Quasicrystals

Homework assignment No. 6 April 11, 2000

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I. Reading

• The paper I handed out in class: R. L., "The symmetry of quasiperiodic crystals," Physica A **232** (1996) 633–647.

II. Problems

1. **Phase functions.** Because the point group G is defined to leave the density indistinguishable, we can associate with each point group operation g a gauge function $\Phi_g(\mathbf{k})$, called a *phase function*, which relates $\rho(g\mathbf{k})$ and $\rho(\mathbf{k})$:

$$\rho(g\mathbf{k}) = e^{2\pi i \Phi_g(\mathbf{k})}\rho(\mathbf{k}) \ . \tag{1}$$

To illustrate the use of phase functions, consider a 2-dimensional density constructed as a sum of five plane waves separated by angles of $\frac{2\pi}{5}$:

$$\rho(\mathbf{r}) = \sum_{n=1}^{5} \cos(\mathbf{k}_n \cdot \mathbf{r} + \phi) \ , \tag{2}$$

where $\mathbf{k}_n = (\cos(n\frac{2\pi}{5}), \sin(n\frac{2\pi}{5}))$. For which values of ϕ does the density have 10-fold symmetry? [Hint: Express the density as a sum of plane waves $e^{i\mathbf{k}\cdot\mathbf{r}}$ and require that the phase function be linear.] Plot $\rho(\mathbf{r})$ for different values of ϕ to convince yourself of your result.

2. **Gauge transformations.** A centrosymmetric crystal is one whose point group contains the inversion operation i which takes every wave vector to its negative, $i\mathbf{k} = -\mathbf{k}$.

(a) Show that for such point groups there exists a gauge in which the phase function $\Phi_i(\mathbf{k})$, associated with the inversion, is zero everywhere. You can do this by assuming a certain phase function ${\Phi_i}'(\mathbf{k})$, and then performing a *gauge transformation*

$$\Phi_i(\mathbf{k}) \equiv {\Phi_i}'(\mathbf{k}) + \chi(i\mathbf{k} - \mathbf{k}). \tag{3}$$

(b) Show that in this gauge all the density Fourier coefficients $\rho(\mathbf{k})$ are real and therefore all other phase functions are restricted to the values 0 or 1/2.

3. **Group compatibility conditions.** Using the point group condition (1) and the identity $[gh]\mathbf{k} = g[h\mathbf{k}]$ we showed in class that all the phase functions must satisfy the *group compatibility condition:*

$$\forall g,h \in G: \qquad \Phi_{gh}(\mathbf{k}) \equiv \Phi_g(h\mathbf{k}) + \Phi_h(\mathbf{k}). \tag{4}$$

(a) Show that if the two sets of phase functions $\phi_{g_i}(\mathbf{k})$ and $\psi_{g_i}(\mathbf{k})$, for all the elements $g_i \in G$, both satisfy all the group compatibility conditions, then so does their sum $\phi_{g_i}(\mathbf{k}) + \psi_{g_i}(\mathbf{k})$.

(b) Show that if g and h commute ($gh = hg$) their phase functions must satisfy

$$\Phi_g(h\mathbf{k} - \mathbf{k}) \equiv \Phi_h(g\mathbf{k} - \mathbf{k}) \ . \tag{5}$$

(c) Let $\phi_{g_i}(\mathbf{k})$ be a set of phase functions satisfying all the group compatibilty conditions. Any particular element $h \in G$ can be used to "rotate" all the phase functions by applying the transformation

$$h: \ \phi_{g_i}(\mathbf{k}) \longrightarrow \phi_{hg_ih^{-1}}(h\mathbf{k}). \tag{6}$$

Show that the "rotated" phase functions differ from the original ones by no more than a gauge transformation.

4. **Glide planes and screw axes.**

(a) Use the group compatibility condition (4) to show that a phase function associated with a mirror m can only assume the values 0 and 1/2 in the invariant plane of the mirror. [Hint: Use the relation $m^2 = e$, where the identity e has by definition $\Phi_e \equiv 0$.]

(b) Show that a phase function associated with an n-fold rotation r can only assume the values j/n on the axis of rotation.

(c) If an axis of n-fold rotation r lies in the plane of a mirror m then the product rm is also a mirror. Show that $\Phi_r(\mathbf{k})$ can only assume the values 0 and 1/2 on the axis of rotation. This establishes that only screw axes of order 2 can exist in mirror planes.

We call the plane of a mirror m a *glide plane* if $\Phi_m(\mathbf{k}) \not\equiv 0$ for any lattice vector in the plane. We call the axis of a rotation r a *screw axis* if $\Phi_r(\mathbf{k}) \not\equiv 0$ for any lattice vector on the axis. These results regarding glide planes and screw axes, though geometrically trivial in the periodic case, are valid for quasiperiodic crystals of arbitrary (not necessarily finite) rank.