



Figure 2.3: The computational box (shaded) and its nearest periodic images. The box is centered at the origin and has area one.

Lemma 2.2.3 (Translation of a Local Expansion) *For any complex z_0, z and $\{a_k\}$, $k = 0, 1, 2, \dots, n$,*

$$\sum_{k=0}^n a_k (z - z_0)^k = \sum_{l=0}^n \left(\sum_{k=l}^n a_k \binom{k}{l} (-z_0)^{k-l} \right) z^l \quad (2.41)$$

2.3 The Fast Multipole Algorithm

In this section, we present an algorithm for the rapid evaluation of the potentials and/or electrostatic fields due to distributions of charges. The central strategy used is that of clustering particles at various spatial lengths and computing interactions with other clusters which are sufficiently far away by means of multipole expansions. Interactions with particles which are nearby are handled directly.

To be more specific, let us consider the geometry of the computational box, depicted in Figure 2.3. It is a square with sides of length one, centered about the origin of the coordinate system, and is assumed to contain all N particles of the system under consideration. The eight nearest neighbor boxes are also shown, and will be needed in the next section when considering various boundary