M09T.2

We’re given the Hamiltonian

\[ H = \frac{p_1^2}{2m} + U(x_1) - f x_N + \sum_{i=2}^{N} \frac{p_i^2}{2m} + U(x_n - x_{n_1}) \]  

(1)

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

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

(2)

We can begin by first performing the integration of \( x_n \), denoted by \( Z_n \), which gives

\[ Z_n \propto \int_{x_{n-1}}^{x_{n-1}+a} dx_n e^{\beta u_0} e^{\beta f x} + \int_{x_{n-1}+a}^{x_{n-1}+Q} dx_n e^{\beta f x} \]

\[ = \frac{1}{\beta f} \left[ e^{\beta u_0} \left( e^{\beta f(x_{n-1}+a)} - e^{\beta f(x_{n-1})} \right) + \left( e^{\beta f(x_{n-1}+Q)} - e^{\beta f(x_{n-1}+a)} \right) \right] \]

\[ = \frac{e^{\beta f x_{n-1}}}{\beta f} \left( e^{\beta f a + u_0} + e^{\beta f Q} - e^{\beta u_0} - e^{\beta f a} \right). \]

where we'll later take the limit \( Q \to \infty \).

From here, it is clear that after performing the integration over all coordinates (when \( x_0 = 0 \)), we arrive at

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

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
\[ \langle x_N \rangle = \frac{\int d^N x \, x_N e^{-\beta H}}{Z} \]

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

However, note that

\[ \int d^N x_N e^{-\beta H} = \frac{1}{\beta} \int \frac{\partial}{\partial f} e^{-\beta H} = \frac{1}{\beta} \frac{\partial}{\partial f} \int e^{-\beta H} = \frac{1}{\beta} \frac{\partial Z}{\partial f} \]

So

\[ \langle x_N \rangle = \frac{N}{\beta} \left[ \frac{1}{\beta f} \left( e^{\beta(fa+u_0)} + e^{\beta fQ} - e^{\beta u_0} - e^{\beta fa} \right) \right]^{N-1} \frac{\partial Z_0}{\partial f} \]

\[ = -\frac{N}{\beta f} + Na \frac{e^{\beta(fa+u_0)} - e^{\beta fa}}{e^{\beta(fa+u_0)} + e^{\beta fQ} - e^{\beta u_0} - e^{\beta fa}} + \frac{NQe^{\beta fQ}}{e^{\beta(fa+u_0)} + e^{\beta fQ} - e^{\beta u_0} - e^{\beta fa}} \]

\[ = Na - \frac{Nk_B T}{f} + \frac{Na}{e^{\beta fa} + e^{\beta f(Q-u_0)} - e^{\beta(fa-u_0)} - 1} \]

\[ + \frac{N(Q-a)e^{\beta fQ}}{e^{\beta(fa+u_0)} + e^{\beta fQ} - e^{\beta u_0} - e^{\beta fa}} \]

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

\[ \langle x_N \rangle = Na - \frac{Nk_B T}{f} + \frac{Na}{e^{\beta fa} - e^{\beta(fa-u_0)} - 1} \]

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

One thought on “M09T.2”
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.