n z^n e^{-n\beta\varepsilon_p}$$

$$z e^{-\beta\varepsilon_p} < 1$$

Fermions do not converge

$$\langle n(p)\rangle = \sum_0^\infty n\,(\mp)^n z^{n+1} e^{-(n+1)\beta\varepsilon_p}$$

$$\rho(r) = \frac{1}{Z}\sum_0^\infty n\,(\mp)^n z^{n+1}\frac{1}{\lambda^3_{n+1}} e^{-\frac{\pi r^2}{\lambda^2_{n+1}}}$$

$$\lambda_n = \frac{h}{\sqrt{2\pi m k_B T}}\sqrt{n}$$

$\beta \to n\beta \quad T \to T/n$

for Bosons at $\mu = 0$

$$\rho(r) = \frac{1}{Z}\sum_0^\infty n\,\frac{1}{\lambda^3_{n+1}} e^{-\frac{\pi r^2}{\lambda^2_{n+1}}}$$

$$= \frac{1}{Z}\sum_0^\infty n\left(\frac{\lambda_1}{\lambda_{n+1}}\right)^3 \frac{1}{\lambda_1^3} e^{-\frac{\pi r^2}{\lambda_1^2}\frac{\lambda_1^2}{\lambda^2_{n+1}}}$$

De Broglie WL

$$\rho(r) = \frac{1}{V} \sum_{0}^{\infty} {}_n \frac{1}{(n+1)^{3/2}} e^{-\frac{\pi r^2}{\lambda^2} \frac{1}{n+1}}$$

$$\sum_{1}^{\infty} {}_n \frac{1}{n^{3/2}} e^{-\frac{\pi r^2}{\lambda^2} \frac{1}{n}} < \sum_{1}^{\infty} {}_n \frac{1}{n^{3/2}} = \zeta(3/2) = 2.6124 = \rho(0)$$

$\rho(r)$ tends to be indeependent on r

$$\frac{1}{1-x} = \sum_{0}^{\infty} {}_n x^n \qquad |x| < 1$$

but as $\mu \to 0$ and $p \to \infty$

$$z e^{-\beta \epsilon_p} \to 1$$

for any finite μ

$$\rho(r) = \frac{1}{Z} \sum_{0}^{\infty} {}_n (\mp)^n z^{n+1} \frac{1}{\lambda^3_{n+1}} e^{-\frac{\pi r^2}{\lambda^2_{n+1}}}$$

$$\rho(r) = \frac{1}{z\lambda^3} \sum_{1}^{\infty} {}_n \frac{z^n}{n^{3/2}} e^{-\frac{\pi r^2}{\lambda^2} \frac{1}{n}} \qquad z < 1$$

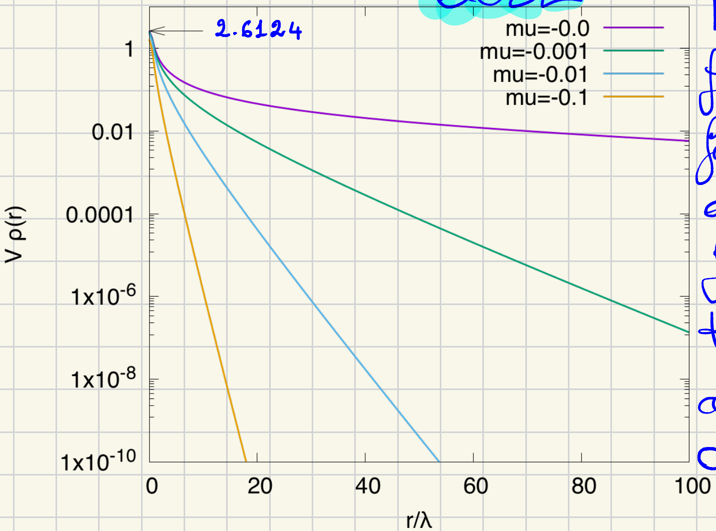
$$z^n = e^{-n\beta|\mu|}$$

guarantee an exponential convergence of the sum

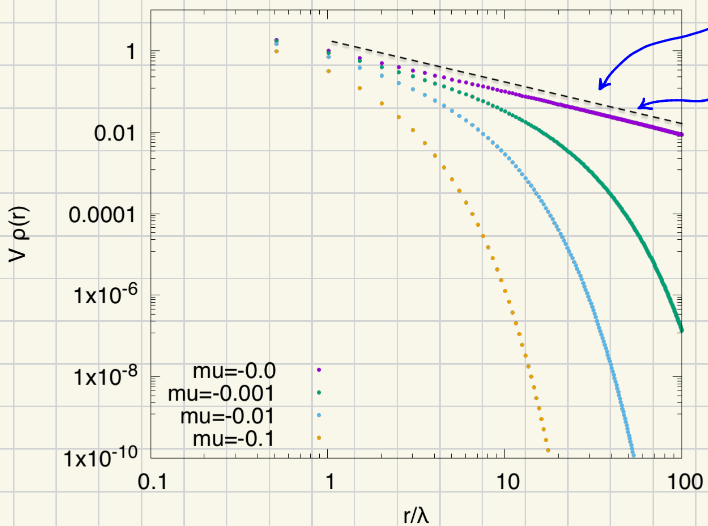
$$f(\beta|\mu|, r/\lambda)$$

for fermions $\mu > 0$ and the serie does not converge for any $\mu > 0$

BOSE



here the $\rho(r)$ for Bose system for different values of $-\beta\mu$ as a function of r/λ the progressive approach to ODLRO is shown



$1/r$

from exponential to power-law