<u>Example:</u>

Ensemble of silver atoms

60 % in $S_z = \frac{\hbar}{2}$ eigenstate of $\hat{S}_z$

40 % in $S_x = -\frac{\hbar}{2}$ eigenstate of $\hat{S}_x$

external field B in y direction

$\Rightarrow \hat{H} = \mu \hat{S}_y \cdot B$

Find $\hat{\rho}(t)$ and $\langle S_z(t) \rangle$

In eigenbasis of S_z:

$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\quad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

EV: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$ $\quad$ EV: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm i \end{pmatrix}$ $\quad$ EV: $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

In eigenbasis of S_y ($\hat{H}$ diagonal !)

$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\quad S_y = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ $\quad S_z = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

EV: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm i \end{pmatrix}$ $\quad$ EV: $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\quad$ EV: $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$

$$\hat{\rho}(0) = \frac{3}{5} |z_+\rangle\langle z_+| + \frac{2}{5} |x_-\rangle\langle x_-|$$

$$= \frac{3}{5}\frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}(1\ 1) + \frac{2}{5}\frac{1}{2}\begin{pmatrix} 1 \\ -i \end{pmatrix}(1\ +i)$$

$$= \frac{3}{10}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{5}\begin{pmatrix} 1 & +i \\ -i & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{3+2i}{10} \\ \frac{3-2i}{10} & \frac{1}{2} \end{pmatrix}$$

$$\hat{\rho}(t) = e^{-i\mathcal{L}t}\hat{\rho}(0) = e^{-\frac{i}{\hbar}\hat{H}t}\hat{\rho}(0)\, e^{\frac{i}{\hbar}\hat{H}t}$$

$$= e^{-\frac{i}{\hbar}\frac{\hbar}{2}\mu B t\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}} \cancel{\hat{\rho}(0)} \begin{pmatrix} \frac{1}{2} & \frac{3+2i}{10} \\ \frac{3-2i}{10} & \frac{1}{2} \end{pmatrix} e^{\frac{i}{\hbar}\frac{\hbar}{2}\mu B t\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

$$= \begin{pmatrix} e^{-\frac{i}{2}\mu B t} & 0 \\ 0 & e^{\frac{i}{2}\mu B t} \end{pmatrix}\begin{pmatrix} \frac{1}{2} & \frac{3+2i}{10} \\ \frac{3-2i}{10} & \frac{1}{2} \end{pmatrix}\begin{pmatrix} e^{\frac{i}{2}\mu B t} & 0 \\ 0 & e^{-\frac{i}{2}\mu B t} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2} e^{-\frac{i}{2}\mu B t} & \frac{3+2i}{10} e^{-\frac{i}{2}\mu B t} \\ \frac{3-2i}{10} e^{\frac{i}{2}\mu B t} & \frac{1}{2} e^{\frac{i}{2}\mu B t} \end{pmatrix} \begin{pmatrix} e^{\frac{i}{2}\mu B t} & 0 \\ 0 & e^{-\frac{i}{2}\mu B t} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2} & \frac{3+2i}{10} e^{-i\mu B t} \\ \frac{3-2i}{10} e^{i\mu B t} & \frac{1}{2} \end{pmatrix}$$

$$\langle S_z(t) \rangle = \mathrm{tr}\left(\hat{S}_z \hat{\rho}(t)\right) = \mathrm{tr}\, \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{3+2i}{10} e^{-i\mu B t} \\ \frac{3-2i}{10} e^{i\mu B t} & \frac{1}{2} \end{pmatrix}$$

$$= \frac{\hbar}{2}\left(\frac{3-2i}{10} e^{i\mu B t} + \frac{3+2i}{10} e^{-i\mu B t} \right)$$

$$= \frac{3}{10}\hbar \cos \mu B t + \frac{1}{5}\hbar \sin \mu B t$$

Individual states:

$$e^{-\frac{i}{\hbar}\hat{H}t}|z_+\rangle = e^{-\frac{i}{2}\mu B t \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-\frac{i}{2}\mu B t} & 0 \\ 0 & e^{\frac{i}{2}\mu B t} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-\frac{i}{2}\mu B t} \\ e^{\frac{i}{2}\mu B t} \end{pmatrix}$$

$$\langle z_+ | e^{\frac{i}{\hbar}\hat{H}t} \hat{S}_z e^{-\frac{i}{\hbar}\hat{H}t} | z_+ \rangle =$$

$$\frac{\hbar}{4}\left(e^{\frac{i}{2}\mu B t} \quad e^{-\frac{i}{2}\mu B t} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-\frac{i}{2}\mu B t} \\ e^{\frac{i}{2}\mu B t} \end{pmatrix} = \frac{\hbar}{4}\left[e^{-i\mu B t} + e^{i\mu B t} \right] = \frac{\hbar}{2}\cos \mu B t$$

$$e^{-\frac{i}{\hbar}\hat{H}t}|x_-\rangle = e^{-\frac{i}{2}\mu B t \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-\frac{i}{2}\mu B t} \\ -i e^{\frac{i}{2}\mu B t} \end{pmatrix}$$

$$\langle x_- | e^{\frac{i}{\hbar}\hat{H}t} \hat{S}_z e^{-\frac{i}{\hbar}\hat{H}t} | x_- \rangle =$$

$$\frac{\hbar}{4}\left(e^{\frac{i}{2}\mu B t} \quad i e^{-\frac{i}{2}\mu B t} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-\frac{i}{2}\mu B t} \\ -i e^{\frac{i}{2}\mu B t} \end{pmatrix} = \frac{\hbar}{4}\left[i e^{-i\mu B t} - i e^{i\mu B t} \right]$$

$$= \frac{\hbar}{2} \sin \mu B t$$

21(9) $\langle \hat{S}_z(t) \rangle = \frac{6}{10}\frac{\hbar}{2}\cos \mu B t + \frac{4}{10}\frac{\hbar}{2}\sin \mu B t$ | no interference between classes of atoms!

VI.3 Warm-up: a three particle system

$$\hat{H} = \frac{\hat{P}_1^2}{2m} + \frac{\hat{P}_2^2}{2m} + \frac{\hat{P}_3^2}{2m}$$

try to understand quantum effects.

cubic box of volume L^3

$\Rightarrow$ single particle wave function

$$\psi_{n_x, n_y, n_z}(x,y,z) = A \sin\frac{n_x \pi x}{L} \sin\frac{n_y \pi y}{L} \sin\frac{n_z \pi z}{L}$$

with n_x, n_y, n_z integers ≥ 1

n_x, n_y, n_z describe wave vector

$$\vec{k} = \frac{n_x \pi}{L}\hat{x} + \frac{n_y \pi}{L}\hat{y} + \frac{n_z \pi}{L}\hat{z}$$

single particle energy eigenvalue is $\frac{\hbar^2 \vec{k}^2}{2m}$

<u>single particle partition function:</u>

$$Z_1(T) = \mathrm{Tr}\, e^{-\beta\hat{H}} = \sum_{\vec{k}} \langle \vec{k} | e^{-\beta\hat{H}} | \vec{k} \rangle$$

$$= \sum_{\vec{k}} \langle \vec{k} | \vec{k} \rangle e^{-\frac{\beta\hbar^2 \vec{k}^2}{2m}} = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} e^{-\frac{\beta\hbar^2\pi^2}{2mL^2}(n_x^2+n_y^2+n_z^2)}$$

if $\frac{\beta\hbar^2\pi^2}{2mL^2} \ll 1$ (i.e. high temperatures, large volume or low density)

$$\approx \frac{1}{8}\int d^3n\, e^{-\frac{\beta\hbar^2\pi^2}{2mL^2}\vec{n}^2} = \frac{1}{8}\left(\frac{2\pi m L^2 k_B T}{\hbar^2\pi^2}\right)^{3/2} = V\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} = \frac{V}{\lambda_T^3}$$

for low temperatures or high density find quantum effects already for <u>one</u> particle all three particles:

bosons:

basis of three particle Hilbert space:

$$|k_1 k_2 k_3\rangle^{(+)} \equiv \frac{1}{\sqrt{3!}}\big(|k_1 k_2 k_3\rangle + |k_1 k_3 k_2\rangle + |k_2 k_1 k_3\rangle + |k_2 k_3 k_1\rangle + |k_3 k_1 k_2\rangle + |k_3 k_2 k_1\rangle\big)$$

for k_1, k_2, k_3 all different

$$|k_1 k_2 k_2\rangle^{(+)} \equiv \frac{1}{\sqrt{3}}\big(|k_1 k_2 k_2\rangle + |k_2 k_1 k_2\rangle + |k_2 k_2 k_1\rangle\big) \quad \text{for } k_1 \neq k_2$$

$$|k\,k\,k\rangle^{(+)} \equiv |k\,k\,k\rangle$$

$$Z_3^{(+)}(T) = \mathrm{Tr}_{3+}\, e^{-\beta \hat{H}}$$

$$= \frac{1}{3!}\sum_{\substack{k_1,k_2,k_3 \\ \text{all different}}} {}^{(+)}\langle k_1 k_2 k_3| e^{-\beta \hat{H}} |k_1 k_2 k_3\rangle^{(+)}$$

$$+ \sum_{k_1 \neq k_2} {}^{(+)}\langle k_1 k_2 k_2| e^{-\beta \hat{H}} |k_1 k_2 k_2\rangle^{(+)}$$

$$+ \sum_{k} {}^{(+)}\langle k\,k\,k| e^{-\beta \hat{H}} |k\,k\,k\rangle$$

$$= \frac{1}{3!}\sum_{\substack{k_1,k_2,k_3 \\ \text{all different}}} e^{-\frac{\beta\hbar^2}{2m}(k_1^2+k_2^2+k_3^2)} + \sum_{k_1\neq k_2} e^{-\frac{\beta\hbar^2}{2m}(k_1^2+2k_2^2)}$$

$$+ \sum_k e^{-\frac{\beta\hbar^2}{2m}3k^2}$$

$$= \frac{1}{3!}\sum_{k_1,k_2,k_3} e^{-\frac{\beta\hbar^2}{2m}(k_1^2+k_2^2+k_3^2)} + \frac{1}{2}\sum_{k_1\neq k_2} e^{-\frac{\beta\hbar^2}{2m}(k_1^2+2k_2^2)}$$

$$+ \Big(1-\frac{1}{3!}\Big)\sum_k e^{-\frac{\beta\hbar^2}{2m}3k^2}$$

$$= \frac{1}{3!}\left(Z_1(T)\right)^3 + \frac{1}{2}\sum_{k_1,k_2} e^{-\frac{\beta\hbar^2}{2m}(k_1^2+2k_2^2)} + \left(1-\frac{1}{6}-\frac{1}{2}\right)\sum_k e^{-\frac{\beta\hbar^2}{2m}3k^2}$$

$$= \underbrace{\frac{1}{3!}\left(Z_1(T)\right)^3}_{\text{"classical" result}} + \underbrace{\frac{1}{2} Z_1(T) Z_1\left(\frac{T}{2}\right) + \frac{1}{3} Z_1\left(\frac{T}{3}\right)}_{\text{quantum corrections}}$$

fermions:

basis of three particle Hilbert space

$$|k_1\, k_2\, k_3\rangle^{(-)} \equiv \frac{1}{\sqrt{3!}}\big(|k_1\, k_2\, k_3\rangle - |k_1\, k_3\, k_2\rangle - |k_2\, k_1\, k_3\rangle + |k_2\, k_3\, k_1\rangle + |k_3\, k_1\, k_2\rangle - |k_3\, k_2\, k_1\rangle\big)$$

for k_1, k_2, k_3 all different

$$Z_3^{(-)}(T) = \mathrm{Tr}_{3-}\, e^{-\beta\hat{H}} =$$

$$\frac{1}{3!}\sum_{\substack{k_1,k_2,k_3\\ \text{different}}} {}^{(-)}\langle k_1\, k_2\, k_3|\, e^{-\beta\hat{H}}\, |k_1\, k_2\, k_3\rangle^{(-)}$$

$$= \frac{1}{3!}\sum_{\substack{k_1,k_2,k_3\\ \text{different}}} e^{-\frac{\beta\hbar^2}{2m}(k_1^2+k_2^2+k_3^2)}$$

$$= \frac{1}{3!}\sum_{k_1,k_2,k_3} e^{-\frac{\beta\hbar^2}{2m}(k_1^2+k_2^2+k_3^2)} - \frac{1}{2}\sum_{k_1\neq k_2} e^{-\frac{\beta\hbar^2}{2m}(k_1^2+2k_2^2)} - \frac{1}{6}\sum_k e^{-\frac{\beta\hbar^2}{2m}3k^2}$$

$$= \frac{1}{3!}\left(Z_1(T)\right)^3 - \frac{1}{2}\sum_{k_1,k_2} e^{-\frac{\beta\hbar^2}{2m}(k_1^2+2k_2^2)} + \left(\frac{1}{2}-\frac{1}{6}\right)\sum_k e^{-\frac{\beta\hbar^2}{2m}3k^2}$$

$$= \frac{1}{3!}\left(Z_1(T)\right)^3 - \frac{1}{2} Z_1(T) Z_1\left(\frac{T}{2}\right) + \frac{1}{3} Z_1\left(\frac{T}{3}\right)$$

combined: $$Z_3^{(\pm)}(T) = \frac{1}{3!}\left(Z_1(T)\right)^3 \pm \frac{1}{2} Z_1(T) Z_1\left(\frac{T}{2}\right) + \frac{1}{3} Z_1\left(\frac{T}{3}\right)$$

↓ 2/19