11.2.2: Path integrals for N-particle systems

If particle spin statistics must be treated in a given problem, the formulation of the path integral is more complicated, and we will not treat this subject here. The extension of path integrals to N-particle systems in which spin statistics can safely be ignored, however, is straightforward, and we will give the expressions below.

The partition function for an N-particle system in the canonical ensemble without spin statistics can be formulated essentially by analogy to the one-particle case. The partition function that one obtains is

$$Q(N,V,T) =$$
$$\lim_{P\to\infty}\left[\prod_{I=1}^{N}\left(\frac{m_I P}{2\pi\beta\hbar^2}\right)^{3P/2}\int d\mathbf{r}_I^{(1)}\cdots d\mathbf{r}_I^{(P)}\right] exp\left[-\beta\sum_{i=1}^{P}\left(\sum_{I=1}^{N}\frac{1}{2}m_I\omega_P^2(\mathbf{r}_I^{(i+1)}-\mathbf{r}_I^{(i)})^2+\frac{1}{P}U(\mathbf{r}_1^{(i)},\ldots,\mathbf{r}_N^{(i)})\right)\right]$$

Thus, it can be seen that the N-particle potential must be evaluated for each imaginary time discretization, however, there is no coupling between separate imaginary time slices due arising from the potential. Thus, interactions occur only between particles in the *same* time slice. From a computational point of view, this is advantageous, as it allows for easily parallelization over imaginary time slices.

The corresponding energy and pressure estimators for the N-particle path integral are given by

$\epsilon_P(\{\mathbf{r}^{(1)},\ldots,\mathbf{r}^{(P)})$	=	$\frac{3NP}{2\beta}-\sum_{i=1}^{P}\sum_{I=1}^{N}\frac{1}{2}m_I\omega_P^2\left(\mathbf{r}_I^{(i)}-\mathbf{r}_I^{(i+1)}\right)^2+\frac{1}{P}\sum_{i=1}^{P}U(\mathbf{r}_1^{(i)},\ldots,\mathbf{r}_N^{(i}$
$p_P(\{\mathbf{r}^{(1)},\ldots,\mathbf{r}^{(P)})$	=	$\frac{NP}{\beta V}-\frac{1}{3V}\sum_{i=1}^{P}\sum_{I=1}^{N}\left[m_I\omega_P^2\left(\mathbf{r}_I^{(i)}-\mathbf{r}_I^{(i+1)}\right)^2+\frac{1}{P}\mathbf{r}_I^{(i)}\cdot\nabla_{\mathbf{r}_I^{(i)}}U\right]$