

We compute the expectation value of an arbitrary pairwise potential

$$V_{\text{pair}} = \sum_{l < m} V(\vec{x}_l, \vec{x}_m)$$

where $V(\vec{x}_l, \vec{x}_m) = V(\vec{x}_m, \vec{x}_l)$, for an N -particle system in a Slater determinant state:

$$\Psi = \frac{1}{\sqrt{N!}} \sum_{i_1, \dots, i_N} \varepsilon_{i_1, \dots, i_N} \prod_{k=1}^N \phi_{i_k}(\vec{x}_k).$$

$$\langle V_{\text{pair}} \rangle = \int \prod_{k=1}^N d^3x_k \left(\frac{1}{\sqrt{N!}} \sum_{j_1, \dots, j_N} \varepsilon_{j_1, \dots, j_N} \phi_{j_k}^*(\vec{x}_k) \right)$$

$$\left(\sum_{l < m} V(\vec{x}_l, \vec{x}_m) \right) \left(\frac{1}{\sqrt{N!}} \sum_{i_1, \dots, i_N} \varepsilon_{i_1, \dots, i_N} \phi_{i_k}(\vec{x}_k) \right) =$$

$$\frac{1}{N!} \sum_{\substack{i_1, \dots, i_N \\ j_1, \dots, j_N}} \varepsilon_{j_1, \dots, j_N} \varepsilon_{i_1, \dots, i_N} \sum_{l < m} \int \prod_{k=1}^N d^3x_k \phi_{j_k}^*(\vec{x}_k) V(\vec{x}_l, \vec{x}_m) \phi_{i_k}(\vec{x}_k).$$

We now remark that, for all $i \neq j$, $V(\vec{x}_i, \vec{x}_j)$ appears in V_{pair} . Moreover, $\langle V_{\text{pair}} \rangle$ is invariant under arbitrary interchanges $\vec{x}_i \leftrightarrow \vec{x}_j$. It follows that each integral of $V(\vec{x}_i, \vec{x}_j)$ will have the same value, so we only perform one such integral. Without loss of generality, we choose $V(\vec{x}_1, \vec{x}_2)$. We multiply this result by the total number of terms in V_{pair} , $N(N-1)/2$. Thus, the

previous line simplifies to

$$\frac{1}{N!} \sum_{\substack{i_1 \dots i_N \\ j_1 \dots j_N}} \epsilon_{j_1 \dots j_N} \epsilon_{i_1 \dots i_N} \frac{N(N-1)}{2}.$$

$$\left(\int d^3x_1 d^3x_2 \phi_{j_1}^*(\vec{x}_1) \phi_{j_2}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2) \right).$$

$$\left(\prod_{k=3}^N \int d^3x_k \phi_{j_k}^*(\vec{x}_k) \phi_{i_k}(\vec{x}_k) \right) =$$

$$\frac{1}{2(N-2)!} \sum_{\substack{i_1 \dots i_N \\ j_1 \dots j_N}} \epsilon_{j_1 \dots j_N} \epsilon_{i_1 \dots i_N} \left(\prod_{k=3}^N \delta_{i_k j_k} \right).$$

$$\left(\int d^3x_1 d^3x_2 \phi_{j_1}^*(\vec{x}_1) \phi_{j_2}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2) \right) =$$

$$\frac{1}{2(N-2)!} \sum_{\substack{i_1 \dots i_N \\ j_1, j_2}} \epsilon_{j_1 j_2 i_3 \dots i_N} \epsilon_{i_1 i_2 \dots i_N}.$$

$$\left(\int d^3x_1 d^3x_2 \phi_{j_1}^*(\vec{x}_1) \phi_{j_2}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2) \right).$$

Now, suppose we fix i_1, i_2, j_1, j_2 . The remaining permutations of i_3, \dots, i_N will contribute $(N-2)!$ copies of the same terms.

All that remains is to compute the sums over $i_1, i_2, j_1,$ and j_2 . With i_3, \dots, i_N fixed, there are two cases: $(i_1 = j_1, i_2 = j_2)$ and $(i_1 = j_2, i_2 = j_1)$. Of course, $i_1 \neq i_2$ and $j_1 \neq j_2$ because of the Levi-Civita symbols. We treat each case separately.

Case 1: $i_1 = j_1$ and $i_2 = j_2$

$$\frac{1}{2(N-2)!} \sum_{\substack{i_1, \dots, i_N \\ j_1, j_2}} \epsilon_{j_1 j_2 i_3 \dots i_N} \epsilon_{i_1 i_2 \dots i_N}$$

$$\left(\int d^3x_1 d^3x_2 \phi_{j_1}^*(\vec{x}_1) \phi_{j_2}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2) \right) =$$

$$\frac{1}{2(N-2)!} \sum_{i_1, \dots, i_N} (\epsilon_{i_1 i_2 \dots i_N})^2$$

$$\left(\int d^3x_1 d^3x_2 \phi_{i_1}^*(\vec{x}_1) \phi_{i_2}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2) \right) =$$

$$\frac{1}{2(N-2)!} \cdot (N-2)! \sum_{i_1 \neq i_2} \left(\int d^3x_1 d^3x_2 \phi_{i_1}^*(\vec{x}_1) \phi_{i_2}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2) \right)$$

$$= \sum_{i_1 < i_2} \int d^3x_1 d^3x_2 \phi_{i_1}^*(\vec{x}_1) \phi_{i_2}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2),$$

where the final equality comes from the fact that $i_1 \leftrightarrow i_2$ leaves the integral unchanged, and thus we have overcounted by a factor of two.

Case 2: $i_1 = j_2$ and $i_2 = j_1$.

$$\frac{1}{2(N-2)!} \sum_{\substack{i_1 \dots i_N \\ j_1, j_2}} \epsilon_{j_1 j_2 i_3 \dots i_N} \epsilon_{i_1 i_2 \dots i_N}.$$

$$\left(\int d^3x_1 d^3x_2 \phi_{j_1}^*(\vec{x}_1) \phi_{j_2}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2) \right) =$$

$$\frac{1}{2(N-2)!} \sum_{i_1 \dots i_N} \epsilon_{i_2 i_1 i_3 \dots i_N} \epsilon_{i_1 i_2 \dots i_N}$$

$$\left(\int d^3x_1 d^3x_2 \phi_{i_2}^*(\vec{x}_1) \phi_{i_1}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2) \right) =$$

$$\frac{1}{2(N-2)!} \cdot (N-2)! \sum_{i_1 \neq i_2} (-1).$$

$$\left(\int d^3x_1 d^3x_2 \phi_{i_2}^*(\vec{x}_1) \phi_{i_1}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2) \right) =$$

$$- \sum_{i_1 < i_2} \int d^3x_1 d^3x_2 \phi_{i_2}^*(\vec{x}_1) \phi_{i_1}^*(\vec{x}_2) V(\vec{x}_1, \vec{x}_2) \phi_{i_1}(\vec{x}_1) \phi_{i_2}(\vec{x}_2).$$

Finally, we add these two cases together (and clean up our variable names), and we get

$$\langle V_{pair} \rangle = \left\langle \sum_{l \leq m} V(\vec{x}_l, \vec{x}_m) \right\rangle =$$

$$\sum_{l \leq m} \int d^3x d^3y \left[\phi_l^*(\vec{x}) \phi_m^*(\vec{y}) V(\vec{x}, \vec{y}) \phi_l(\vec{x}) \phi_m(\vec{y}) - \phi_m^*(\vec{x}) \phi_l^*(\vec{y}) V(\vec{x}, \vec{y}) \phi_l(\vec{x}) \phi_m(\vec{y}) \right] =$$

$$\sum_{l \leq m} \left\langle \phi_l \phi_m | V | \phi_l \phi_m \right\rangle - \left\langle \phi_m \phi_l | V | \phi_l \phi_m \right\rangle$$

if you define the matrix elements in a sensible way.