Assignment 8

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1 Kadar Ch. 6 Problem 8

We have a density operator $\hat{\rho}$. Recall that classically we would have some probability density $p(t)$ for being in a certain state (position and momentum). Integrating the probability dnesiyt over all phase space must result in 1. Likewise, the density operator describes the statistics of a quantum system and must have $\mathrm{tr}\left[\hat{\rho}\right] = 1$.

1.1 Part a)

Classically

$$S = -\sum_{i=1}^{M} p_i \ln p_i$$

so we expect quantum mechanically

$$S = -\mathrm{tr}\left[\hat{\rho}(t) \ln \hat{\rho}(t)\right]. \tag{1}$$

Classically the probability density evolves with time by obeying the Liouville's Theorem

$$\frac{d\hat{\rho}}{dt} = \frac{\partial \hat{\rho}}{\partial t} - \left\{\hat{\mathcal{H}}, \hat{\rho}\right\}$$

where $\{\quad,\quad\}$ are Poisson brackets and $\hat{\mathcal{H}}$ is the Hamiltonian operator. By chosing the eigenstates as the basis Kadar demonstrates that indepedent of basis

$$i\hbar \frac{\partial}{\partial t}\hat{\rho} = \left[\hat{\mathcal{H}}, \hat{\rho}\right] \tag{2}$$

where $[\quad,\quad]$ are commutators.

So the rate of change of entropy (applied directly to the operator and independent of basis) is

$$\begin{aligned}\frac{\partial S}{\partial t} &= -\frac{\partial}{\partial t}\mathrm{tr}\left[\hat{\rho}(t)\ln\hat{\rho}(t)\right]\\ &= -\mathrm{tr}\left[\frac{\partial}{\partial t}\hat{\rho}(t)\ln\hat{\rho}(t)\right]\\ &= -\mathrm{tr}\left[\ln\hat{\rho}(t)\frac{\partial\hat{\rho}}{\partial t}+\hat{\rho}\frac{1}{\hat{\rho}}\frac{\partial\hat{\rho}}{\partial t}\right]\\ &= -\mathrm{tr}\left[(1+\ln\hat{\rho}(t))\left(\frac{1}{i\hbar}\right)i\hbar\frac{\partial\hat{\rho}}{\partial t}\right]\\ &= -\left(\frac{1}{i\hbar}\right)\mathrm{tr}\left[(1+\ln\hat{\rho}(t))\left[\hat{\mathcal{H}},\hat{\rho}\right]\right]\end{aligned}$$

$$\boxed{i\hbar\frac{\partial S}{\partial t} = \mathrm{tr}\left[(1+\ln\hat{\rho}(t))\left[\hat{\rho},\hat{\mathcal{H}}\right]\right]} \tag{3}$$

which I suppose should be writen

$$\left[\hat{\mathcal{H}},S\right] = \mathrm{tr}\left[(1+\ln\hat{\rho}(t))\left[\hat{\rho},\hat{\mathcal{H}}\right]\right]$$

1.2 Part b)

Find the density operator that maximizes the quantum mechanical entropy. The energy is fixed at $\mathrm{tr}\left[\hat{\rho}\hat{\mathcal{H}}\right] = E$ and we also must remember normalization $\mathrm{tr}\left[\hat{\rho}\right]$.

So we want to use Lagrange multipliers α and β for these two conditions

$$\begin{aligned}S &= -\mathrm{tr}\left[\hat{\rho}\ln\hat{\rho}\right]\\ &= \mathrm{tr}\left[-\hat{\rho}\left(\ln\hat{\rho}+\alpha+\beta\hat{\mathcal{H}}\right)\right]+\alpha+\beta E.\end{aligned}$$

We search for the extrema.

$$\begin{aligned}\left.\frac{\partial S}{\partial\hat{\rho}}\right|_{\hat{\rho}_{\max}} &= 0\\ &= \frac{\partial}{\partial\hat{\rho}}\left\{\mathrm{tr}\left[-\hat{\rho}\left(\ln\hat{\rho}+\alpha+\beta\hat{\mathcal{H}}\right)\right]+\alpha+\beta E\right\}\\ &= -\mathrm{tr}\left[\frac{\partial}{\partial\hat{\rho}}\hat{\rho}\left(\ln\hat{\rho}+\alpha+\beta\hat{\mathcal{H}}\right)\right]\\ &= -\left(\ln\hat{\rho}+\alpha+\beta\hat{\mathcal{H}}+1\right)\end{aligned}$$

$$\boxed{\hat{\rho}_{\max} = \exp\left(-\alpha-1-\beta\hat{\mathcal{H}}\right)} \tag{4}$$

1.3 Part c)

The maximizing density operator is stable if it doesn't change with time:

$$\begin{aligned}\left[\hat{\mathcal{H}}, \hat{\rho}_{\max}\right] &= i\hbar\frac{\partial \hat{\rho}_{\max}}{\partial t} \\ &= i\hbar\frac{\partial}{\partial t}\exp\left(-\alpha - 1 - \beta\hat{\mathcal{H}}\right) \\ &= e^{-(\alpha+1)}\left(-\beta\right)e^{-\beta\hat{\mathcal{H}}} i\hbar\frac{\partial}{\partial t}\hat{\mathcal{H}} \\ &= -\beta\hat{\rho}_{\max}\left[\hat{\mathcal{H}}, \hat{\mathcal{H}}\right] \\ &= 0.\end{aligned}$$

We've shown it explicitly for this case but:

- Since the commutator of $\hat{\mathcal{H}}$ with any function of $\hat{\mathcal{H}}$ will undoubtably include the commutator of $\hat{\mathcal{H}}$ with itself, it must be zero.

2 Kadar Ch. 7 Problem 16

Consider a gas of non-interaction bosons in d dimensions. I'll use Kadar's notation without introducing variables in this question.

2.1 Part a)

We find the grand potential by setting $\eta = +$ and find

$$\mathcal{Q}_+ = \prod_{\vec{k}} \frac{1}{1 - \exp\left[\beta\left(\mu - \epsilon_k\right)\right]}.$$

2.1.1 Grand Potential

If we take the logarithm then the product series becomes a summation

$$\ln \mathcal{Q}_+ = -\sum_k \ln\left(1 - \exp\left[\beta\left(\mu - \epsilon_k\right)\right]\right). \tag{5}$$

We take the series to the continuous limit in d-dimensions and get an integral (see pg. 106 of Kadar for a refresher if you need or for notation)

$$\sum_k \to \int_0^\infty \frac{V d^d k}{\left(2\pi\right)^d} = \frac{V S_d}{\left(2\pi\right)^d}\int_0^\infty k^{d-1} dk$$

Using this limit

$$\begin{aligned}\ln \mathcal{Q}_+ &= -\sum_k \ln\left(1 - \exp\left[\beta\left(\mu - \epsilon_k\right)\right]\right) \\ &= -\frac{V S_d}{\left(2\pi\right)^d}\int_0^\infty k^{d-1}\ln\left(1 - \exp\left[\beta\left(\mu - \epsilon_k\right)\right]\right) dk\end{aligned}$$

Let's let

$$
\begin{aligned}
z &= e^{\beta\mu} && \text{(6a)}\\
\epsilon_k &= \hbar ck && \text{(6b)}\\
x &= \beta\hbar ck. && \text{(6c)}
\end{aligned}
$$

So then the logarithm of the grand partition function looks like

$$
\begin{aligned}
\ln \mathcal{Q}_+ &= -\frac{VS_d}{(2\pi)^d}\int_0^\infty k^{d-1}\ln\left(1-ze^{-x}\right)dk\\
&= -\frac{VS_d}{(2\pi)^d}\int_0^\infty \left(\frac{x}{\beta\hbar c}\right)^{d-1}\ln\left(1-ze^{-x}\right)\left(\frac{1}{\beta\hbar c}\right)dx\\
&= -\left(\frac{k_\mathrm{B}T}{2\pi\hbar c}\right)^d VS_d\int_0^\infty x^{d-1}\ln\left(1-ze^{-x}\right)dx.
\end{aligned}
$$

we're going to do integration by parts so let's let

$$
\begin{aligned}
\xi &= -\left(\frac{k_\mathrm{B}T}{2\pi\hbar c}\right)^d VS_d && \text{(7a)}\\
u &= \ln\left(1-ze^{-x}\right) && \text{(7b)}\\
v &= x^d && \text{(7c)}
\end{aligned}
$$

These varaibles make it more clear that

$$
\begin{aligned}
\ln \mathcal{Q}_+ &= \xi\int_0^\infty \frac{1}{d}\frac{dv}{dx}udx\\
&= \frac{\xi}{d}\left[uv-\int_0^\infty v\frac{du}{dx}udx\right]\\
&= \frac{\xi}{d}\left[x^d\ln\left(1-ze^{-x}\right)\Big|_0^\infty-\int_0^\infty\frac{zx^de^{-x}}{1-ze^{-x}}dx\right]\\
&= \frac{\xi}{d}\left[0-\int_0^\infty\frac{x^d}{z^{-1}e^x-1}dx\right]\\
&= \frac{\xi}{d}\int_0^\infty\frac{x^d}{1-z^{-1}e^x}dx.
\end{aligned}
$$

From pg. 189 of Kadar we see

$$
\ln \mathcal{Q}_+ = \left(\frac{k_\mathrm{B}T}{2\pi\hbar c}\right)^d\frac{VS_d}{d}d!f_{d+1}^+(z) \tag{8}
$$

and if we use $\lambda_c = hc/k_\mathrm{B}T$ then

$$
\boxed{\mathcal{G} = -k_\mathrm{B}T\frac{V}{\lambda_c^d}\frac{\pi^d/2d!}{(d/2)!}f_{d+1}^+(z)} \tag{9}
$$

2.1.2 Density

The density is then

$$\begin{aligned} n &= \frac{N}{V} \\ &= -\frac{1}{V}\frac{\partial \mathcal{G}}{\partial \mu} \\ &= -\frac{\beta z}{V}\frac{\partial \mathcal{G}}{\partial z} \\ &= -\frac{\beta}{V}\left(-k_{\mathrm{B}}T\frac{V}{\lambda_c^d}\frac{\pi^{d/2}d!}{(d/2)!}\right) z\frac{\partial}{\partial z} f_{d+1}^{+}(z)\,. \end{aligned}$$

The important thing to notice is on of the nice properties of $f_{d+1}^{+}(z)$ whcih can be found on pg 194 of Kadar, namely

$$z\frac{\partial}{\partial z} f_{d+1}^{+}(z) = f_d^{+}(z)\,.$$

That means that the density is

$$\boxed{n = \left(\frac{1}{\lambda_c^d}\frac{\pi^{d/2}d!}{(d/2)!}\right) f_d^{+}(z)}. \tag{10}$$

2.2 Part b)

The pressure is simply

$$\boxed{P = -\frac{\mathcal{G}}{V}} \tag{11}$$

and the energy is

$$\begin{aligned} E &= \beta\frac{\partial \mathcal{G}}{\partial \beta} \\ &= -\frac{\partial}{\partial \beta}\ln \mathcal{Q} \\ &= -\frac{\partial}{\partial \beta}\left(\left(\frac{1}{\beta 2\pi\hbar c}\right)^d \frac{VS_d}{d} d! f_{d+1}^{+}(z)\right) \\ &= \frac{d}{\beta}\ln \mathcal{Q} \end{aligned}$$

$$\boxed{E = -d\mathcal{G}}. \tag{12}$$

So then the ratio is

$$\boxed{\frac{E}{PV} = d} \tag{13}$$

as expected.

2.3 Part c)

We know that at high temperatures in the classical limit μ is a large negative number. As the temperature goes to zero, so does the chemical potential. We assume that the chemical potential goes to zero faster than the temperature and the limit is

$$\lim_{T\to 0} z = 1 \tag{14}$$

i.e. the chemical potential is approximately zero but the temperature is small but finite.

So then given a density n, at what temperature does the Eq. 14 apply? Taking the limit of z but not T we solve Eq. 10 for the resulting critical temperatures

$$\begin{aligned} n &= \left(\frac{1}{\lambda_c^d}\frac{\pi^{d/2}d!}{(d/2)!}\right) f_d^+(1) \\ &= \left(\frac{k_{\mathrm{B}}T_c}{hc}\right)^d \frac{\pi^{d/2}d!}{(d/2)!}\zeta(d) \\ \left(\frac{k_{\mathrm{B}}T_c}{hc}\right)^d &= \frac{n}{\zeta(d)}\frac{(d/2)!}{\pi^{d/2}d!} \end{aligned}$$

$$\boxed{k_{\mathrm{B}}T_c = hc\sqrt[d]{\frac{n}{\zeta(d)}\frac{(d/2)!}{\pi^{d/2}d!}}} \tag{15}$$

where we have used that $f_d^+(1) = \zeta(d)$ is the Riemann zeta function which has tabulated solutions. There called critical because in $T < T_c$ $\mu = 0$ while for $T > T_c$ μ is finite and negative.

For example

$$\begin{aligned} \zeta(4) &= \frac{\pi^2}{90} \\ \zeta(3) &\approx 1.2 \\ \zeta(2) &= \frac{\pi^2}{6} \end{aligned}$$

but

$$\zeta(1) = \infty$$

which means that $T_c = 0$ for $d = 1$ *i.e.* in 1-D there is no critical temperature.

2.4 Part d)

Below T_c the chemical potential is zero and $z = 1$. The heat capacity is

$$\begin{aligned} C &= \frac{\partial E}{\partial T} \\ &= -d\frac{\partial \mathcal{G}}{\partial T} \\ &= -d\,(d+1)\,\frac{\mathcal{G}}{T} \end{aligned}$$

and in the region of interest

$$\boxed{C = d\,(d+1)\,\frac{k_{\mathrm{B}}T}{T}\,\frac{V}{\lambda_c^d}\,\frac{\pi^d/2d!}{(d/2)!}\zeta(d+1)}$$

2.5 Part e)

The dimensionless heat capacity at $z = 1$ is

$$\boxed{\frac{C}{Nk_{\mathrm{B}}} = \frac{d\,(d+1)\,\zeta(d+1)}{\zeta(d)}}$$

3 Kadar Ch. 7 Problem 17

We want to talk about the electrons in graphene. So they are relativistic 2-D fermions of spin 1/2 giving $g = 2$ and an energy of

$$\epsilon_{\pm}(\vec{k}) = \pm\hbar v \left|\vec{k}\right| \tag{16}$$

3.1 Part a)

At $T = 0$ all the negative energy states are occupied and all the positive states are empty. So we can imagine the system to be made up of two *phases.* Electrons in the negative state and holes in the positive state. At $T = 0$ the two phases coexist indefinately. Whenever, two phases coexist in equalibrium the chemical potential is

$$\boxed{\mu = 0}. \tag{17}$$

3.2 Part b)

Let's talk about the total energy as an average *i.e.* in terms of the sum all states of the energy in that state times the average occupation number in that state

$$E(T) = \sum_{k,s}\left[\langle n_{k,-}\rangle_{-}\,\epsilon_{+} + \langle n_{k,-}\rangle_{-}\,\epsilon_{-}\right]$$

Since they are fermions only one electron can be in each state and so the average occupation numbers must be simply $\langle n_k\rangle_{-} = 1 - \langle n_k\rangle_{+}$ meaning

$$\begin{aligned}
E(T) &= \sum_{k,s}\left[\langle n_{k,+}\rangle_{-}\,\epsilon_{+} + \Big(1 - \langle n_{k,+}\rangle_{-}\Big)\,\epsilon_{-}\right] \\
&= \sum_{k,s}\left[\langle n_{k,+}\rangle_{-}\,\epsilon_{+} - \langle n_{k,+}\rangle_{-}\,\epsilon_{-}\right] + \sum_{k,s}\epsilon_{-}
\end{aligned}$$

The question told us that when the temperature is zero all the negative states are occupied which meanst that the sum of all the negative energy states is the energy at $T = 0$ *i.e.* $\sum_{k,s}\epsilon_{-} = E(T = 0)$. Plus we know that $\epsilon_{-} = -\epsilon_{+}$ and that the degeneracy is two. Using these three pieces of information the energy is

$$\begin{aligned} E(T) &= \sum_{k,s}\left[\langle n_{k,+}\rangle_- \epsilon_+ - \langle n_{k,+}\rangle_- \epsilon_-\right] + \sum_{k,s}\epsilon_- \\ &= 2\sum_{k}\left[\langle n_{k,+}\rangle_- \epsilon_+ + \langle n_{k,+}\rangle_- \epsilon_+\right] + E(0) \\ E(T) - E(0) &= 4\sum_{k}\langle n_{k,+}\rangle_- \epsilon_+ \end{aligned}$$

If we take the sum to the continuous limit (exactly as was done in the last problem) and substitute in the standard function for $\langle n_{\vec{k}}\rangle_-$ then the energy is

$$\boxed{E(T) - E(0) = 4A\int \frac{d^2\vec{k}}{(2\pi)^2}\frac{\epsilon_+}{e^{\beta\epsilon_+}+1}} \tag{18}$$

3.3 Part c)

We can determin the value of $E(T) - E(0$ by letting $\epsilon_+ = \hbar v\left|\vec{k}\right| = \hbar v k$ and integrating in polar coordinates.

$$\begin{aligned} E(T) - E(0) &= 4A\int \frac{2\pi k dk}{(2\pi)^2}\frac{\hbar v k}{e^{\beta\hbar v k}+1} \\ &= \frac{4A}{2\pi}\hbar v\int dk\frac{k^2}{e^{\beta\hbar v k}+1} \\ &= \frac{4A}{2\pi}\hbar v\int\left(\frac{1}{\beta\hbar v}\right)dx\left(\frac{1}{\beta\hbar v}\right)^2\frac{x^2}{e^x+1} \\ &= \frac{2A}{\pi\beta}\left(\frac{1}{\beta\hbar v}\right)^2\int_0^\infty dx\frac{x^2}{e^x+1} \end{aligned}$$

There's our magical integral function again with $\eta = -1$, $m = 3$ and $z = 1$ meaning that it's another Riemann zeta function.

$$\begin{aligned} E(T) - E(0) &= \frac{2A}{\pi}k_{\mathrm{B}}T\left(\frac{1}{\beta\hbar v}\right)^2 2! f_3^-(1) \\ &= \frac{2A}{\pi}k_{\mathrm{B}}T\left(\frac{k_{\mathrm{B}}T}{\hbar v}\right)^2 2\left(\frac{3}{4}\zeta(3)\right) \end{aligned}$$

$$\boxed{E(T) - E(0) = \frac{3A}{\pi}\zeta(3)\left(\frac{k_{\mathrm{B}}T}{\hbar v}\right)^2 k_{\mathrm{B}}T} \tag{19}$$

3.4 Part d)

Calculate the heat capacity

$$\begin{aligned} C_V &= \left.\frac{\partial E}{\partial T}\right|_V \\ &= \frac{\partial}{\partial T}\left(E(0) + \frac{3A}{\pi}\zeta(3)\left(\frac{k_\mathrm{B}T}{\hbar v}\right)^2 k_\mathrm{B}T\right) \\ &= \frac{3A}{\pi}\zeta(3)\frac{\partial}{\partial T}\left(\frac{k_\mathrm{B}T}{\hbar v}\right)^2 k_\mathrm{B}T \end{aligned}$$

$$\boxed{C_V = \frac{9A}{\pi}k_\mathrm{B}\zeta(3)\left(\frac{k_\mathrm{B}T}{\hbar v}\right)^2} \tag{20}$$

3.5 Part d)

We've been considering electrons with a velocity of $v \approx 10^6 m/s$ but now we would like to know if we need to consider the phonons' contribution to the heat capacity. Now phonons are bosons but they do have the same form of energy

$$\varepsilon = \hbar\nu\,|k|$$

where $\nu \approx 2\times 10^4 m/s$ is the speed of sound in graphite and also have no chemical potential. The fact that they are bosons means the occupation number changes but if just for a qualitative investigation say it doesn't matter than the treatment of the phonons would be exactly the same and they would have the same form for energy and the same form for heat capacity. The only difference is $v \to \nu$. Since $C_V \propto v^-2$ the ratios of their heat capacity would be

$$\begin{aligned} \frac{C_V^\text{phonon}}{C_V^\text{electron}} &\approx \left(\frac{\nu}{v}\right)^2 \\ &= \left(\frac{2\times 10^4}{10^6}\right)^2 \\ &= 4\times 10^{-4}. \end{aligned}$$

So we expect the phonon contribution to be neglible.