Advanced Statistical Physics Homework

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1. Please calculate the average ensemble of a free particle placed in a cube with sides of length L.

Answer 1. *For this free particle, Hamiltonian is formed in* $\hat{\boldsymbol{H}} = -\dfrac{\hbar^2}{2m}\nabla^2$ *, and its eigenfunctions is defined by* $\phi_{\boldsymbol{k}}(x, y, z) = \langle \boldsymbol{r}|\boldsymbol{k}\rangle = \dfrac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{L^{3/2}}$ *. Besides that* $\phi_{\boldsymbol{k}}(x, y, z)$ *shall satisfy periodic boundary condition, we can get eigenenergy by solving Schrödinger equation :*

$$\hat{\boldsymbol{H}}\phi_{\boldsymbol{k}} = E_{\boldsymbol{k}}\phi_{\boldsymbol{k}} \longrightarrow E_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m},\ \boldsymbol{k} = (k_x + k_y + k_z) = \frac{2\pi}{L}(n_x + n_y + n_z) \tag{0.1}$$

which

$$\begin{aligned} E_{\boldsymbol{k}} &= \frac{\hbar^2 k^2}{2m} \\ \boldsymbol{k} &\equiv (k_x, k_y, k_z) = \frac{2\pi}{L}(n_x, n_y, n_z) \\ (n_x, n_y, n_z) &= 0, \pm 1, \pm 2, \cdots \end{aligned}$$

Free particle partition function :

$$Z = Tre^{-\beta\hat{\boldsymbol{H}}} = \sum_k \int e^{-\beta E_k}\phi^*_{\boldsymbol{k}}(\boldsymbol{r})\phi_{\boldsymbol{k}}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = V\left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} \tag{0.2}$$

Operational representation of canonical ensemble :

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{\boldsymbol{H}}} = \sum_{\boldsymbol{k}} |\boldsymbol{k}\rangle \frac{1}{Z} e^{-\beta \hat{\boldsymbol{H}}} \langle \boldsymbol{k}| = \sum_{\boldsymbol{k}} |\boldsymbol{k}\rangle \frac{1}{Z} e^{-\beta E_k} \langle \boldsymbol{k}| \tag{0.3}$$

Under coordinate representation, we can describe matrix elements by :

$$\begin{aligned}\langle \boldsymbol{r}| \hat{\rho} |\boldsymbol{r'}\rangle &= \sum_{\boldsymbol{k}} \langle \boldsymbol{r}|\boldsymbol{k}\rangle \frac{1}{Z} e^{-\beta \hat{\boldsymbol{H}}} \langle \boldsymbol{k}|\boldsymbol{r'}\rangle = \sum_{\boldsymbol{k}} \phi^*_{\boldsymbol{k}}(\boldsymbol{r}) \frac{1}{Z} e^{-\beta \hat{\boldsymbol{H}}} \phi_{\boldsymbol{k}}(\boldsymbol{r}) \\ &= \frac{1}{V} \exp\left(-\frac{m(r-r')^2}{2\hbar^2\beta}\right)\end{aligned} \tag{0.4}$$

The average ensemble of Hamiltonian is :

$$\begin{aligned}\left\langle \hat{\boldsymbol{H}} \right\rangle &= Tr(\hat{\rho}\hat{\boldsymbol{H}}) = -\frac{\partial}{\partial\beta} \ln\left[Tr(e^{-\beta\hat{\boldsymbol{H}}})\right] = -\frac{\partial}{\partial\beta}\ln Z \\ &= \frac{3}{2} k_B T\end{aligned} \tag{0.5}$$

2. Please calculate the relationship between average population number c with temperature and specific heat capacity of Bose-Einstein condensation.

Answer 2. *The equation of state for ideal Boson gas :*

$$\begin{cases} \dfrac{P}{k_B T} = \dfrac{1}{\lambda^3} g_{5/2}(z) - \dfrac{1}{V}\ln(1-z) \\ \\ \dfrac{1}{v} = \dfrac{1}{\lambda^3} g_{3/2}(z) + \dfrac{1}{V}\dfrac{z}{1-z} \end{cases} \tag{0.6}$$

For specific capacity is $v = \dfrac{V}{N}$ *, mean thermal wavelength is* $\lambda = \sqrt{\dfrac{2\pi\hbar^2}{mk_BT}}$ *, and fugacity* $z = e^{\beta\mu}$ *, which* μ

is chemical potential. For Boson gas we have : $0 \leq z \leq 1$ *, it's obvious that* $z \geq 0$ *, and we can confirm it by average population number* $\langle n_0 \rangle = \dfrac{z}{1-z} \geq 0$ *.* $g_n(z)$ *is generated by :*

$$g_n(z) = \sum_{l=1}^{\infty} \frac{z^l}{l^n} \tag{0.7}$$

when z *valued from* 0 *to* 1 *,* $g_n(z)$ *is positive monotone increasing and it's a limited function. If* $n > 1$ *,* $g_n(z)$ *would turn into Riemann-*ζ *function :*

$$g_n(1) = \sum_{l=1}^{\infty} \frac{1}{l^n} = \zeta(n) \quad (n > 1) \tag{0.8}$$

And $g_n(z)$ *diverged when* $n \leq 1$ *, so we have :*

$$g_{3/2}(z) \leq g_{3/2}(1) = \zeta(3/2) = 2.612... \tag{0.9}$$

Now we'll continue to discuss conditions that produce condensation. First, we can rewrite the second formula of Equ.0.6 :

$$\lambda^3 \frac{\langle n_0 \rangle}{V} = \frac{\lambda^3}{v} - g_{3/2}(z) \tag{0.10}$$

When $\dfrac{\langle n_0 \rangle}{V} > 0$ *, the condensation achieved, and it must be true when* $\dfrac{\lambda^3}{v} > g_{3/2}(1)$ *.*

Discuss the critical condition :

$$\frac{\lambda_c^3}{v} = g_{3/2}(z) \tag{0.11}$$

then we will get critical temperature and critically specific heat capacity :

$$T_c = \frac{2\pi\hbar^2}{mk_B[v g_{3/2}(1)]^{2/3}} \qquad v_c = \frac{\lambda^3}{g_{3/2}(1)} \tag{0.12}$$

When $T < T_c$ *(* v *is constant) or* $v < v_c$ *(* T *is constant) , Bose-Einstein condensation occurred. That is to say creation conditions of Bose-Einstein condensation are low temperature and high density.*

Besides, when $V \to \infty$ *, fugacity* z *tends to*

$$z = \begin{cases} 1 & \left(\frac{\lambda^3}{v} \geq g_{3/2}(1)\right) \\ \textit{The roots of } g_{3/2}(z) = \frac{\lambda^3}{v} & \left(\frac{\lambda^3}{v} \leq g_{3/2}(1)\right) \end{cases} \tag{0.13}$$

And from Equ.0.10 , we have

$$\frac{\langle n_0 \rangle}{N} = \begin{cases} 1 - \left(\frac{T}{T_c}\right)^{\frac{3}{2}} = 1 - \frac{v}{v_c} & \left(\frac{\lambda^3}{v} \geq g_{3/2}(1)\right) \\ 0 & \left(\frac{\lambda^3}{v} \leq g_{3/2}(1)\right) \end{cases} \tag{0.14}$$