Statistical Mechanics and Density Functional Theory

The total potential energy of a system of N interacting particles is:

$$\Phi = \sum_{i<j} \phi(|\mathbf{r_i} - \mathbf{r_j}|) + 3body + ...,$$

where $\mathbf{r_i}$ is the position of the ith particle and ϕ is the two-body interaction potential. The form of ϕ depends on the type of system described. For example, for ideal gasses, a common choice is the Lennard-Jones potential. The Hamiltonian of the system is:

$$H = \sum_{i=1}^{N} \frac{\mathbf{p_i}^2}{2m} + \sum_{i=1}^{N} V_{ext}(\mathbf{r_i}) + \Phi,$$

where the first term corresponds to kinetic energy, with momenta $\mathbf{p_i}$, the second to external potential V_{ext} acting on the particles, and the third to particle interactions.