4·2. *Energy relations in solid helium at* 0 °K

For the interaction between two helium atoms we assume the de Boer–Michels potential† (de Boer & Michels 1938)

$$\phi = (Br^{-12} - Cr^{-6})\, 10^{-12}\,\text{erg}, \tag{15}$$

where $B = 447$, $C = 1{\cdot}59$, and r, the distance between the centres of both atoms, is measured in ångströms. We further assume that the energy in a system of many atoms can be calculated by simply superimposing the two-body potential of equation (15). In order to define the *static* lattice energy, Φ, we assume that the atoms are held rigidly at their average positions (the lattice sites). The energy Φ can then be calculated from equation (15) by taking account of all interactions:

$$\Phi = \tfrac{1}{2} \sum_{i \neq j} \phi(r_{ij}), \tag{16}$$

where the sum extends over all lattice sites. According to quantum theory this is not the ground state. In classical terms we can say that even at 0 °K the atoms vibrate around their average positions. This can be seen as a consequence of the uncertainty principle. Owing to this zero-point motion the internal energy at 0 °K, U_0, is higher than the static lattice energy, and the difference between these energies is defined as zero-point energy U_z,

$$U_z = U_0 - \Phi. \tag{17}$$

(In this relation, all the quantities depend on volume.)

Because the definition of U_z involves Φ, which can be only obtained through consideration of a hypothetical classical model of the solid, the zero-point energy cannot be determined directly from experiment. The concept of zero-point energy is, however, valuable because it provides a convenient measure of the influence of quantum corrections.

In figure 13 we have given the static lattice potential, Φ, calculated from the de Boer–Michels potential (equation (15)), the internal energy, U_0, at 0 °K for solid ^{4}He and ^{3}He, and the zero-point energy U_z, for both isotopes. It will be noticed that U_0 is positive over most of the volume range of our experiments.

Several calculations of the ground state of solid helium have been published. London (1954) and Hurst & Levelt (1961) used a cell model of the solid. London considered a spherical rigid box, whereas Hurst & Levelt used a sphericalized potential derived from the actual interatomic potential and the observed lattice structure. The cell model is essentially a one-particle model and corresponds to the Einstein approximation in the theory of specific heats.

Quantum-mechanical variational methods have been used by Bernardes (1960), by Saunders (1962), and by Nosanow & Shaw (1962) to obtain an estimate of the energy of the ground state of solid helium. Nosanow & Shaw review the previous variational treatments and conclude that such a method using spherically symmetric, single-particle wave functions is not adequate for calculating the ground states of solid ^{3}He or ^{4}He.

† We have chosen this version of the helium interatomic potential because it is derived from low-temperature gas data; these data emphasize the low energy part of the potential curve, which is important here. For a more detailed discussion see Hooton (1955).