Histogram reweighting For Rods

In this report, I examine the Rod-like particle with K=8,L=32,Z=14

- Pick a specific μ_2 as to be in the coexistence region of the case of K=8,L=32, which in our case: $\mathbf{Z_2 = 14}$ thus that we would expect to obtain two peaks in our N distribution;
- Following the Wang-Laudau algorithm demonstrated on page 16 of *the Biased sampling and related free energy technique lecture notes*, M.S.Shell 2009, we did a simulation for generating our weighting function $\eta_{\mu 2}(N;\mu_1=0)$, or equivalently, $\eta_{z2}(N;Z_1=1)$ since in our simulation we define

$$Z_i \equiv e^{\beta\mu i} \dots (1)$$

In addition, this time, since we now have 2 species, we fix $\mathbf{Z_2 = 14}$ and we then set $\mathbf{Z_1 = 1}$ as to generate the weighting function $\eta_{z2}(N_1;Z_1=1)$. In other words, our acceptance probabilities would now looks like:

For Addition : $P_{acc1} = \min[1, (Z_1 * V/((N_1 + 1)*K)*\exp(\eta_{z2}[N_1 + 1] - \eta_{z2}[N_1])];$

$P_{acc2} = \min[1, (Z_2 * V/((N_2 + 1)*K)];$

For Deletion : $P_{del1} = \min[1, (N_1*K/(Z_1*V))*\exp(\eta_{z2}[N_1 -1] - \eta_{z2}[N_1])];$

$P_{del2} = \min[1, N_2*K/(Z_2*V)];$

- In RLC Vink's notation:

$$g_{\beta,z2}(N_1;Z_1=1) = e^{-\eta_{z2}(N_1;Z1=1)} \dots (2).$$

Thus that we directly obtained our "integrated" DOS: $g_{\beta,z2}(N_1;Z_1=1)$.

- Then, Instead of doing multiple long MC runs for obtaining the distribution depending on different **Z**s, the N distribution for example, we can easily generate the distribution/probability distribution of the number of particles $P_i(N;Z_i)$ by just applying the histogram reweighting method onto the "integrated" DOS we just got for Z=1: $g_\beta(N;Z_1=1)$. More precisely, It's the equation.4 on Page 10, *Lecture 7 and 8 RLC Vink*:

$$P(N) \propto g_\beta(N)e^{\beta\kappa N} \dots (3)$$

- Where in Vink's notation K stands for chemical potential (the μ in M.S.Shell's notation) and therefore in our notation: $e^{\beta\kappa N} \equiv e^{\beta\mu N} \equiv Z^N$; Hence, combining equation (1), (2) ,(3) we got the final equation to do the histogram reweighting:

$$P_i(N_1;Z_1=Z_i) \propto e^{-\eta_{z2}(N_1;Z1=1)}Z_i^N \dots (4)$$

Histogram reweighting for Rod: K=8,L=32, Z=14