Statistical Mechanics - Class Exercise 1

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Exercise 0080 - The spreading of a free particle

Given a free classic particle $H = \frac{p^2}{2m}$, that has been prepared in time $t = 0$ in a state represented by the probability function

$$\rho_{t=0}(x,p) \propto \exp\left(-a(x-x_0)^2 - b(p-p_0)^2\right)$$

1. Normalize $\rho_{t=0}(x,p)$.
2. Calculate $\langle x \rangle$, $\langle p \rangle$, σ_x, σ_p, E
3. Express the random variables $\hat{x}_t, \hat{p}_t$ with $\hat{x}_{t=0}, \hat{p}_{t=0}$
4. Express $\rho_t(x,p)$ with $\rho_{t=0}(x,p)$. (Hint: 'variables replacement').
5. Mention two ways to calculate the sizes appeared in paragraph b in time t. use the simple one to express $\sigma_x(t), \sigma_p(t)$ with $\sigma_x(t=0), \sigma_p(t=0)$ (that you've calculated in b).

Answer

1. We know that $\rho_{t=0}(x,p) = Ne^{-a(x-x_0)^2-b(p-p_0)^2}$

$$\begin{aligned}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\rho_{t=0}(x,p)\frac{dxdp}{2\pi} =&1\\ =&N\int_{-\infty}^{\infty}e^{-a(x-x_0)^2}dx\int_{-\infty}^{\infty}e^{-b(p-p_0)^2}\frac{dp}{2\pi} = N\frac{1}{2\sqrt{ab}} = 1\\ &\to N = 2\sqrt{ab}\end{aligned}$$

2. $\langle A(x,p)\rangle = \int\int \rho_{t=0}(x,p)\, A(x,p)\, \frac{dxdp}{2\pi}$

$$\begin{aligned}\langle x\rangle =&2\sqrt{ab}\int\int e^{-a(x-x_0)^2-b(p-p_0)^2}x\frac{dxdp}{2\pi}\\ =&\sqrt{\frac{a}{\pi}}\int e^{-a(x-x_0)^2}xdx = \sqrt{\frac{a}{\pi}}\int e^{-ax^2}(x+x_0)\,dx\\ =&x_0\sqrt{\frac{a}{\pi}}\int e^{-ax^2}dx + \sqrt{\frac{a}{\pi}}\int e^{-ax^2}xdx = x_0\end{aligned}$$

In the same way $\langle p\rangle = p_0$

$$\sigma_x^2 = \left\langle (x-\langle x\rangle)^2 \right\rangle = \left\langle x^2\right\rangle - \langle x\rangle^2$$

$$\begin{aligned}\left\langle x^2\right\rangle =&\sqrt{\frac{a}{\pi}}\int e^{-a(x-x_0)^2}x^2dx = \sqrt{\frac{a}{\pi}}\int e^{-ax^2}\left(x^2+2xx_0+x_0^2\right)dx = \\ =&x_0^2 - \sqrt{\frac{a}{\pi}}\frac{d}{da}\int e^{-ax^2}dx = x_0^2 - \sqrt{\frac{a}{\pi}}\frac{d}{da}\sqrt{\frac{\pi}{a}} = x_0^2 + \frac{1}{2a}\end{aligned}$$

$$\sigma_x = \sqrt{\left\langle x^2\right\rangle - x_0^2} = \sqrt{\frac{1}{2a}}$$

In the same way $\sigma_p = \sqrt{\frac{1}{2b}}$

$$\begin{aligned}E = \langle \mathcal{H}(x,p)\rangle =& 2\sqrt{ab}\int\int e^{-a(x-x_0)^2-b(p-p_0)^2}\frac{p^2}{2m}\frac{dxdp}{2\pi} \\ =&\frac{1}{2m}\sqrt{\frac{b}{\pi}}\int e^{-b(p-p_0)^2}p^2d = \frac{1}{2m}\left(p_0^2+\frac{1}{2b}\right) = \frac{p_0^2}{2m}+\frac{\sigma_p^2}{2m}\end{aligned}$$

3. The equations of motion are

$$\begin{aligned}\dot{x} &= \frac{\partial\mathcal{H}}{\partial p} = \frac{p}{m} \\ \dot{p} &= -\frac{\partial\mathcal{H}}{\partial x} = 0\end{aligned}$$

$$\begin{aligned}x &= x_0 + \frac{p}{m}t \\ p &= p_0\end{aligned}$$

So

$$\begin{aligned}\hat{x_t} &= \hat{x}_{t=0} + \frac{\hat{p}_{t=0}}{m}t \\ \hat{p}_t &= \hat{p}_{t=0}\end{aligned}$$

4. we change the variables from Hizenberg picture to Schrodinger picture

$$\rho_t(x,p)\frac{dxdp}{2\pi} = \rho_{t=0}(x',p')\frac{dx'dp'}{2\pi} = \rho_{t=0}\left(x-\frac{p}{m}t,p\right)\left(\frac{dx'}{dx}\frac{dp'}{dp}\right)\frac{dxdp}{2\pi}$$

$$\rightarrow \rho_t(x,p) = \rho_{t=0}\left(x-\frac{p}{m}t,p\right)$$

5. We can calculate directly with $\rho_t(x,p)$

$$\begin{aligned}\langle x\rangle_t =&2\sqrt{ab}\int\int e^{-a\left(x-\left(x_0+\frac{p_0}{m}t\right)\right)^2-b(p-p_0)^2}x\frac{dxdp}{2\pi} \\ =&\sqrt{\frac{a}{\pi}}\int e^{-a\left(x-\left(x_0+\frac{p_0}{m}t\right)\right)^2}xdx = \sqrt{\frac{a}{\pi}}\int e^{-ax^2}\left(x+\left(x_0+\frac{p_0}{m}t\right)\right)dx \\ =&\left(x_0+\frac{p_0}{m}t\right)\sqrt{\frac{a}{\pi}}\int e^{-ax^2}dx + \sqrt{\frac{a}{\pi}}\int e^{-ax^2}xdx = x_0+\frac{p_0}{m}t\end{aligned}$$

Or we can use the the characteristics of random variables

$$\langle x\rangle_t = \langle x_t\rangle = \left\langle x_{t=0} + \frac{p_{t=0}}{m}t\right\rangle = x_0 + \frac{p_0}{m}t$$

In the same way $\langle p\rangle_t = p_0$

$$\sigma_x^2(t) = \left\langle (x - \langle x\rangle)^2\right\rangle_t = \left\langle x_t^2\right\rangle - \langle x_t\rangle^2$$

$$=\left\langle x_{t=0}^2 + 2x_{t=0}\frac{p_{t=0}}{m}t + \left(\frac{p_{t=0}}{m}t\right)^2\right\rangle - \left(x_0 + \frac{p_0}{m}t\right)^2$$
$$=\left\langle x_{t=0}^2\right\rangle + 2\langle x_{t=0}\rangle\frac{\langle p_{t=0}\rangle}{m}t + \left(\frac{t}{m}\right)^2\left\langle p_{t=0}^2\right\rangle - \left(x_0 + \frac{p_0}{m}t\right)^2$$
$$=x_0^2 + \frac{1}{2a} + 2x_0\frac{p_0}{m}t + \left(\frac{t}{m}\right)^2\left(p_0^2 + \frac{1}{2b}\right) - \left(x_0^2 + 2x_0\frac{p_0}{m}t + \left(\frac{t}{m}\right)^2 p_0^2\right) = \frac{1}{2a} + \left(\frac{t}{m}\right)^2\frac{1}{2b}$$

$$\sigma_x(t) = \sqrt{\frac{1}{2a} + \left(\frac{t}{m}\right)^2\frac{1}{2b}} = \sqrt{\sigma_x^2(0) + \left(\frac{t}{m}\right)^2\sigma_p^2(0)}$$

σ_p stay $\sigma_p = \sqrt{\frac{1}{2b}}$

$$E(t) = \left\langle\frac{p_t^2}{2m}\right\rangle = \frac{1}{2m}\left(p_0^2 + \sigma_p^2\right)$$

micro-canonical state and spectral functions

For the Hamiltonian $H(x,p)$ the distribution function

$$\rho(x,p)\frac{dxdp}{2\pi}$$

is the probability to the system to be in $x < \hat{x} < x + dx, p < \hat{p} < p + dp$
In equilibrium the distribution function is a function of the energy and it constant in time

$$\rho(x,p) = F(H(x,p))$$

For micro-canonical state, the energy is given and the distribution function

$$\rho(x,p) = C\delta(E - H(x,p)) = \frac{1}{g(E)}\delta(E - H(x,p))$$

where $g(E)$ is the density of states.
For canonical state, the temperature is given and the distribution function

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

or, for discrete state

$$\rho(r) = \frac{1}{Z}e^{-\beta E_r}$$

where Z is the partition function

$$Z(\beta) = \int e^{-\beta H(x,p)} \frac{dxdp}{2\pi}$$

or

$$Z(\beta) = \sum_r e^{-\beta E_r} = \int g(E) e^{-\beta E} dE$$

Also, we can see that

$$E = \langle H \rangle = \sum_r \rho(r) E_r = \sum_r \frac{1}{Z} e^{-\beta E_r} E_r = -\sum_r \frac{1}{Z} \frac{\partial}{\partial \beta} e^{-\beta E_r} = -\frac{1}{Z} \frac{\partial}{\partial \beta} \sum_r e^{-\beta E_r}$$

$$= -\frac{1}{Z} \frac{\partial}{\partial \beta} Z = -\frac{\partial}{\partial \beta} \ln(Z)$$

Exercise 0060 - Oscillator in a micro-canonical state

Assume that a harmonic oscillator with frequency Ω and mass m is prepared in a micro-canonical state with energy E.

1. Write the probability distribution $\rho(x,p)$
2. Find the projected probability distribution $\rho(x)$

Answer

1.

$$H = \frac{p^2}{2m} + \frac{m\Omega^2}{2} x^2$$

so the probability distribution is

$$\rho(x,p) = \frac{1}{g(E)} \delta\left(\frac{p^2}{2m} + \frac{m\Omega^2}{2} x^2 - E\right)$$

2. to find $\rho(x)$ we calculate

$$\rho(x) = \int \rho(x,p) \frac{dp}{2\pi} = \frac{1}{g(E)} \int_{-\infty}^{\infty} \delta\left(\frac{p^2}{2m} + \frac{m\Omega^2}{2} x^2 - E\right) \frac{dp}{2\pi} =$$

we use $\delta(g(x)) = \sum_i \frac{\delta(x-x_i)}{|g'(x_i)|}$

$$= \frac{1}{g(E)} \int_{-\infty}^{\infty} \frac{1}{\left|\frac{p}{m}\right|} \left[\delta\left(p + \sqrt{2mE - m^2\Omega^2 x^2}\right) + \delta\left(p - \sqrt{2mE - m^2\Omega^2 x^2}\right)\right] \frac{dp}{2\pi} = \frac{1}{\pi\Omega g(E)} \frac{1}{\sqrt{\frac{2E}{m\Omega^2} - x^2}}$$

$$\rho(x) = \begin{cases} \frac{1}{\pi\Omega g(E)} \frac{1}{\sqrt{\frac{2E}{m\Omega^2} - x^2}} & x^2 < \frac{2E}{m\Omega^2} \\ 0 & \text{else} \end{cases}$$

To find $g(E)$ we calculate

$$\int \rho(x) dx = 1$$

$$\frac{1}{\pi\Omega g(E)}\int_{-\sqrt{\frac{2E}{m\Omega^2}}}^{\sqrt{\frac{2E}{m\Omega^2}}}\frac{1}{\sqrt{\frac{2E}{m\Omega^2}-x^2}}dx=\frac{1}{\pi\Omega g(E)}\int_{-1}^{1}\frac{1}{\sqrt{1-u^2}}du$$

$$=\frac{1}{\pi\Omega g(E)}\arcsin(u)\,|_{-1}^{1}=\frac{1}{\Omega g(E)}=1$$

$$g(E)=\frac{1}{\Omega}$$

$$\rho(x)=\begin{cases}\frac{1}{\pi\sqrt{\frac{2E}{m\Omega^2}-x^2}} & x^2<\frac{2E}{m\Omega^2}\\ 0 & \text{else}\end{cases}$$

$$\rho(x,p)=\Omega\delta\left(\frac{p^2}{2m}+\frac{m\Omega^2}{2}x^2-E\right)$$

Exercise 0150 - Spectral functions for N spins

Consider an N spin system:

$$\hat{H}=\sum_{\alpha=1}^{N}\frac{\varepsilon}{2}\hat{\sigma}_z^{(\alpha)}$$

Calculate $Z_N(\beta)$ in two different ways:

1. The short way - Calculate $Z_N(\beta)$ by factoring the sum.
2. The long way - Write the energy levels E_n of the system. Mark with $n=0$ the ground level, and with $n=1,2,3,...$ the excited levels. Find the degeneracy g_n of each level. Use these results to express $Z_N(\beta)$, and show the that the same result is obtained.

Answer

1. The short way

$$\hat{H}_1=\frac{\varepsilon}{2}\hat{\sigma}_z$$

$$Z_1(\beta)=e^{-\beta\left(\frac{\varepsilon}{2}\right)}+e^{-\beta\left(-\frac{\varepsilon}{2}\right)}=2\cosh\left(\frac{\beta\varepsilon}{2}\right)$$

$$Z_N(\beta)=\sum_{\sigma^1=\pm1}\cdots\sum_{\sigma^N=\pm1}e^{-\beta\sum_{\alpha=1}^{N}\frac{\varepsilon}{2}\sigma^\alpha}=\prod_{\alpha=1}^{N}\sum_{\sigma^\alpha=\pm1}e^{-\beta\frac{\varepsilon}{2}\sigma^\alpha}=(Z_1(\beta))^N=2^N\cosh^N\left(\frac{\beta\varepsilon}{2}\right)$$

2. The long way
n is the number of spin "up"

$$E_n=\frac{\varepsilon}{2}n-\frac{\varepsilon}{2}(N-n)$$

the degeneracy of n "up" and $N-n$ "down"

$$g_n=\frac{N!}{(N-n)!n!}$$

$$Z_N(\beta) = \sum_{n=0}^{N} g_n e^{-\beta E_n} = \sum_{n=0}^{N} \frac{N!}{(N-n)!n!} e^{-\beta\left[\frac{\varepsilon}{2}n - \frac{\varepsilon}{2}(N-n)\right]} =$$

$$= \sum_{n=0}^{N} \frac{N!}{(N-n)!n!} \left(e^{-\beta\frac{\varepsilon}{2}}\right)^{n} \left(e^{\beta\frac{\varepsilon}{2}}\right)^{(N-n)}$$

from the binomial theorem $(a+b)^N = \sum_{n=0}^{N} \frac{N!}{(N-n)!n!} a^n b^{N-n}$ we get

$$Z_N(\beta) = \left(e^{-\beta\frac{\varepsilon}{2}} + e^{\beta\frac{\varepsilon}{2}}\right)^N = 2^N \cosh^N\left(\frac{\beta\varepsilon}{2}\right)$$