Hexagonal phase field lattice

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1 Hexagonal lattice phase-field and free energy

To begin, we create a scalar phase field ψ, which roughly corresponds to a time-average of the mass-density of atoms in the lattice. Hence, we would like to write down a form which has mass concentrated in a hexagonal lattice pattern. This looks like:

$$\psi(\mathbf{r}) = \psi_0 + \sum_n A_0 e^{i\,\mathbf{q}_n \cdot \mathbf{r}} \tag{1}$$

with ψ_0 some constant, A_0 an amplitude, and each $\mathbf{q}_n$ a lattice vector, given by:

$$\mathbf{q}_1 = \hat{\mathbf{y}}, \quad \mathbf{q}_2 = \tfrac{\sqrt{3}}{2}\hat{\mathbf{x}} - \tfrac{1}{2}\hat{\mathbf{y}}, \quad \mathbf{q}_3 = -\tfrac{\sqrt{3}}{2}\hat{\mathbf{x}} - \tfrac{1}{2}\hat{\mathbf{y}} \tag{2}$$