2. Densities in Coordinate Space

$P(\underline{R}) = W(\underline{R},\underline{R}) =$ the probability density of the $3N$-dimensional configuration $\underline{R}$.

Bosons

These are particles with spin $0,1,2,3,...$.

The wavefunction

$$\phi_n\left(\underline{r}_1,\underline{r}_2,...,\underline{r}_i,...,\underline{r}_j,...,\underline{r}_N\right) = \phi_n\left(\underline{r}_1,\underline{r}_2,...,\underline{r}_j,...,\underline{r}_i,...,\underline{r}_N\right)$$

i.e. the many-body wavefunction of identical bosons is symmetric, or 'even', under the interchange of any two particles.

Fermions

These are particles with spin $\frac{1}{2},\frac{3}{2},\frac{5}{2},\frac{7}{2},...$.

The wavefunction

$$\phi_n\left(\underline{r}_1,\underline{r}_2,...,\underline{r}_i,...,\underline{r}_j,...,\underline{r}_N\right) = -\phi_n\left(\underline{r}_1,\underline{r}_2,...,\underline{r}_j,...,\underline{r}_i,...,\underline{r}_N\right)$$

i.e. the many-body wavefunction of identical fermions is antisymmetric, or 'odd', under the interchange of any two particles.

For both fermionic and bosonic many-body systems, the probability density

$$\phi_n^*(\underline{R})\phi_n(\underline{R})$$

is always symmetric (i.e. even) under interchange of any two particles. So the total probability density

$$P(\underline{R}) = W(\underline{R},\underline{R}) = \frac{1}{Z}\sum_n e^{-\beta E_n}\left|\phi_n(\underline{R})\right|^2$$

is always symmetric under the interchange of particles.

$$P\left(\underline{r}_1,\underline{r}_2,...,\underline{r}_i,...,\underline{r}_j,...,\underline{r}_N\right) = P\left(\underline{r}_1,\underline{r}_2,...,\underline{r}_j,...,\underline{r}_i,...,\underline{r}_N\right) \quad (26)$$

So $P(\underline{R})$ does not change under interchange of any number of particles (in any order) because any permutation $\left(\underline{r}_1,\underline{r}_2,...,\underline{r}_N\right)$ may be obtained as a succession of interchanges of two particles.

$$P\left(\underline{r}_3,\underline{r}_1,\underline{r}_2\right) = P\left(\underline{r}_1,\underline{r}_3,\underline{r}_2\right) = P\left(\underline{r}_1,\underline{r}_2,\underline{r}_3\right)$$
$$P\left(\underline{r}_3,\underline{r}_1,\underline{r}_2\right) = P\left(\underline{r}_2,\underline{r}_1,\underline{r}_3\right) = P\left(\underline{r}_1,\underline{r}_2,\underline{r}_3\right)$$

2.1 The One-Body Density

The one-body density operator is given by $\hat{\rho}(\underline{x})$. $\underline{x} = (x,y,z)$ is any position in 3D space in the volume V that is occupied by the many-body system.

If particles were rigidly fixed to their places $\underline{r}_1,\underline{r}_2,...,\underline{r}_N$, then the classical density $\rho_c(\underline{x})$ would be given by

$$\rho_c(\underline{x}) = \sum_{i=1}^{N}\delta\left(\underline{x}-\underline{r}_i\right)$$

which would be the probability density that a particle is at $\underline{x}$.

$$\delta\left(\underline{x}-\underline{r}_i\right) = \delta\left(x-x_i\right)\delta\left(y-y_i\right)\delta\left(z-z_i\right) \quad (27)$$

is the three-dimensional Dirac delta function.

The normalization of the delta function is

$$\int_V \delta(\underline{x}-\underline{r}_i)d\underline{r}_i = \int_V \delta(x-x_i)\delta(y-y_i)\delta(z-z_i)dx_idy_idz_i = 1 \quad (28)$$

We also have that (for a single particle)

$$\int_V \delta(\underline{x}-\underline{r}_i)d\underline{x} = \int_V \delta(x-x_i)\delta(y-y_i)\delta(z-z_i)dxdydz = 1 \quad (29)$$

i.e. the particle must be present in either coordinate system. So

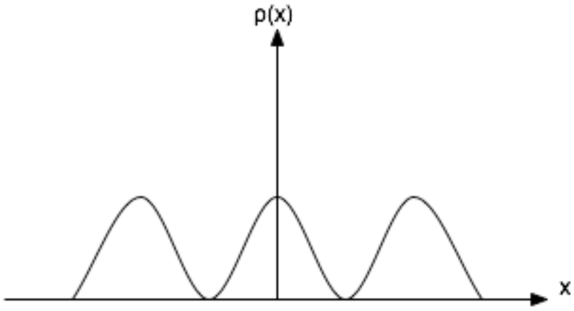
$$\int_V \rho_c(\underline{x})d\underline{x} = \sum_{i=1}^{N}\int_V \delta(\underline{x}-\underline{r}_i)d\underline{x} = \sum_{i=1}^{N} 1 = N$$

because we have N particles.

$\rho(\underline{x})$ is the one-body density, and is also known as the one-body distribution function. It is the probability density for a particle to be at $\underline{x}$.

$\rho(\underline{x})d\underline{x} = \rho(\underline{x})dxdydz$ is the probability of a particle being in an infinitesimal 3D volume element of size $d\underline{x} = dxdydz$ centered at $\underline{x}$.

Quantum



Turn $\rho_c(\underline{x})$ into operator $\hat{\rho}(\underline{x})$, which is the operator of multiplication with $\sum_{i=1}^{N}\delta(\underline{x}-\underline{r}_i)$.

$$\hat{\rho}(\underline{x})+(\underline{R}) = \left(\sum_{i=1}^{N}\delta(\underline{x}-\underline{r}_i)\right)\times\psi(\underline{R}) = \sum_{i=1}^{N}\delta(\underline{x}-\underline{r}_i)\psi(\underline{R}) \quad (31)$$

Multiply $(\underline{R})$ with $\sum_{i=1}^{N}\delta(\underline{x}-\underline{r}_i)$.

Take equation (15): the one-body density $\rho(\underline{x})$ is the thermodynamic expectation value of the one-body density operator $\hat{\rho}(\underline{x})$.

$$\langle\hat{\rho}(\underline{x})\rangle = Tr\left\{\hat{\rho}(\underline{x})\hat{W}\right\} = \rho(\underline{x}) \quad (32)$$

Take equation (24):

$$\begin{aligned}\int_{V^N}\left[\hat{O}_{\underline{R}}W(\underline{R},\underline{R}')\right](\underline{R}'=\underline{R})d\underline{R} &= \int_{V^N}\left[\hat{\rho}(\underline{x})W(\underline{R},\underline{R}')\right](\underline{R}'=\underline{R})d\underline{R}\\ &= \int_{V^N}\left[\sum_{i=1}^{N}\delta(\underline{x}-\underline{r}_i)W(\underline{R},\underline{R}')\right](\underline{R}'=\underline{R})d\underline{R}\\ &= \int_{V^N}\sum_{i=1}^{N}\delta(\underline{x}-\underline{r}_i)W(\underline{R},\underline{R})d\underline{R}\\ &= \sum_{i=1}^{N}\int_{V^N}\delta(\underline{x}-\underline{r}_i)W(\underline{R},\underline{R})d\underline{R}\end{aligned}$$

$$\begin{aligned}\int_{V^N}\delta(\underline{x}-\underline{r}_i)P(\underline{R})d\underline{R} &= \int_{V^N}\delta(\underline{x}-\underline{r}_i)P(\underline{r}_1,\underline{r}_2,...,\underline{r}_i,...,\underline{r}_N)d\underline{r}_1,d\underline{r}_2,...,d\underline{r}_i,...,d\underline{r}_N\\ &= \int_{V^N}\delta(\underline{x}-\underline{r}_i)P(\underline{r}_i,\underline{r}_2,...,\underline{r}_1,...,\underline{r}_N)d\underline{r}_i,d\underline{r}_2,...,d\underline{r}_1,...,d\underline{r}_N\end{aligned}$$

Because every 3D particle coordinate $\underline{r}_1,\underline{r}_2,..,\underline{r}_i,...,\underline{r}_N$ is integrated over V, we may relabel the integration variables $\underline{r}_i \to \underline{y}$ and $\underline{r}_1 = \underline{z}$. Hence

$$\begin{aligned}\int_{V^N}\delta(\underline{x}-\underline{r}_i)P(\underline{R})d\underline{R} &= \int_{V^N}\delta(\underline{x}-\underline{y})P(\underline{y},\underline{r}_2,...,\underline{z},...,\underline{r}_N)d\underline{y},d\underline{r}_2,...,d\underline{z},...,d\underline{r}_N\\ &= \int_V\cdots\int_V\cdots\int_V\underbrace{\left\{\int_V\delta(\underline{x}-\underline{y})P(\underline{y},\underline{r}_2,...,\underline{z},...,\underline{r}_N)d\underline{y}\right\}}_{=P(\underline{x},\underline{r}_2,...,\underline{z},...,\underline{r}_N)}d\underline{r}_2...d\underline{z}...d\underline{r}_N\\ &= \int_{V^{N-1}}P(\underline{x},\underline{r}_2,...,\underline{z},...,\underline{r}_N)d\underline{r}_2...d\underline{z}...d\underline{r}_N\end{aligned}$$

which is a $3(N-1)$ dimensional integration, where we have used

$$\int_V\delta(\underline{x}-\underline{y})f(\underline{y})d\underline{y} = f(\underline{x}) \quad (33)$$

which applies for any function $f(\underline{y})$. We can now relabel the integration variable $\underline{z}\to\underline{r}_i$. It follows that:

$$\int_{V^N}\delta(\underline{x}-\underline{r}_i)P(\underline{R})d\underline{R} = \int_{V^{N-1}}P(\underline{x},\underline{r}_2,\underline{r}_3,...,\underline{r}_N)d\underline{r}_2d\underline{r}_3,...,d\underline{r}_N$$

We get the same result for all i. Hence (remembering that $W(\underline{R},\underline{R}) = P(\underline{R})$),

$$\sum_{i=1}^{N}\int_{V^N}\delta(\underline{x}-\underline{r}_i)P(\underline{R})d\underline{R} = \rho(\underline{x}) = N\int_{V^{N-1}}P(\underline{x},\underline{r}_2,\underline{r}_3,...,\underline{r}_N)d\underline{r}_2d\underline{r}_3...d\underline{r}_N$$

$$\begin{aligned}\rho(\underline{x}) &= N\int_{V^{N-1}}W(\underline{x},\underline{r}_2,\underline{r}_3,...,\underline{r}_N,\underline{x},\underline{r}_2,\underline{r}_3,...,\underline{r}_N)d\underline{r}_2d\underline{r}_3...d\underline{r}_N\\ &= N\int_{V^{N-1}}P(\underline{x},\underline{r}_2,\underline{r}_3,...,\underline{r}_N)d\underline{r}_2d\underline{r}_3...d\underline{r}_N\\ &= \left\langle\sum_{i=1}^{N}\delta(\underline{x}-\underline{r}_i)\right\rangle \quad (34)\end{aligned}$$

$$\int_V\rho(\underline{x})d\underline{x} = N\int_{V^N}P(\underline{x},\underline{r}_2,\underline{r}_3,...,\underline{r}_N)d\underline{r}_2d\underline{r}_3...d\underline{r}_N$$

Relabel the integration variable $\underline{x}\to\underline{r}_1$, and using equation 23,

$$\begin{aligned}\int_V\rho(\underline{x})d\underline{x} &= N\int_{V^N}P(\underline{r}_1,\underline{r}_2,\underline{r}_3,...,\underline{r}_N)d\underline{r}_2d\underline{r}_3...d\underline{r}_N\\ &= N\int_{V^N}P(\underline{R})d\underline{R} = N\int_{V^N}W(\underline{R},\underline{R})d\underline{R} = N\end{aligned}$$

$$\int_V \rho(\underline{x})d\underline{x} = N \quad (35)$$

This is particle number conservation.

2.2 The Two-Body Density

For all particles rigidly fixed to their positions $\underline{r}_i$, $1 \le i \le N$, the probability density for a particle to be at $\underline{x}_1 = (x_1, y_1, z_1)$ and another particle is simultaneously at $\underline{x}_2 = (x_2, y_2, z_2)$

$$\delta(\underline{x}_1 - \underline{r}_i)\delta(\underline{x}_2 - \underline{r}_2) \text{ for } i \ne j$$

as the probabilities for i to be at $\underline{x}_1$ and j to be at $\underline{x}_2$ multiply. The total probability density $\sum_{i=1}^{N}\sum_{\substack{j=1 \\ j\ne i}}^{N}\delta(\underline{x}_1 - \underline{r}_i)\delta(\underline{x}_1 - \underline{r}_i)$, because the probabilities add up for the $N(N-1)$ distinct ordered pairs (i, j) of particles. For the quantum expression, convert to the two-body density operator $\hat{\rho}_2(\underline{x}_1, \underline{x}_2)$.

$$\hat{\rho}_2(\underline{x}_1, \underline{x}_2) = \sum_{i=1}^{N}\sum_{\substack{j=1 \\ j\ne i}}^{N}\delta(\underline{x}_1 - \underline{r}_i)\delta(\underline{x}_2 - \underline{r}_j)$$

$$= \sum_{i\ne j=1}^{N}\delta(\underline{x}_1 - \underline{r}_i)\delta(\underline{x}_2 - \underline{r}_j) \quad (36)$$

$\hat{\rho}_2(\underline{x}_1, \underline{x}_2)$ is the operator of multiplication with $\sum_{i\ne j=1}^{N}\delta(\underline{x}_1 - \underline{r}_i)\delta(\underline{x}_2 - \underline{r}_j)$.

$$\hat{\rho}_2(\underline{x}_1, \underline{x}_2)\psi(\underline{R}) = \left[\sum_{i\ne j=1}^{N}\delta(\underline{x}_1 - \underline{r}_i)\delta(\underline{x}_2 - \underline{r}_j)\right]\psi(\underline{R}) \quad (37)$$