May 2006 #1 (SM)

Particles on a line, classical particles

a. $H = \frac{p_1^2}{2m} + U(x_1) + \sum_{i=2}^{N}\left(\frac{p_i^2}{2m} + U(x_i - x_{i-1})\right) + f x_N$

(constant force $-f$ on the $N^{th}$ particle)

$$U(y) = \begin{cases} \infty & y<0 \\ -U_0 & 0 \le y \le a \\ 0 & y > a \end{cases}$$

— particle $i$ is to the right of $i-1$

— particles want to be within a distance

$$Z = \frac{1}{h^N}\int e^{-\frac{\beta}{2m}p_1^2}dp_1 \cdots \int e^{-\frac{\beta}{2m}p_N^2}dp_N \int e^{-\beta U_+(x_1,\dots,x_N)}dx_1 \dots dx_N$$

$$\int_{-\infty}^{\infty} e^{-\frac{\beta}{2m}p^2}dp = \sqrt{\frac{2\pi m}{\beta}}$$

$$Z = \frac{1}{h^N}\left(\frac{2\pi m}{\beta}\right)^{N/2} A \qquad A = \int e^{-\beta U_+(x_1,\dots,x_N)}dx_1 \dots dx_N$$

$$\ln Z = N\left(\frac{1}{2}\ln\left(\frac{2\pi m}{\beta}\right) - \ln h\right) + \ln A$$

To compute $\langle x_n \rangle$, use $\langle x_n \rangle = \sum_r x_{nr} P_r(\text{state } r)$

$$\langle x_n \rangle = \frac{\sum_r e^{-\beta E_r} x_{nr}}{\sum_r e^{-\beta E_r}} = \frac{\sum_r e^{-\beta E_r} x_{nr}}{Z}$$

$$A = \int dx_1 \cdots dx_N \, e^{-\beta U(x_1)} e^{-\beta U(x_2 - x_1)} e^{-\beta U(x_3 - x_2)} \cdots e^{-\beta U(x_{N-1} - x_{N-2})} e^{-\beta U(x_N - x_{N-1})} e^{-\beta f x_N}$$

$$A = \int_0^{\infty} dx_1 \, e^{-\beta U(x_1)} \int_{x_1}^{\infty} dx_2 \, e^{-\beta U(x_2 - x_1)} \cdots \int_{x_{N-2}}^{\infty} dx_{N-1} \, e^{-\beta U(x_{N-1} - x_{N-2})} \int_{x_{N-1}}^{\infty} dx_N \, e^{-\beta U(x_N - x_{N-1})} e^{-\beta f x_N}$$

Can get a factor of $x_n$ by applying $-\frac{1}{\beta}\frac{\partial}{\partial f}$

$\rightarrow \langle x_n \rangle = -\frac{1}{\beta}\frac{1}{Z}\frac{\partial}{\partial f}Z = -\frac{1}{\beta}\frac{\partial}{\partial f}\ln Z = -\frac{1}{\beta}\frac{\partial}{\partial f}\ln A$ (only $A$ depends on $f$)

Can evaluate $A$ directly: First Integral:

$$\int_{x_{N-1}}^{\infty} dx_N \, e^{-\beta U(x_N - x_{N-1})} e^{-\beta f x_N} = \int_{x_{N-1}}^{x_{N-1}+a} dx_N \, e^{\beta U_0} e^{-\beta f x_N} + \int_{x_{N-1}+a}^{\infty} dx_N \, e^{-\beta f x_N}$$

$$= -\frac{1}{\beta f}\left(e^{\beta U_0} e^{-\beta f x_N}\Big|_{x_{N-1}}^{x_{N-1}+a}\right) - \frac{1}{\beta f} e^{-\beta f x_N}\Big|_{x_{N-1}+a}^{\infty}$$

$$= \frac{1}{\beta f}\left[e^{-\beta f a} + e^{\beta U_0}(1 - e^{-\beta f a})\right] e^{-\beta f x_{N-1}} \equiv C e^{-\beta f x_{N-1}}$$

$$C = \frac{1}{\beta f}\left[e^{-\beta f a} + e^{\beta U_0}(1 - e^{-\beta f a})\right]$$

Second integral: $C \underbrace{\int_{x_{N-2}}^{\infty} dx_{N-1}\, e^{-\beta U(x_{N-1}-x_{N-2})} e^{-\beta f x_{N-1}}}_{\text{same as first integral, except } x_{N-1} \to x_{N-2}}$

$$= C^2 e^{-\beta f x_{N-2}}$$

This continues until the last integral, where "$x_0$" $= 0$

$$A = C^N$$

$$\ln A = N \ln C = N \ln\left(e^{-\beta f a} + e^{\beta U_0}(1 - e^{-\beta f a})\right) - N\ln f - N \ln \beta$$

$$\langle x_n \rangle = -\frac{1}{\beta}\frac{\partial}{\partial f}\ln A = -\frac{N}{\beta}\left[-\frac{1}{f} + \frac{-\beta a e^{-\beta f a} + \beta a e^{\beta U_0} e^{-\beta f a}}{e^{-\beta f a} + e^{\beta U_0}(1 - e^{-\beta f a})}\right]$$

$$\langle x_n \rangle = N\left[\frac{1}{\beta f} - \frac{a e^{-\beta f a}(e^{\beta U_0} - 1)}{e^{-\beta f a} + e^{\beta U_0}(1 - e^{-\beta f a})}\right]$$

b. High temperature limit: $\beta f a \ll 1$, $\beta U_0 \ll 1$

$$\langle x_N \rangle \to N\left[\frac{1}{\beta f} - \frac{a(\beta U_0)}{1 - \beta f a + 1(\beta f a)}\right] = N\left[\frac{1}{\beta f} - a\beta U_0\right] = Na\left[\frac{1}{\beta f a} - \beta U_0\right]$$

$$\langle x_N \rangle \to \frac{NkT}{f} = Na\left(\frac{kT}{fa}\right)$$ $(Na) \times$ a large number

Low temperature limit: $\beta f a \gg 1$, $\beta U_0 \gg 1$

$$\langle x_N \rangle \to N\left[\frac{1}{\beta f} - \frac{a e^{-\beta f a} e^{\beta U_0}}{e^{\beta U_0}}\right] = N\left[\frac{1}{\beta f} - a e^{-\beta f a}\right] = Na\left[\frac{1}{\beta f a} - e^{-\beta f a}\right]$$

$\beta f a$ is large, so $\frac{1}{\beta f a} \gg e^{-\beta f a}$

$$\langle x_N \rangle \to \frac{NkT}{f} = Na\left(\frac{kT}{fa}\right)$$ $(Na) \times$ a small number