# One body density matrix

for a single particle we have seen that

$\hat{\psi}^+(x)\hat{\psi}(x)$ represent the density at point x

for a pure state the diagonal element of

$\hat{\rho} = |\psi\rangle\langle\psi|$ in the coordinate representation

is $\langle x|\hat{\rho}|x\rangle = |\psi(x)|^2$

The operator $\hat{\rho}^D_{2Q} = \hat{\psi}^+(x)\hat{\psi}(x)$ written in the

single particle subspace reads

$\hat{\rho}^D_{2Q} = \hat{\psi}^+(x)|0\rangle\langle 0|\hat{\psi}(x) = |x\rangle\langle x|$

its average over a one particle state gives

$\langle\psi|\hat{\rho}^D_{2Q}|\psi\rangle = |\psi(x)|^2$

Now consider non-diagonal elements

of the density matrix for a pure state

$\hat{\rho} = |\psi\rangle\langle\psi| \rightarrow \langle x|\hat{\rho}|y\rangle = \psi^*(y)\psi(x)$

and consider the operator

$\hat{\rho}^{OD}_{2Q} = \hat{\psi}^+(y)\hat{\psi}(x)$

on a single particle state $\hat{\rho}^{OD}_{2Q} = \hat{\psi}^+(y)|0\rangle\langle 0|\hat{\psi}(x)$

its average over a single particle state gives

$$\langle\psi|\hat{\rho}^{OD}_{2q}|\psi\rangle = \langle\psi|y\rangle\langle x|\psi\rangle = \psi^*(y)\psi(x)$$

Therefore on single particle state the density matrix for a pure state have

diagonal elements

$$\langle x|\hat{\rho}|x\rangle = \langle\psi|\hat{\psi}^\dagger(x)\hat{\psi}(x)|\psi\rangle$$

off diagonal elements

$$\langle x|\hat{\rho}|y\rangle = \langle\psi|\hat{\psi}^\dagger(y)\hat{\psi}(x)|\psi\rangle$$

are averages of $\hat{\psi}^\dagger(y)\hat{\psi}(x)$

The one body density matrix operator can be defined in 2Q as $\hat{\rho}(x,y) = \hat{\psi}^\dagger(y)\hat{\psi}(x)$

Now consider 2 distinguishable particles a pure state have the density

$$\langle x_2 x_1|\psi\rangle\langle\psi|x_1 x_2\rangle = |\psi(x_1,x_2)|^2$$

Now consider the average of diagonal terms of $\hat{\rho}^D_{2a} = \hat{\psi}^\dagger(x)\hat{\psi}(x)$ on such a state

$$\langle\psi|\hat{\psi}^\dagger(x)\hat{\psi}(x)|\psi\rangle$$

$$|\psi\rangle = \int dx_1 dx_2\, \psi(x_1,x_2)\,|x_1 x_2\rangle$$

$$\langle \hat{\rho}^{D}_{2Q}(x)\rangle = \int dx_1' dx_2' dx_1 dx_2 \, \langle x_2' x_1' | \hat{\psi}^{\dagger}(x)\hat{\psi}(x) | x_1 x_2\rangle \times$$
$$\times \, \psi^*(x_1' x_2')\, \psi(x_1 x_2)$$

$$\hat{\psi}^{\dagger}(x)\hat{\psi}(x) = \int dy \, \hat{\psi}^{\dagger}(x) \overbrace{|y\rangle\langle y|}^{\text{identity in one particle states!}} \psi(x) =$$
$$= \int dy \, |x\, y\rangle\langle y\, x|$$

(here I assume that particles are distinguishable and $\psi$ creates particle 1 $\quad |\underset{1}{x_1}\, \underset{2}{x_2}\rangle$

$$\langle \rho^{D}_{2Q}(x)\rangle = \int dx_1' dx_2' dx_1 dx_2 \int dy \, \underbrace{\langle x_2' x_1' | x\, y\rangle}_{\delta(x_1'-x)\delta(x_2'-y)} \underbrace{\langle y\, x | x_1 x_2\rangle}_{\delta(x-x_1)\delta(y-x_2)}$$
$$\times \, \psi^*(x_1' x_2')\, \psi(x_1 x_2)$$

$$= \int dx_1' dx_2' dx_1 dx_2 \, \delta(x_1'-x)\delta(x-x_1)\delta(x_2'-x_2) \times \psi^*(x_1' x_2')\, \psi(x_1 x_2)$$
$$= \int dx_2' dx_2 \, \delta(x_2'-x_2)\, \psi^*(x, x_2')\, \psi(x, x_2)$$
$$= \int dx_2 \, \psi^*(x, x_2)\, \psi(x, x_2)$$
$$= \int dx_2 \, |\psi(x, x_2)|^2$$

Thus the average of one body density operator represents in its diagonal element the reduced one body density

This can be generalised to off diagonal term

$$\hat{\rho}(x,y) = \hat{\psi}^{+}(y)\,\hat{\psi}(x)$$

$$\hat{\rho}(x,y) = \sum_{\alpha\beta} u_\alpha^*(y)\, u_\beta(x)\, a_\alpha^+ a_\beta$$

lets consider its thermal average on a free Hamiltonian e.g. that of ideal quantum gas the one particle states are eigenstates of momentum $\alpha \equiv \vec{k}$

$$a_{\vec{k}}^+ |0\rangle = |\vec{k}\rangle$$

$$\boxed{\hat{\rho}(\vec{r},\vec{r}\,') = \sum_{\vec{k}\vec{k}'} u^*_{\vec{k}'}(\vec{r}\,')\, u_{\vec{k}}(\vec{r})\, a^+_{\vec{k}'} a_{\vec{k}}}$$

general

off diagonal d.m. operator

The one body density matrix is thus its average

$$\langle \hat{\rho}(\vec{r}, \vec{r}\,') \rangle = \sum_{\vec{k}\,\vec{k}'} u^*_{\vec{k}'}(\vec{r}\,')\, u_{\vec{k}}(\vec{r})\, \underbrace{\langle a^+_{\vec{k}'} a_{\vec{k}} \rangle}_{\delta_{\vec{k}',\vec{k}} \langle \hat{n}_k \rangle}$$

$$\langle \hat{\rho}(\vec{r}, \vec{r}\,') \rangle = \sum_{\vec{k}} \underbrace{u^*_k(\vec{r}\,')\, u_k(\vec{r})}_{e^{i\vec{k}(\vec{r}-\vec{r}\,')}} \underbrace{\langle \hat{n}_k \rangle}$$

periodic boundary cond

$$n_k = \frac{1}{e^{\beta(\epsilon_n - \mu)} \pm 1}$$

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$$n_k = e^{\beta(\epsilon_n - \mu)}$$ Boltzmann

for Boltzmann particles

$$\langle \hat{\rho}(\vec{r}, \vec{r}\,') \rangle \propto e^{-\underbrace{a}_{\text{numerical constant}} \frac{|\vec{r}-\vec{r}\,'|^2}{\lambda^2}}$$

$\lambda$ = De Broglie wavelength

numerical constant $\Rightarrow$ exercise

The one body density matrix for a perfect gas has only diagonal elements in $\vec{k}$-space

$$\hat{\rho}_{\vec{k}} = \hat{a}^+_k \hat{a}_k = \hat{n}_k$$

indeed

$$\langle \hat{\rho}_{\vec{k}'\vec{k}} \rangle = \langle \hat{a}^+_{\vec{k}'} \hat{a}_{\vec{k}} \rangle = \delta_{\vec{k}'\vec{k}} \langle \hat{n}_k \rangle$$

# Normalization of one body density matrix

the OBDM defined above have the following normalization

$$\mathrm{tr}\langle \hat{\rho}_{kk} \rangle = \Sigma_k \langle \hat{n}_k \rangle = \langle \hat{N} \rangle$$

its trace equals to $\langle \hat{N} \rangle$ _

In the classical limit $z \ll 1$

$$\mathrm{tr}\langle \hat{\rho}_{kk} \rangle = \Sigma_k \frac{1}{e^{\beta(\epsilon_k - \mu)} \pm 1} \longrightarrow z \Sigma_k e^{-\beta \epsilon_k}$$

and $z = e^{\beta\mu}$ _

the classical limit of OBDM is thus

$$\langle \hat{\rho}_{kk} \rangle \delta_{kk'} = z e^{-\beta \epsilon_k} \delta_{kk'}$$

In the classical limit $\langle N \rangle = z \Sigma_k e^{-\beta \epsilon_k}$

therefore $z = \dfrac{\langle N \rangle}{\Sigma_k e^{-\beta \epsilon_k}}$ and

$$\langle \hat{\rho}_{kk'} \rangle = \frac{\langle N \rangle}{\Sigma_k e^{-\beta \epsilon_k}} e^{-\beta \epsilon_k} \delta_{kk'}$$

As defined above

$$\langle \hat{\rho}_{kk'} \rangle = \frac{\langle N \rangle}{Z^{(1)}} e^{-\beta \epsilon_k} \delta_{k,k'}$$

where $Z^{(1)} = \sum_k e^{-\beta \epsilon_k} = \frac{L^3}{h^3} \int d^3p \, e^{-\beta \frac{p^2}{2m}} = \frac{V}{\lambda^3}$

One can define for Boltzmann's particle

$$\hat{\rho}^{(1)} = \frac{e^{-\beta \hat{H}^{(1)}}}{Z^{(1)}}$$

and it is possible to show that

$$\langle \vec{r} | \hat{\rho}^{(1)} | \vec{r}' \rangle = \frac{1}{Z^{(1)}} e^{-a \frac{|\vec{r} - \vec{r}'|^2}{\lambda^2}} \frac{1}{\lambda^2}$$

dimensionless constant

Notice that the normalization is in this case

$$\frac{1}{Z^{(1)}} \operatorname{tr} e^{-\beta H^{(1)}} = 1$$

but one has to consider finite volume

since $\langle \vec{r} | e^{-\beta H^{(1)}} | \vec{r} \rangle = \frac{1}{\lambda^2} \frac{1}{Z^{(1)}}$

then performing the trace over position eigenstates means

$$\mathrm{tr}\,\frac{e^{-\beta H^{(1)}}}{Z^{(1)}} = \int_V d^3r\, \langle \vec r | e^{-\beta H^{(1)}} | \vec r \rangle \frac{1}{Z^{(1)}} =$$

!!

$$= \frac{V}{\lambda^3}\,\frac{1}{Z^{(1)}} = 1$$