group theory - week 8

Graphene

Georgia Tech PHYS-7143

Homework HW8 due Tuesday, March 8, 2016

== show all your work for maximum credit,
== put labels, title, legends on any graphs
== acknowledge study group member, if collective effort
== if you are LaTeXing, here is the source code

Exercise 8.1 *Space group*	2 points
Exercise 8.2 *Band structure of a square lattice*	8 points

Bonus points

Exercise 8.3 *Tight binding model*	8 points

Total of 10 points = 100 % score. Extra points accumulate, can help you later if you miss a few problems.

2016-03-01 Boris Lecture 15 Space groups

Gutkin lecture notes Lecture 7 *Applications III. Energy Band Structure*, Sects. *1. Lattice symmetries* and *2. Band structure*.

2016-03-01 Boris Lecture 16 Graphene

Gutkin lecture notes Lecture 7 *Applications III. Energy Band Structure*, Sect. 7.3 *Band structure of graphene*.

8.1 Literature

2016-02-22 Predrag To understand the order of the full group O_h of symmetries of the cube, exercise 5.1 a.ii), it is instructive to look at figure 8.1 (figs. 8.8 and 8.12 in Joshi [8]). When a cube is a building block that tiles a $3D$ cubic lattice, it is referred to as the 'elementary' or 'Wigner-Seitz' cell, and its Fourier transform is called 'the first Brillouin zone' in 'the reciprocal space'. The special points and the lines of symmetry in the Brillouin zone are shown in figure 8.1 a). The tetrahedron $\Gamma X M R$, an $1/48$th part of the Brillouin zone, is the fundamental domain, as the action of the 48 elements of the point group O_h on it tiles the Brillouin zone without any gaps or overlaps. We will return to this when we discuss space groups (symmetries of discrete lattices).

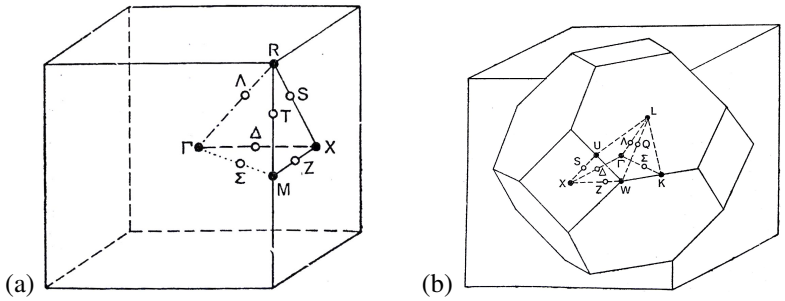

Figure 8.1: (a) The special points and the lines of symmetry in the first Brillouin zone of a simple cubic lattice define its fundamental domain, the tetrahedron $\Gamma X M R$. (b) Just not to get any ideas that this is easy: the fundamental domain for the first Brillouin zone of a bcc lattice. (From Joshi [8].)

2016-02-22 Predrag OK, I'll confess. The reason why it is lovely to teach graduate level physics is that one is allowed to learn new things while doing it. I'll now sketch one, perhaps wild, direction that you are completely free to ignore.

Here is the problem of space groups in the nutshell. The Euclidean invariance on Newtonian space-time (including its subgroups, such as the discrete space groups), and the Poincaré invariance of special-relativistic space-time is a strange brew: the space is non-compact (homogeneity), while rotations are compact (isotropy). That leads to the conceptually awkward situation of mixing a

group of additions (translations) with a group of multiplications (rotations). To work with such group we *first* translate objects to the *origin* and *then* rotate them with the respect to the origin. That's not nice, because by translation invariance any point is as good as any other, there is no preferred origin. There is no reason why one should translate first, rotate second. What one needs is a formalism that implements translations and rotations on the same footing.

If I understand Hestenes [5] right (also David Finkelstein and perhaps Holger Beck Nielsen have told me things in this spirit) a way to accomplish that is to replace the flat translational directions by a compact manifold where translations and rotations are non-commuting multiplicative group operations.

A part of the Hestenes program is redoing crystallography. I have read Hestenes [6] paper (but not the follow up om Hestenes and Holt [7]). It looks very interesting, but I will spare you from my comments here, as I do not know how to make this formalism work for our purposes (character; explicit computations), so I should not waste your time on that. If you do have a look at his, or at Coxeter [4] discussion of planar tilings, please do report back to Boris and me.

2016-02-24 Predrag Graphene is a two-dimensional sheet of carbon in which the carbon atoms are arranged in a honeycomb lattice: each carbon atom is connected to three neighbors. It was exfoliated by Schafhaeutl [2, 9] in 1840 (more recently, a con man got a Nobel Prize for that), and formally defined for chemists by Boehm [3] in 1986. In 1947 Wallace [10] calculated the electronic structure of graphene, as a preliminary exercise to calculating electronic structure of graphite, and noted that the velocity of the electrons was independent of their energies: they all travel at the same speed (about 100 km per second, about 1/3000 of the speed of light): plot of the energy of the electrons in graphene as a function of its momentum (which is inversely proportional to its wavelength) is V shaped since the energy of the electron is linearly proportional to its momentum (Wallace1 Eq. 3.1). The energy of a free electron is proportional to the square of its momentum, but not so in a crystal. As this is reminiscent of massless elementary particles like photons and neutrino's, it has been renamed since 'Dirac cones', but Dirac has nothing whatsoever to do with that. To learn more, talk to people from the Claire Berger and Walt De Heer's group [1] - I have extracted above history of graphene from De Heer's notes.

References

[1] C. Berger, Z. Song, T. Li, X. Li, A. Y. Ogbazghi, R. Feng, Z. Dai, A. N. Marchenkov, E. H. Conrad, P. N. First, and W. A. De Heer, "Ultrathin epitaxial graphite: 2D electron gas properties and a route toward graphene-based nanoelectronics", J. Phys. Chem. B **108**, 19912–19916 (2004).

[2] H. P. Boehm., A. Clauss, G. O. Fischer, and U. Hofmann, "Dünnste Kohlenstoff-Folien", Z. Naturf. B **17**, 150–153 (1962).

[3] H. Boehm, R. Setton, and E. Stumpp, "Nomenclature and terminology of graphite intercalation compounds", Carbon **24**, 241–245 (1986).

[4] H. S. M. Coxeter, *Introduction to Geometry*, 2nd ed. (Wiley, New York, 1989).

[5] D. Hestenes, *Space-time Algebra*, 2nd ed. (Springer, 1966).

[6] D. Hestenes, "Point groups and space groups in geometric algebra", in *Applications of Geometric Algebra in Computer Science and Engineering*, edited by L. Dorst, C. Doran, and J. Lasenby (Birkhäuser, Boston, MA, 2002), pp. 3–34.

[7] D. Hestenes and J. W. Holt, "Crystallographic space groups in geometric algebra", J. Math. Phys. **48**, 023514 (2007).

[8] A. Joshi, *Elements of Group Theory for Physicists* (New Age International, New Delhi, India, 1997).

[9] C. Schafhaeutl, "LXXXVI. On the combinations of carbon with silicon and iron, and other metals, forming the different species of cast iron, steel, and malleable iron", Philos. Mag. Ser. 3 **16**, 570–590 (1840).

[10] P. R. Wallace, "The band theory of graphite", Phys. Rev. **71**, 622–634 (1947).

Exercises

8.1. **Space group.**

(a) Show that for any space group, the translations by vectors from Bravais lattice form a normal subgroup.

(b) Can rotations of the lattice at a fixed point constitute a normal subgroup of a space group?

(B. Gutkin)

8.2. **Band structure of a square lattice.** A charged particle (without spin) moves in a potential created by an infinite square lattice of atoms, see figure 8.2.

(a) What are the symmetry groups of the Bravais and reciprocal lattices?

(b) Plot the 1st Brillouin zone. What is its symmetry? What is the corresponding fundamental domain?

Let $\boldsymbol{k}$ be quasi-momentum and $E_n(\boldsymbol{k})$ the energy of the nth band.

(c) At which points of the Brillouin zone is the group $G^{(\boldsymbol{k})}$ (the group which leaves vector $\boldsymbol{k}$ invariant) nontrivial? What is it?

(d) What is the symmetry of $E_n(\boldsymbol{k})$ as a function of $\boldsymbol{k}$? At which points of the Brillouin zone is the group velocity $\nabla E_n(\boldsymbol{k})$ equal 0?

(e) At which points of the Brillouin zone neighboring bands (generically) stick to each other? How many bands can stick? Explain from the group theory prospective.

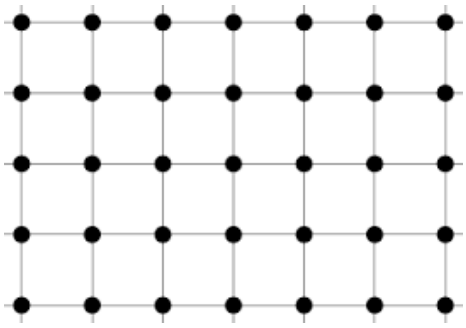

Figure 8.2: Square lattice of atoms

(f) Assume now that the lattice is slightly squeezed along one of the axis. What will be the new symmetry of the system and its 1st Brillouin zone? Will the sticking between bands be lifted or persiss?

(B. Gutkin)

8.3. **Tight binding model.** Verify your solution of exercise 8.2 within the 2-state tight binding model. Assume that particle can hop either from corner to corner of the square lattice with coefficient t_1 or from corner to the middle of the square with coefficient t_2 (and vice versa).

(a) Show the obtained energy bands $E_i(\boldsymbol{k})$ as both contour- and 3-dimensional plots.

(b) Compare with the results from exercise 8.2.