M09T.2

We're given the Hamiltonian

$$H=\frac{p_1^2}{2m}+U(x_1)-fx_N+\sum_{i=2}^{N}\frac{p_1^2}{2m}+U(x_n-x_{n_1}) \tag{1}$$

We need not worry about the momentum, in this problem. We calculate the partition function Z,

$$Z\propto\int e^{-\beta H}=\int d^N x\exp\left[-\beta U(x_1)+\beta f x_N-\beta\sum_{i=2}^{N}U(x_n-x_{n_1})\right] \tag{2}$$

We can begin by first perfoming the integration of x_n, denoted by Z_n , which gives

$$\begin{aligned}Z_n &\propto\int_{x_{n-1}}^{x_{n-1}+a}dx_n e^{\beta u_0}e^{\beta fx}+\int_{x_{n-1}+a}^{x_{n-1}+Q}dx_n e^{\beta fx}\\ &=\frac{1}{\beta f}\left[e^{\beta u_0}\left(e^{\beta f(x_{n-1}+a)}-e^{\beta f(x_{n-1})}\right)+\left(e^{\beta f(x_{n-1}+Q)}-e^{\beta f(x_{n-1}+a)}\right)\right]\\ &=\frac{e^{\beta f x_{n-1}}}{\beta f}\left(e^{\beta(fa+u_0)}+e^{\beta fQ}-e^{\beta u_0}-e^{\beta fa}\right).\end{aligned}$$

where we'll later take the limit $Q\rightarrow\infty$.
From here, it is clear that after performing the integration over all coordinates (when $x_0=0$), we arrive at

$$Z\propto\left[\frac{1}{\beta f}\left(e^{\beta(fa+u_0)}+e^{\beta fQ}-e^{\beta u_0}-e^{\beta fa}\right)\right]^N=Z_0^N.$$

Interestingly, the partition function is the same as the single particle partition function raised to the power of N. Most of the work is now done. The average length of the system is given by

$$\langle x_N\rangle = \frac{\int d^N x\, x_N e^{-\beta H}}{Z} \tag{3}$$
$$= \frac{\int d^N x\, x_N \exp\left[-\beta U(x_1) + \beta f x_N - \beta \sum_{i=2}^{N} U(x_n - x_{n_1})\right]}{Z}$$

However, note that

$$\int d^N x_N e^{-\beta H} = \frac{1}{\beta}\int \frac{\partial}{\partial f} e^{-\beta H} = \frac{1}{\beta}\frac{\partial}{\partial f}\int e^{-\beta H} = \frac{1}{\beta}\frac{\partial Z}{\partial f} \tag{4}$$

So

$$\langle x_N\rangle = \frac{N}{\beta}\frac{\left[\frac{1}{\beta f}\left(e^{\beta(fa+u_0)} + e^{\beta f Q} - e^{\beta u_0} - e^{\beta f a}\right)\right]^{N-1}}{\left[\frac{1}{\beta f}\left(e^{\beta(fa+u_0)} + e^{\beta f Q} - e^{\beta u_0} - e^{\beta f a}\right)\right]^{N}}\frac{\partial Z_0}{\partial f}$$
$$= -\frac{N}{\beta f} + Na\frac{e^{\beta(fa+u_0)} - e^{\beta f a}}{e^{\beta(fa+u_0)} + e^{\beta f Q} - e^{\beta u_0} - e^{\beta f a}} + \frac{NQe^{\beta f Q}}{e^{\beta(fa+u_0)} + e^{\beta f Q} - e^{\beta u_0} - e^{\beta f a}}$$
$$= -\frac{N}{\beta f} + Na + \frac{e^{\beta u_0}}{e^{\beta(fa+u_0)} + e^{\beta f Q} - e^{\beta u_0} - e^{\beta f a}} + \frac{N(Q-a)e^{\beta f Q}}{e^{\beta(fa+u_0)} + e^{\beta f Q} - e^{\beta u_0} - e^{\beta f a}}$$
$$= Na - \frac{Nk_{\mathrm{B}}T}{f} + \frac{Na}{e^{\beta f a} + e^{\beta f(Q-u_0)} - e^{\beta(fa-u_0)} - 1}$$
$$+ \frac{N(Q-a)e^{\beta f Q}}{e^{\beta(fa+u_0)} + e^{\beta f Q} - e^{\beta u_0} - e^{\beta f a}}$$

If $f < 0$, then taking the limit of $Q \to \infty$ gives

$$\langle x_N\rangle = Na - \frac{Nk_{\mathrm{B}}T}{f} + \frac{Na}{e^{\beta f a} - e^{\beta(fa-u_0)} - 1} \tag{5}$$

otherwise the length diverges. As $T \to 0$, $\langle x_N\rangle \to Na$.

One thought on “M09T.2”

December 11, 2013 at 10:43 pm

The idea is right.
In (5) when taking the $T \to 0$ limit you forgot that $f < 0$. Taking that into account you would get $\langle x_N \rangle \to 0$, which makes more sense than Na.
Also, you were supposed to consider the high-T limit too.
Also there are several typos in your formulas which would be better to correct.