Derivation of the relation between $U(r)$ and observed single particle and pair position distributions

The pair interaction potential, $U(r)$, can be determined by measurement of both $p_{\text{obs}}(r)$, the observed distribution of separations, and $p_0(x)$, the distribution of positions, $x_i$ of a single particle trapped in the line.

Denoting the confining potential of the trap as $U_{\text{ext}}(x)$, this potential and $p_0(x)$ are related by a Boltzmann relation: $p_0(x) \propto \exp \left( -\frac{U_{\text{ext}}(x)}{k_B T} \right)$. Consider a line trap of length $L$ centered at $x = 0$ with two trapped, interacting particles with position distribution functions $p_1(x_1)$ and $p_2(x_2)$. The probability distribution of their separations is

$$\left[ \text{Eq. S1} \right] \quad p_{\text{obs}}(r) = A \int_{-L/2}^{L/2} p_1(x_1) p_2(x_1 - x) dx_1 ,$$

where the first factor indicates the probability of finding particle 1 at $x = x_1$ and the second indicates the probability of finding particle 2 at $x = x_2$ given the position of particle 1, and $A$ is a normalization constant. Particle 2 experiences a total energy $U(x_1, x_2) = U_{\text{ext}}(x_2) + U(r)$, where $r = x_2 - x_1$. Therefore

$$\left[ \text{Eq. S2} \right] \quad p_2(x_2) = \exp \left( -\frac{U_{\text{ext}}(x_2)}{k_B T} \right) = \exp \left( -\frac{U_{\text{ext}}(x_2)}{k_B T} \right) \exp \left( -\frac{U(r)}{k_B T} \right) = p_0(x) p(r) ,$$

neglecting normalization factors, where $p(r)$ is the “true” (not observed) distribution function for the pair separations. Combining Eqs. S1 and S2:

$$\left[ \text{Eq. S3} \right] \quad p_{\text{obs}}(r) = A \int_{-L/2}^{L/2} p_0(x_1) p_0(x_1 + r) p(r) dx_1 = A p(r) \int_{-L/2}^{L/2} p_0(x_1) p_0(x_1 + r) dx_1 .$$

Therefore, $p(r)$ is related to the observed $p_{\text{obs}}(r)$ by:

$$\left[ \text{Eq. S4} \right] \quad p(r) = \frac{p_{\text{obs}}(r)}{\int_{-L/2}^{L/2} p_0(x) p_0(x + r) dx} ,$$

which gives $U(r)$ via the Boltzmann relation

$$\left[ \text{Eq. S5} \right] \quad U(r) = -k_B T \ln p(r) .$$