A crystal is a material with a simple and repetitive nuclear arrangement. In reality, crystals are not perfect, it is common to find imperfections in the crystal arrangement. The introduction of a local defect disturbs the nuclear arrangement throughout the crystal. Understanding defects is important to gain a deeper insight into the properties of crystals.

My interest is in understanding the rearrangement of nuclei that is caused by the introduction of a defect into an otherwise perfect crystal. We use the Thomas-Fermi-Weizäcker model to associate an energy to each nuclear arrangement. This leads to a variational problem for finding the minimising displacement.

The Thomas-Fermi-Weizäcker Model

To describe the system, we use $n, \rho, \omega : \mathbb{R}^3 \to \mathbb{R}$, where
- $n$ - the root electron density, $\omega \geq 0$.
- $\rho$ - the Coulomb potential generated by $n$ and $\omega$.

Using these, the Thomas-Fermi-Weizäcker energy of this system is defined by

$$E_{TFW}(n, \rho, \omega) = \int \frac{1}{2} \nabla u^2 + \int \frac{1}{2} \mu_{10} \rho + \frac{1}{2} \int \phi (\omega - u^2).$$

The first two terms describe the kinetic energy and the last term describes the Coulomb energy of the system due to the charged particles.

We consider an infinite system, so given a nuclear distribution $\omega$, by minimising the energy per unit volume, we obtain a ground-state $(n, \phi)$, which solves

- $\Delta u + \frac{5}{3} \rho^{2/3} - \phi u = 0$,
- $\Delta \phi = 4\pi (\omega - u^2)$.

The existence and uniqueness of a solution to this system is guaranteed under broad assumptions on $\omega$ and is shown in [1].

The Periodic System

Let $\Lambda \subset \mathbb{R}^3$ be a Bravais lattice, so $\Lambda = \mathbb{Z}a_1 + \mathbb{Z}a_2 + \mathbb{Z}a_3$, where $a_1, a_2, a_3 \in \mathbb{R}^3$ are linearly independent vectors and $\min_{i,j,k} |a_i^\ast a_j a_k| = 1$. Below are three examples of Bravais lattices.

- Primitive cubic
- Body-centred cubic
- Face-centred cubic

To define the nuclear distribution, let $0 < \delta < \frac{1}{2}$ and choose $\eta \in C_c^\infty ([0,1])$ such that $\eta$ is non-negative, radial and satisfies $\int \eta(x) \, dx = 1$. This function is used to describe an individual nucleus. Using this, the periodic ground state is defined by

$$m_{\text{per}}(x) = \sum_{l \in \Lambda} \eta(x - l).$$

The periodic ground state $(\mu_{\text{per}}, \phi_{\text{per}})$ is the unique, $\Lambda$-periodic solution to

- $\Delta \mu_{\text{per}} + \frac{5}{3} \rho_{\text{per}}^{2/3} - \phi_{\text{per}} \mu_{\text{per}} = 0$,
- $\Delta \phi_{\text{per}} = 4\pi (\mu_{\text{per}} - u_{\text{per}}^2)$.

References


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