Problem 1:

(a) We have a frequency distribution function $D(\omega)$:

$$D(\omega) = \frac{A}{\omega} \quad \text{for} \quad \omega_a \le \omega \le \omega_b$$

If we know the energy of an oscillator for a given temperature, then we can average that energy over the frequency distribution fct.

For 1D osc. with frequency ω at temperature T, we have

$$U_\omega = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2kT}\right)$$

we can use our result from class for canonical ensemble (see class notes p. 168)

$$\Rightarrow U = \int_{\omega_a}^{\omega_b} D(\omega) U_\omega \, d\omega$$

$$= A \frac{\hbar}{2} \int_{\omega_a}^{\omega_b} \coth\left(\frac{\hbar\omega}{2kT}\right) d\omega$$

$\int \coth(x\omega) d\omega = \frac{1}{x} \log(\sinh(x\omega))$

$$= \frac{A}{\beta} \log\left(\frac{\sinh\left(\frac{\hbar\omega_b}{2kT}\right)}{\sinh\left(\frac{\hbar\omega_a}{2kT}\right)}\right)$$

But : we also need to make sure that we are accounting for all the particles.

$$N = \int_{\omega_a}^{\omega_b} \mathcal{D}(\omega)\, d\omega = A \int_{\omega_a}^{\omega_b} \frac{1}{\omega}\, d\omega$$

$$= A \log\left(\frac{\omega_b}{\omega_a}\right)$$

$$\Rightarrow \quad A = N \log\left(\frac{\omega_a}{\omega_b}\right)$$

$\uparrow$

"A" can really be interpreted as a normalization constant

$$\frac{U}{N} = \frac{kT}{\log\left(\frac{\omega_b}{\omega_a}\right)} \log\left(\frac{\sinh\left(\frac{\hbar\omega_b}{2kT}\right)}{\sinh\left(\frac{\hbar\omega_a}{kT}\right)}\right)$$

chain rule

specific heat: per particle $\quad \frac{d\left(\frac{U}{N}\right)}{dT} = \frac{k}{\log\left(\frac{\omega_b}{\omega_a}\right)} \log\left(\frac{\sinh\left(\frac{\hbar\omega_b}{2kT}\right)}{\sinh\left(\frac{\hbar\omega_a}{2kT}\right)}\right)$

$$+ \frac{\hbar\omega_a}{2T} \frac{\coth\left(\frac{\hbar\omega_a}{2kT}\right)}{\log\left(\frac{\omega_b}{\omega_a}\right)}$$

$$\boxed{\frac{d}{dT}\left[\log\left(\sinh\left(\frac{x}{T}\right)\right)\right] = -\frac{x\coth\left(\frac{x}{T}\right)}{T^2}}$$

$$- \frac{\hbar\omega_b}{2T} \frac{\coth\left(\frac{\hbar\omega_b}{2kT}\right)}{\log(\omega_b/\omega_a)}$$

(b)

for large T: $2kT \gg \hbar\omega_a$ and $2kT \gg \hbar\omega_b$

Note: the low T regime would imply

$2kT \ll \hbar\omega_a$ and $2kT \ll \hbar\omega_b$ (of course, the factor of 2 can be dropped).

Back to large T: $\sinh x \approx x$ for small $\frac{\hbar\omega}{2kT} = x$

$\coth x \approx x^{-1}$ for small x

$$\Rightarrow \frac{d\left(\frac{E}{N}\right)}{dT} \longrightarrow \frac{k}{\log\left(\frac{\omega_b}{\omega_a}\right)} \log\left(\frac{\omega_b}{\omega_a}\right) = k$$

specific heat per particle

note: the second and third terms cancel to a good approximation

So: specific heat per particle $\longrightarrow k$ in high T limit $\rightsquigarrow$ the frequency distribution becomes irrelevant

(c) internal energy per particle for single-frequency case:

$$U_\omega = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2kT}\right)$$

$$\frac{d}{dT} \coth\left(\frac{x}{T}\right) = \frac{x}{T^2\left(\sinh\left(\frac{x}{T}\right)\right)^2}$$

$$\Rightarrow \frac{dU_{\hbar\omega}}{dT} = \frac{\hbar\omega}{2} \frac{\hbar\omega}{2k} \frac{1}{T^2} \frac{1}{\sinh^2\left(\frac{\hbar\omega}{2kT}\right)}$$

$$= \frac{(\hbar\omega)^2}{4(kT)^2} \, k \, \frac{1}{\sinh^2\left(\frac{\hbar\omega}{2kT}\right)}$$

in the notebook: $\hbar\omega \to hw$

$\hbar\omega_a \to hwa$

$\hbar\omega_b \to hwb$

$kT \to kT$

In[196]:= CperNw[kT_, hw_] := $\dfrac{\frac{hw^2}{4\,kT^2}}{\text{Sinh}\left[\frac{hw}{2\,kT}\right]^2}$

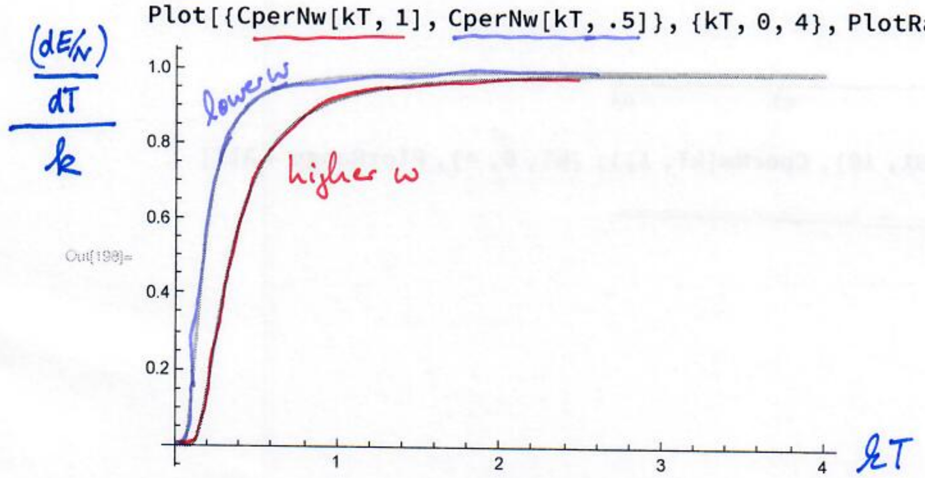
In[199]:=

CperNwave[kT_, hwa_, hwb_] := $\dfrac{1}{\text{Log}\left[\frac{hwb}{hwa}\right]}\text{Log}\left[\dfrac{\text{Sinh}\left[\frac{hwb}{2\,kT}\right]}{\text{Sinh}\left[\frac{hwa}{2\,kT}\right]}\right] + \dfrac{\frac{hwa}{2\,kT}\,\text{Coth}\left[\frac{hwa}{2\,kT}\right]}{\text{Log}\left[\frac{hwb}{hwa}\right]} - \dfrac{\frac{hwb}{2\,kT}\,\text{Coth}\left[\frac{hwb}{2\,kT}\right]}{\text{Log}\left[\frac{hwb}{hwa}\right]}$

In[198]:=

```
Plot[{CperNw[kT, 1], CperNw[kT, .5]}, {kT, 0, 4}, PlotRange → All]
```

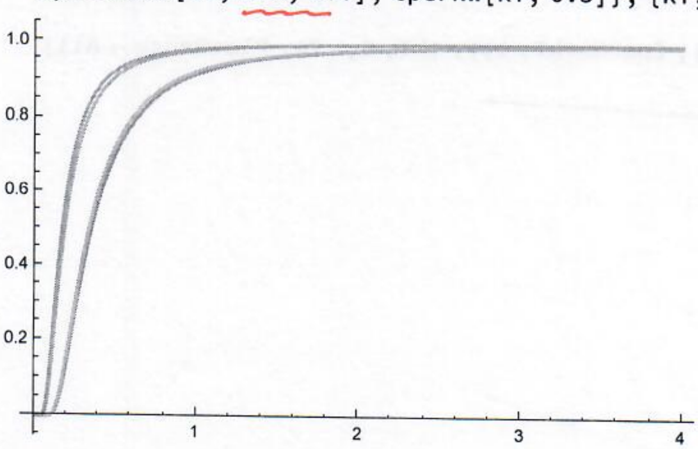
Out[198]=



In[209]:=

```
Plot[{CperNwave[kT, 1., 1.1], CperNw[kT, 1],
  CperNwave[kT, 0.5, 0.6], CperNw[kT, 0.5]}, {kT, 0, 4}, PlotRange → All]
```

Out[209]=



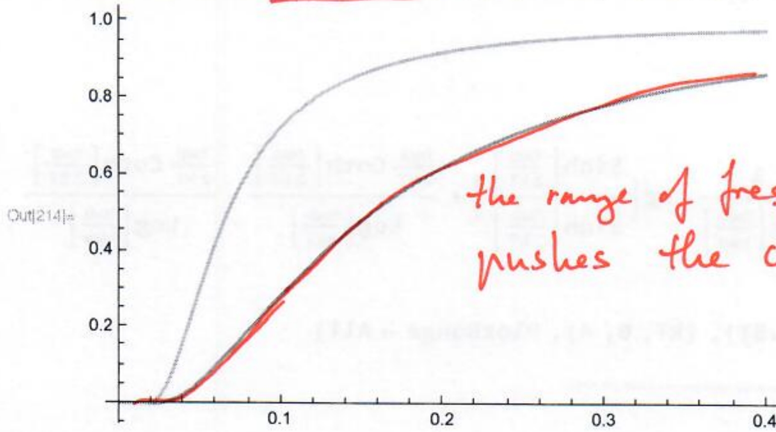
super small range for ω_a, ω_b

$\hookrightarrow \omega_a \approx \omega_b$

agreement with single frequency result (almost...)

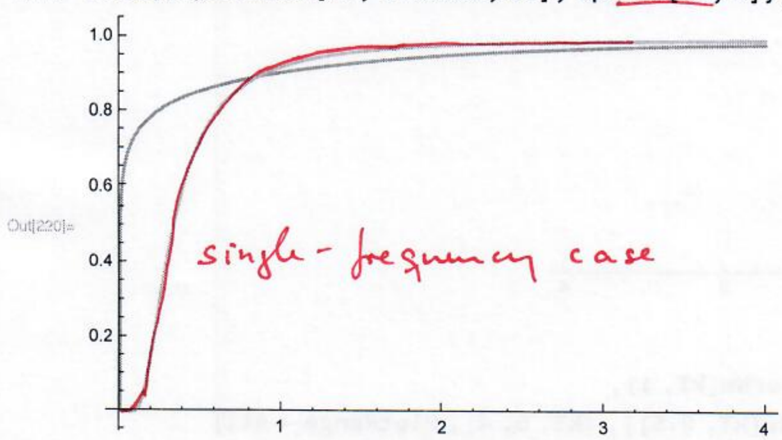
In[214]:= `Plot[{CperNwave[kT, 0.2, 1], CperNw[kT, .2]}, {kT, 0, .4}, PlotRange → All]`

Out[214]=



In[220]:= `Plot[{CperNwave[kT, 0.00001, 10], CperNw[kT, 1]}, {kT, 0, 4}, PlotRange → All]`

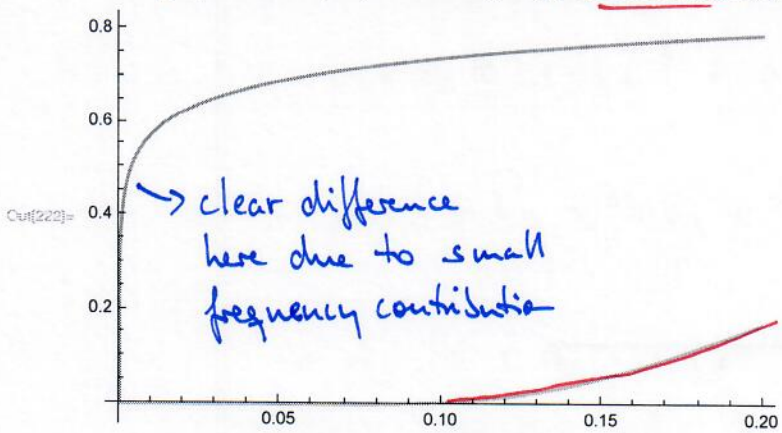
Out[220]=



same plot but blown up

In[222]:= `Plot[{CperNwave[kT, 0.00001, 10], CperNw[kT, 1]}, {kT, 0, .2}, PlotRange → All]`

Out[222]=



single-frequency case

Problem 2:

(a) $B\,|\vec{p}|^4 \rightarrow$ energy

$\downarrow$

$p^2 \rightarrow$ mass · energy

$\Rightarrow p^4 \rightarrow$ mass^2 energy^2

$\Rightarrow B = (\text{mass}^2\ \text{energy})^{-1} = \left(\text{mass}^2\ \text{mass}\ \frac{\text{meter}^2}{\text{time}^2}\right)^{-1}$

(b)

two dimensions $\quad dk_x dk_y \rightarrow 2\pi\, k\, dk$

$$N = 2 \sum_{\vec{k}} \langle n_{\vec{k}} \rangle_{T=0}$$

from spin degree of freedom

assume system is in $\underbrace{\text{"box"}}_{\text{square}}$ of area L^2

$$N = 2 \frac{1}{\left(\frac{2\pi}{L}\right)^2} \iint \langle n_{\vec{k}} \rangle_{T=0}\ d^2k$$

$$= 2 \frac{L^2}{(2\pi)^2} 2\pi \int_0^{k_F} \langle n_{\vec{k}} \rangle_{T=0}\ k\, dk$$

now: $\langle n_{\vec{k}} \rangle$ at $T=0$ is either 1 or 0 for $k < k_F \rightarrow \langle n_{\vec{k}} \rangle = 1$

$$\Rightarrow N = \frac{L^2}{\pi} \underbrace{\int_0^{k_F} k \, dk}_{\frac{1}{2} k_F^2}$$

$$\Rightarrow N = \frac{L^2}{2\pi} k_F^2$$

in 2D, the particle density is $n = \frac{N}{L^2}$

$$\Rightarrow k_F^2 = \frac{2\pi N}{L^2} = 2\pi n$$

We want the Fermi energy $\rightsquigarrow \hbar k_F = p_F$

and $E = B|\vec{p}|^4$

$$\Rightarrow E_F = B p_F^4 = B (\hbar k_F)^4$$

So $\boxed{E_F = B \, \hbar^4 (2\pi n)^2}$

(c) $\frac{1}{\text{mass}^2} \frac{1}{\text{energy}}$ $\quad \text{energy}^4 \quad \text{time}^4 \quad \frac{1}{\text{length}^4}$

$$\text{energy}^{3} \quad \frac{\text{time}^4}{\text{mass}^2\ \text{length}^4}$$

$$\frac{1}{\text{energy}^2}$$

$$E = \frac{1}{2} m v^2$$

$$\Rightarrow \text{mass}\ \frac{\text{length}^2}{\text{time}^2}$$

$\rightarrow$ energy

so, units work out!

Preliminary remarks for Problem 3:

Energy between spin magnetic moment $\vec{\mu}_s$ and uniform magnetic field $\vec{B}$:

$$\hat{V} = - \hat{\vec{\mu}}_s \cdot \vec{B}$$

$$\Rightarrow \quad \hat{\mathcal{H}} = - \hat{\vec{\mu}}_s \cdot \vec{B}$$

For the electron: $\hat{\vec{\mu}}_s = \underbrace{- \frac{2\mu_B}{\hbar}}\hat{\vec{S}}$ and $\hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}}$

Spin and spin magnetic moment of the electron are anti-parallel!

more accurately:

$$\hat{\vec{\mu}}_s = - \frac{g_s \mu_B}{\hbar} \hat{\vec{S}}$$

$$g_s = 2.\underbrace{0023}\ldots$$

small deviation from 2 due to quantum electrodynamics

$$\Rightarrow \quad \hat{\mathcal{H}} = - \hat{\vec{\mu}}_s \cdot \vec{B} = - \left(- \frac{2\mu_B}{\hbar} \right) \hat{\vec{S}} \cdot \vec{B}$$

$$= \frac{2\mu_B}{\hbar} \frac{\hbar}{2} \hat{\vec{\sigma}} \cdot \vec{B} = \mu_B \hat{\vec{\sigma}} \cdot \vec{B}$$

$$= - \mu_B B_z \hat{\sigma}_z$$

Let $\vec{B} = - B_z \hat{e}_z$

We are now ready to tackle the problem.

We want: $\hat{\rho} = \dfrac{e^{-\beta\hat{\mathcal{H}}}}{\mathrm{Tr}\left(e^{-\beta\hat{\mathcal{H}}}\right)}$

in matrix form: $\underset{\substack{\uparrow \\ \text{matrix}}}{\rho} = \begin{pmatrix} \langle\uparrow|\hat{\rho}|\uparrow\rangle & \langle\uparrow|\hat{\rho}|\downarrow\rangle \\ \langle\downarrow|\hat{\rho}|\uparrow\rangle & \langle\downarrow|\hat{\rho}|\downarrow\rangle \end{pmatrix}$

Let's start w/ $e^{-\beta\hat{\mathcal{H}}}$:

$$e^{-\beta\hat{\mathcal{H}}} = e^{-\beta\hat{\mathcal{H}}}\Big(\underbrace{|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|}_{\text{identity}}\Big)$$

$$= e^{-\beta\hat{\mathcal{H}}}|\uparrow\rangle\langle\uparrow| + e^{-\beta\hat{\mathcal{H}}}|\downarrow\rangle\langle\downarrow|$$

look at $e^{-\beta\hat{\mathcal{H}}}|\uparrow\rangle = e^{+\beta\mu_B B_z\hat{\sigma}_z}|\uparrow\rangle$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\beta\mu_B B_z\hat{\sigma}_z\right)^n|\uparrow\rangle$$

Taylor expansion

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\beta\mu_B B_z\right)^n|\uparrow\rangle$$

$$= e^{\beta\mu_B B_z}|\uparrow\rangle$$

Similarly:

$$e^{-\beta \hat{\mathcal{H}}} |\downarrow\rangle = e^{\beta \mu_B B_z \hat{\sigma}_z} |\downarrow\rangle$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} (\beta \mu_B B_z \hat{\sigma}_z)^n |\downarrow\rangle$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} (\beta \mu_B B_z)^n (-1)^n |\downarrow\rangle$$

$\hat{\sigma}_z^n |\downarrow\rangle = (-1)^n |\downarrow\rangle$

$$= e^{-\beta \mu_B B_z} |\downarrow\rangle$$

$$\Rightarrow e^{-\beta \hat{\mathcal{H}}} = e^{\beta \mu_B B_z} |\uparrow\rangle + e^{-\beta \mu_B B_z} |\downarrow\rangle$$

In matrix form:

$$\begin{pmatrix} \langle\uparrow| e^{-\beta \hat{\mathcal{H}}} |\uparrow\rangle & \langle\uparrow| e^{-\beta \hat{\mathcal{H}}} |\downarrow\rangle \\ \langle\downarrow| e^{-\beta \hat{\mathcal{H}}} |\uparrow\rangle & \langle\downarrow| e^{-\beta \hat{\mathcal{H}}} |\downarrow\rangle \end{pmatrix}$$

$$= \begin{pmatrix} e^{\beta \mu_B B_z} & 0 \\ 0 & e^{-\beta \mu_B B_z} \end{pmatrix}$$

What about $\mathrm{Tr}\, e^{-\beta \hat{\mathcal{H}}}$?

$$\mathrm{Tr}\, e^{-\beta \hat{\mathcal{H}}} = e^{\beta \mu_B B_z} + e^{-\beta \mu_z B_z}$$

Summing up the diagonal elements

$$\Rightarrow \quad \hat{\rho} = \frac{1}{e^{\beta \mu_B B_z} + e^{-\beta \mu_B B_z}} \begin{pmatrix} e^{\beta \mu_B B_z} & 0 \\ 0 & e^{-\beta \mu_B B_z} \end{pmatrix}$$

We see: $Tr(\hat{\rho}) = 1$.

Thermal expectation value of $\langle \hat{\sigma}_z \rangle$:

$$\langle \hat{\sigma}_z \rangle = \frac{Tr(\hat{\rho}\,\hat{\sigma}_z)}{Tr(\hat{\rho})} = Tr(\hat{\rho}\,\hat{\sigma}_z)$$

$$= Tr\left(\begin{pmatrix} e^{\beta \mu_B B_z} & 0 \\ 0 & e^{-\beta \mu_B B_z} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \cdot \frac{1}{e^{\beta \mu_B B_z} + e^{-\beta \mu_B B_z}}$$

$$= \frac{e^{\beta \mu_B B_z} - e^{-\beta \mu_B B_z}}{e^{\beta \mu_B B_z} + e^{-\beta \mu_B B_z}}$$

$$= \tanh(\beta \mu_B B_z)$$

Problem 4:

(a) Free particle in a box w/ periodic BCs.

$$E = \frac{\hbar^2 k^2}{2m}$$

$$\phi_{\vec{k}}(\vec{r}) = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{r}} \qquad \text{("box normalization")}$$

$$\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z) \quad \text{where } n_x = 0, \pm 1, \pm 2, \ldots$$

$$n_y = \ldots$$

$$n_z = \ldots$$

So far, we have just collected information from previous homework.

We want the density matrix $\hat{\rho}$ in the canonical ensemble: $\hat{\rho} = \frac{e^{-\beta \hat{\mathcal{H}}}}{Tr(e^{-\beta \hat{\mathcal{H}}})}$

We need to find an expression for $e^{-\beta\hat{\mathcal{H}}}$.

As before, insert a complete set.

We have:

$$\sum_{\vec{k}} |\phi_{\vec{k}}\rangle\langle\phi_{\vec{k}}| = 1$$

$$\Rightarrow \quad e^{-\beta\hat{\mathcal{H}}} = e^{-\beta\hat{\mathcal{H}}} \sum_{\vec{k}} |\phi_{\vec{k}}\rangle\langle\phi_{\vec{k}}|$$

$$= \sum_{\vec{k}} \underbrace{e^{-\beta\hat{\mathcal{H}}} |\phi_{\vec{k}}\rangle}\langle\phi_{\vec{k}}|$$

to evaluate this, we need to perform a Taylor expansion, then act w/ $\hat{\mathcal{H}}^n$ onto $|\phi_{\vec{k}}\rangle$, and then collect terms

This yields $e^{-\beta\hat{\mathcal{H}}}|\phi_{\vec{k}}\rangle = e^{-\beta\frac{\hbar^2k^2}{2m}}|\phi_{\vec{k}}\rangle$

$$= \sum_{\vec{k}} e^{-\beta\frac{\hbar^2k^2}{2m}} |\phi_{\vec{k}}\rangle\langle\phi_{\vec{k}}|$$

$$\Rightarrow \boxed{e^{-\beta\hat{\mathcal{H}}} = \sum_{k} |\phi_{\vec{k}}\rangle \exp\left(-\beta\frac{\hbar^2k^2}{2m}\right)\langle\phi_{\vec{k}}|}$$

$$\Rightarrow \boxed{\langle\vec{r}|e^{-\beta\hat{\mathcal{H}}}|\vec{r}\,'\rangle = \frac{1}{L^3}\sum_{\vec{k}} e^{+i\vec{k}\cdot\vec{r}}\, e^{-\beta\frac{\hbar^2k^2}{2m}}\, e^{-i\vec{k}\cdot\vec{r}\,'}}$$

where we used $\langle\vec{r}|\phi_{\vec{k}}\rangle = \frac{1}{L^{3/2}}e^{i\vec{k}\cdot\vec{r}}$ &

$$\langle \phi_{\vec{k}} | \vec{r}\,' \rangle = \frac{1}{L^{3/2}} e^{-i\vec{k}\cdot\vec{r}\,'}$$

$\frac{1}{\mathrm{Tr}(e^{-\beta\hat{\mathcal{H}}})} \langle \vec{r} \,|\, e^{-\beta\hat{\mathcal{H}}} \,|\, \vec{r}\,' \rangle$ is referred to as density matrix in the coordinate representation.

Now, we want to simplify this → the infinite sum is very inconvenient.

Let's rewrite the sum as an integral over $dk_x\, dk_y\, dk_z$

$$k_x = \frac{2\pi}{L} n_x \qquad \text{where } n_x = 0, \pm 1, \pm 2, \ldots$$

$$\Delta n_x = 1$$

$$\Rightarrow dk_x \mathrel{\hat{=}} \frac{2\pi}{L} \underbrace{\Delta n_x}_{=1}$$

$$\Rightarrow \frac{L\, dk_x}{2\pi} \mathrel{\hat{=}} 1$$

and $$\frac{L^3\, dk_x\, dk_y\, dk_z}{(2\pi)^3} \mathrel{\hat{=}} 1$$

So, we can rewrite our infinite sum as an integral:

$$\langle \vec{r} \,|\, e^{-\beta \hat{\mathcal{H}}} \,|\, \vec{r}\,' \rangle = \frac{1}{(2\pi)^3} \iiint \exp\left(-\frac{\beta \hbar^2 k^2}{2m} + i\vec{k}\cdot(\vec{r}-\vec{r}\,')\right) d^3k$$

$$= \frac{1}{(2\pi)^3} \iiint e^{-\frac{\beta \hbar^2 k^2}{2m}} \cos\left(\vec{k}\cdot(\vec{r}-\vec{r}\,')\right) d^3k$$

$$+ \frac{i}{(2\pi)^3} \iiint \underbrace{e^{-\frac{\beta \hbar^2 k^2}{2m}} \sin\left(\vec{k}\cdot(\vec{r}-\vec{r}\,')\right)}_{=0} d^3k$$

$$= \frac{1}{(2\pi)^3} \left(\sqrt{\frac{\pi}{\frac{\beta\hbar^2}{2m}}}\right)^3 \exp\left(-\frac{|\vec{r}-\vec{r}\,'|}{4\,\frac{\beta\hbar^2}{2m}}\right)$$

$$= \left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} \exp\left(-\frac{m|\vec{r}-\vec{r}\,'|}{2\beta\hbar^2}\right)$$

Next, we want to calculate $\mathrm{Tr}\left(e^{-\beta \hat{\mathcal{H}}}\right)$.

$$\mathrm{Tr}\left(e^{-\beta\hat{\mathcal{H}}}\right) = \iiint \langle \vec{r} | e^{-\beta\hat{\mathcal{H}}} | \vec{r} \rangle \, d^3 r$$

$$= \iiint \sum_{\vec{k}} \langle \vec{r} | \phi_{\vec{k}} \rangle e^{-\beta \frac{\hbar^2 k^2}{2m}} \langle \phi_{\vec{k}} | \vec{r} \rangle \, d^3 r$$

using $e^{-\beta\hat{\mathcal{H}}}$ $= \sum_{\vec{k}} |\phi_{\vec{k}}\rangle e^{-\beta \frac{\hbar^2 k^2}{2m}} \langle \phi_{\vec{k}}|$

$$= \iiint \underbrace{\exp\left(-\frac{m|\vec{r}-\vec{r}|}{2\beta\hbar^2}\right)}_{1} \underbrace{\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2}}_{\text{indep. of } r} d^3 r$$

using our previous results (for sum over $\vec{k}$)

$$\boxed{\mathrm{Tr}\left(e^{-\beta\hat{\mathcal{H}}}\right) = \underbrace{V}_{L^3} \left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2}}$$

$$\Rightarrow \langle \vec{r} | \hat{\rho} | \vec{r}\,' \rangle = \langle \vec{r} | \frac{e^{-\beta\hat{\mathcal{H}}}}{\mathrm{Tr}\left(e^{-\beta\hat{\mathcal{H}}}\right)} | \vec{r}\,' \rangle$$

$$= \frac{\langle \vec{r} | e^{-\beta\hat{\mathcal{H}}} | \vec{r}\,' \rangle}{\mathrm{Tr}\left(e^{-\beta\hat{\mathcal{H}}}\right)}$$

$$= \frac{1}{V} \exp\left(-\frac{m|\vec{r}-\vec{r}\,'|}{2\beta\hbar^2}\right)$$

Finally:

$$\boxed{\langle \vec{r} \,|\, \hat{\rho} \,|\, \vec{r}\,' \rangle = \frac{1}{V} \exp\left(- \frac{m |\vec{r} - \vec{r}\,'|}{2\beta \hbar^2} \right)}$$

(b) $$\boxed{\langle \vec{r} \,|\, \hat{\rho} \,|\, \vec{r} \rangle = \frac{1}{V}}$$

What does this mean?

↳ How can we interpret $\langle \vec{r} | \hat{\rho} | \vec{r} \rangle$?

$$\hat{\rho} = \frac{e^{-\beta \hat{\mathcal{H}}}}{\mathrm{Tr}(e^{-\beta \hat{\mathcal{H}}})}$$

our earlier expression

Look at $\langle \delta(\vec{r}\,'' - \vec{r}) \rangle$: average of finding $\vec{r}$ at position $\vec{r}\,''$ ⟶ it's the operator that tells us where the particle is

$$\langle \delta(\vec{r}\,'' - \vec{r}) \rangle$$

$$= \mathrm{Tr}\left(\hat{\rho}\, \delta(\vec{r}\,'' - \vec{r}) \right) = \frac{\int \langle \vec{r} | e^{-\beta \hat{\mathcal{H}}} \delta(\vec{r}\,'' - \vec{r}) | \vec{r} \rangle d^3\vec{r}}{\mathrm{Tr}(e^{-\beta \hat{\mathcal{H}}})}$$

$$= \frac{\langle \vec{r}\,'' | e^{-\beta \hat{\mathcal{H}}} | \vec{r}\,'' \rangle}{\mathrm{Tr}(e^{-\beta \hat{\mathcal{H}}})} = \langle \vec{r}\,'' | \hat{\rho} | \vec{r}\,'' \rangle$$

$\boxed{\text{So: } \langle \vec{r} | \hat{\varrho} | \vec{r} \rangle \text{ just gives us the density.}}$

The density is independent of $\vec{r}$!
(this is the case because we have a free particle)

(c) Want to calulate $\langle \hat{\mathcal{H}} \rangle = \mathrm{Tr}(\hat{\varrho}\hat{\mathcal{H}})$

$$\mathrm{Tr}(\hat{\varrho}\,\hat{\mathcal{H}}) = \frac{\mathrm{Tr}(e^{-\beta\hat{\mathcal{H}}}\,\hat{\mathcal{H}})}{\mathrm{Tr}(e^{-\beta\hat{\mathcal{H}}})}$$

$$= -\frac{\partial}{\partial\beta}\log \mathrm{Tr}(e^{-\beta\hat{\mathcal{H}}})$$

$$= -\frac{\partial}{\partial\beta}\log\left(V\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2}\right)$$

using our earlier result

$$= \frac{3}{2}\frac{1}{\beta} = \frac{3}{2}kT$$

So: $\boxed{\langle \hat{\mathcal{H}} \rangle = \frac{3}{2}kT}$