

1. Van der Waals attractive interaction

- (a) As suggested in class one can model two adjacent inert gas atoms as linear oscillating electric dipoles. Fill in the mathematics between the following two equations:

$$H_1 = \left[\frac{e^2}{R} + \frac{e^2}{R + x_1 - x_2} - \frac{e^2}{R + x_1} - \frac{e^2}{R - x_2} \right]$$

and

$$H_1 \approx -\frac{2e^2x_1x_2}{R^3}$$

The above equations are in CGS units, to transfer to SI units, multiply by

$$\frac{1}{4\pi\epsilon_0}$$

- (b) As suggested in class, a normal mode transformation can change the coupled oscillating dipole problem into a sum of two independent oscillators with slightly modified energies and spring constants. Do the math which uses the normal mode approximation to go from the coupled oscillator hamiltonian

$$H_o + H_1 = \frac{p_1^2}{2m} + \frac{Cx_1^2}{2} + \frac{p_2^2}{2m} + \frac{Cx_2^2}{2} - \frac{2e^2x_1x_2}{R^3}$$

to two uncoupled oscillators

$$H_o + H_1 = \frac{p_a^2}{2m} + \frac{C_ax_a^2}{2} + \frac{p_s^2}{2m} + \frac{C_sx_s^2}{2}$$

where the normal mode transformation is

$$\begin{aligned} x_s &= \frac{1}{\sqrt{2}}(x_1 + x_2) & p_s &= \frac{1}{\sqrt{2}}(p_1 + p_2) \\ x_a &= \frac{1}{\sqrt{2}}(x_1 - x_2) & p_a &= \frac{1}{\sqrt{2}}(p_1 - p_2) \end{aligned}$$

2. **Quantum Solid** (Kittel 5th ed., p. 102.)

Liquid Helium will not solidify even at the lowest temperatures experimentally accessible unless very high pressures are applied. When it finally solidifies, crystalline Helium is one of the inert gas crystals. In our treatment of these crystals, we neglected the motion of the nuclei. Remember that we used the adiabatic approximation which assumed that the nuclei were fixed. In quantum mechanics, particles are confined to a small region of space cannot be still; they have a zero point ($T=0$) kinetic energy. This zero point kinetic energy is the reason that Helium does not solidify. In effect, it acts like a repulsive force. Consider a crude one-dimensional model of crystalline He^4 with each He atom is confined to a line segment of length L .

- (a) Find the zero-point kinetic energy per particle.
- (b) find an expression for the force needed to keep the line from expanding.
- (c) In equilibrium, the expansive tendency of the kinetic energy is balanced by the van der Waals (VdW) interaction. The vdW energy between nearest neighbours is given very roughly by $U(L) = -1.6L^{-6}10^{-60}$ erg, where L is in cm. Find the equilibrium value of L .

3. **Divalent ionic crystals. (Kittel problem 7, p. 93)**

Barium oxide crystallizes in the NaCl structure. Estimate the cohesive energies per molecule of the hypothetical crystals Ba^+O^- and $\text{Ba}^{++}\text{O}^{--}$ referred to separated neutral atoms. The observed nearest-neighbour internuclear distance is $R_o=2.76\text{\AA}$; the first and second ionization potentials of Ba are 5.19 and 9.96 eV, respectively; and the electron affinities of the first and second electrons added to the neutral oxygen atom are 1.5 and -9.0 eV. Note that energy is released when the first electron is added to an oxygen atom but that it takes energy to put a second electron on oxygen in the reaction $\text{O}^- + e^- \rightarrow \text{O}^{--}$. Which valence state do you predict will occur? Assume that the equilibrium separation R_o is the same for both forms, and neglect the nearest neighbour repulsive energy when calculating the electrostatic energy.