group theory - week 8

Space groups

Georgia Tech PHYS-7143

Homework HW8 due Tuesday 2019-03-05

== 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.

2019-02-26 Predrag Lecture 15 Space groups

There are no classroom meetings this week. Instead, try the online lecture, and read the suggested literature. Gutkin lecture notes Lecture 7 *Applications III. Energy Band Structure*, Sects. *1. Lattice symmetries* and *2. Band structure*. Also good reads: Dresselhaus *et al.* [11] chapter *9. Space Groups in Real Space* (click here), and Cornwell [9] chapter *7. Crystallographic Space Groups* (click here). Walt De Heer learned this stuff from Herzberg [15] *Molecular Spectra and Molecular Structure*. Condensed matter people like Kittel [21] *Introduction to Solid State Physics*, but I am not a fan, because simple group theoretical facts are there presented as condensed matter phenomena.

2019-02-19 Claire Berger has no time to teach this lecture. But if she did, she would: (i) Start with 2D square lattice. (ii) Define Bravais lattice unit cell. (iii) Show that rotation symmetries compatible with a 2D lattice are (none), 2-, 3-, 4-, or 6-fold. (iv) Sketch the resulting 17 wallpaper groups, sect. 8.2.1.

2019-02-28 Predrag Lecture 16 Reciprocal lattice

Suggested reading, beyond Lecture 15 links:

Quinn and Yi [24] *Solid State Physics: Principles and Modern Applications* introduction to space groups looks compact and sensible. *Band structure of graphene*.

2019-02-19 Claire Berger has no time to teach this lecture. But if she did, she would: (i) Start with Bragg diffraction off 2-layer square lattice to motivate the reciprocal lattice. (ii) Show her group's graphene diffraction measurements that identify and distinguish the one- and the two-layer graphene. Reciprocal lattice is not a mathematical construct - it *is* what experimentalists see. (iii) Construct the reciprocal lattice and the first Brillouin zone. (iv) Show the Brillouin zone for graphene, explain what is seen in experiments.

If you are curious about graphene, work out Gutkin lecture notes Lecture 7 *Applications III. Energy Band Structure*, Sect. 7.3

8.1 Thoughts

This week's notes are long, because I'm fascinated why –of all fields of physics where problems are formulated on lattices– only condensed matter utilizes the theory of irreps of space groups. For the course itself, read sect. 8.2 *Space groups* and sect. 8.2.1 *Wallpaper groups* - the rest is speculations, mostly.

Why do I care? In this course we are learning theory of space groups as applied to quantum mechanics of crystals - rather than diagonalizing the Hamiltonian and computing energy levels, one works on the reciprocal lattice, and computes energy bands (continuum limit of finely spaced discrete eigenvalues of finite, periodic lattices). If fluctuations from strict periodicity are small, one can often identify the crystal by measuring the intensities of Bragg peaks.

Then there are other kinds of lattices. In computational field theory (classical and quantum) one discretizes the space-time, often on a cubic lattice; one example is worked out here in sect. 8.3 *Elastodynamic equilibria of 2D solids*. The there are Ising models in one, two, three dimensions, problems like deterministic diffusion on periodic lattices of scatterers, coupled maps lattices. None of that literature *ever* (to best of my knowledge) reduces the computations to the reciprocal space Brilluion zone. Why?

The funny thing is - I *know* the answer since 1976, but the siren song of classical crystallography is so enchanting that it has blinded me with science. I think that is due to a deep and under-appreciated "chaos / turbulence" physics underlying these problems. If deviations from the strict periodic structure are *small* (the basic "long wavelength" assumption of sect. 8.3), the "integrable" thinking in terms of normal modes applies, and you should use the crystallography described here. If the symmetry of the law you are studying is a space group, but the deviations of typical solutions are *large* (our deterministic diffusion, Ising models, ...), we have to think again. One fundamental thing we learned in studies of transitions to chaos is that the traditional Fourier analysis is useless - it just yields broad, shapeless continuous spectra. The powerful way to think about these problems is Poincaré's qualitative theory of solutions of differential equations : analyse the geometry of their flows in their *state space*. I know for a fact (from a study of cat maps and spatiotemporal cat maps - those I would have to explain one-on-one, as the papers are unpublished) that in that case the translational eigenfunctions are hyperbolic sinhes and coshes, rather than the sines and cosines we are used to as C_n eigenfunctions. For finite discrete symmetries you saw that irreps were fine for linear problems, like coupled arrays of springs, but symmetry reduction for a nonlinear problem like Lorenz equations required quite different techniques. For space group symmetries the analogous nonlinear problems seem still quite unexplored.

8.2 Space groups

A space group, a subgroup of the group of rotations and translations in three dimensions, is the set of transformations that leave a crystal invariant. A space group operator is commonly denoted as

$$\{R|\boldsymbol{t}\}\,, \tag{8.1}$$

where $\boldsymbol{t}$ belongs to the infinite set of discrete translations, and R is one of the finite number of discrete orientation (point group) symmetries. Translation symmetry, i.e., the periodicity of a crystal, manifests itself physically through phonons, magnons, and other smooth, long-wavelength deformations. Discrete orientation symmetry manifests itself through macroscopic anisotropies of crystals, and its natural faces. The experimental challenge is to determine the crystal structure, typically by diffraction (study of the *reciprocal lattice*). It is a challenge, as one measures only the intensities of Bragg peaks, not their phases, but the answer should be one of the 230 space groups listed in the *International Tables for Crystallography*, the "Bible" of crystallographers.

Unless you have run into a quasicrystal :). In that case Claire has a story to tell, but it will have to remain private.

Understanding the Bible requires much more detail than what we can cover in a week or two (it could take a lifetime), and has been written up many places. I found Dresselhaus *et al.* [11] Chapter *9. Space Groups in Real Space* quite clear on matrix representation of space groups (click here). (The MIT course 6.734 online version contains much of the same material.) I also found Béatrice Grenier's overview over crystallography helpful. Many online tools are available to ease the task, for example the FullProf suite of crystallographic programs. The Bible was completed in 19th century, but the field is undergoing a revival, as the study of topological insulators requires diving deeper into crystallography than simply looking up the tables.

The translation group T, the set of translations $\boldsymbol{t}$ that put the crystallographic structure in coincidence with itself, constitutes the *lattice*. T is a normal subgroup of G. It defines the *Bravais lattice*. Translations are of the form

$$\boldsymbol{t} = \boldsymbol{t_n} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3\,, \qquad n_j \in \mathbb{Z}\,.$$

The basis vectors $\boldsymbol{a}_j$ span the *unit cell*. There are 6 simple (or primitive) unit cells that contain a single point, specified by the lengths of the unit translations a, b, c and pairwise angles α, β, γ between them. The most symmetric among them is the *cubic* cell, with $a = b = c$ and $\alpha = \beta = \gamma = 90^o$.

The lattice unit cell is always a *generating region* (a tile that tiles the entire space), but the smallest generating region *–the fundamental domain–* may be smaller than the lattice unit. At each lattice point the identical group of "atoms" constitutes the *motif*. A *primitive cell* is a minimal region repeated by lattice translations. The lattice and the motif completely characterize the crystal.

The cosets by translation subgroup T (the set all translations) form the *factor* (AKA *quotient*) group G/T, isomorphic to the point group g (rotations). All irreducible representations of a space group G can be constructed from irreducible representations of g and T. This step, however, is tricky, as, due to the non-commutativity of translations and rotations, the quotient group G/T is not a normal subgroup of the space group G.

The quantum-mechanical calculations are executed by approximating the infinite crystal by a triply-periodic one, and going go to the *reciprocal* space by deploying C_{N_j} discrete Fourier transforms. This implements the G/T quotienting by translations and reduces the calculation to a finite *Brilluoin zone*. That is the content of the *'Bloch theorem'* of condensed matter physics. Further work is then required to reduce the calculations to the point group irreps.

Point symmetry operations leave at least one point fixed. They are (a) inversion through a point, (b) rotation around an axis, (c) roto-inversion around an axis and through a point and (d) reflection through a mirror plane. The rotations have to be compatible with the translation symmetry: in 3 spatial dimensions they can only be of orders 1, 2, 3, 4, or 6. They can be proper $(\det\, = +1)$ or improper $(\det\, = -1)$.

The spectroscopists' Schoenflies notation labels point groups as: cyclic C_n, dihedral $\mathrm{C}_{n'}$, tetrahedral T and octahedral O rotation point groups, of order $n = 1, 2, 3, 4, 6$, respectively. The superscript $'$ refers to either v (parallel mirror plane) or h (perpendicular mirror plane). The crystallographer's preferred classification is, however, the international crystallographic (Hermann-Mauguin) notation.

8.2.1 Wallpaper groups

Pedagogically, it pays to start with a discussion of two-dimensional space groups, or *wallpaper groups* (there are 17 of those).

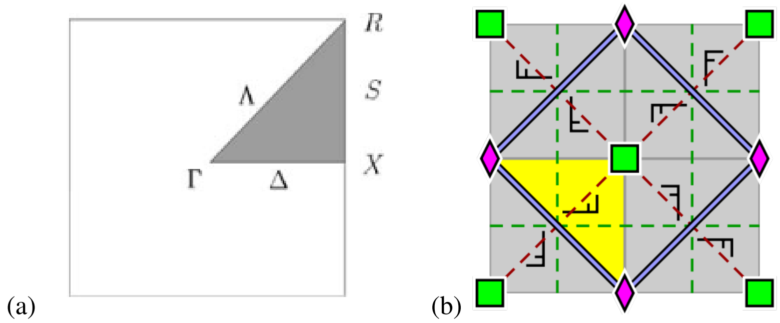

Figure 8.1: The shaded (or yellow) area indicates a *fundamental domain*, i.e., the smallest part of the pattern whose repeats tile the entire plane. (a) For the most symmetric 2D square lattice, with point group $p4mm$, the fundamental domain is indicated by the shaded triangle $\Gamma\Lambda RSX\Delta\Gamma$ which constitutes 1/8 of the Brillouin zone, and contains the basic wave vectors and the high symmetry points (Fig. 10.2 of Dresselhaus *et al.* [11]). (b) For the 2D square lattice with the glide and reflect point group $p4g$ the fundamental domain is indicated by the yellow triangle (Figure drawn by M. von Gagern).

For wallpaper groups the Hermann-Mauguin notation begins with either p or c, for a primitive cell or a face-centred cell. This is followed by a digit, n, indicating the highest order of rotational symmetry: 1-fold (none), 2-fold, 3-fold, 4-fold, or 6-fold. The first, resp. second of the next two symbols indicates the symmetry relative to one translation axis of the pattern, referred to as the main, resp. second one. The symbols are either m, g, or 1, for mirror, glide reflection, or none.

Section *9.3 Two-Dimensional Space Groups* of Dresselhaus *et al.* [11] discusses the most symmetric of the wallpaper groups, the tiling of a plane by squares, which in the international crystallographic notation is denoted by #11, with point group $p4mm$. We work out this space group in exercise 8.2. The largest invariant subgroup of C_{4v} is C_4. In that case, the space group is $p4$, or #10. Prefix p indicates that the unit cell is primitive (not centered). This is a 'simple', or *symmorphic* group, which makes calculations easier. There is, however, the third, non-symmorphic two-dimensional square space group $p4g$ or #12 ($p4gm$), see Table B.10 of ref. [11]. If someone can explain its 'Biblical' diagram to me, I would be grateful. The wiki explanation, reproduced here as figure 8.1 (b), is the best one that I have found so far, but I'm still scratching my head:) The Bravais lattice 'unit cell' is a square in all three cases. In the crystallographic literature the ChaosBook's 'fundamental domain' makes an appearance only in the reciprocal lattice, as the Brilloun zone depicted for $p4mm$ in figure 8.1 (a). However, the 'wallpaper groups' wiki does call 'fundamental domain' the smallest part of the configuration pattern that, when repeated, tiles the entire plane.

The quantum-mechanical calculations are carried out in the reciprocal space, in our case with the full Γ point, $k = 0$, wave vector symmetry (see Table 10.1 of ref. [11]), and 'Large Representations'.

Sect. *10.5 Characters for the Equivalence Representation* look like those for the point group, sort of.

8.2.2 One-dimensional line groups

One would think that the one-dimensional *line groups*, which describe systems exhibiting translational periodicity along a line, such as carbon nanotubes, would be simpler still. But even they are not trivial – there are 13 of them.

The normal subgroup of a line group L is its translational subgroup T, with its factor group L/T isomorphic to the *isogonal point group* P of discrete symmetries of its 1-dimensional unit cell $x \in (-a/2, a/2]$. In the reciprocal lattice k takes on the values in the first Brillouin zone interval $(-\pi/a, \pi/a]$e. In *Irreducible representations of the symmetry groups of polymer molecules. I*, Božović, Vujičić and Herbut [7] construct all the reps of the line groups whose isogonal point groups are $C_n, C_{nv}, C_{nh}, S_{2n}$, and D_n. For some of these line groups the irreps are obtained as products of the reps of the translational subgroup and the irreps of the isogonal point group.

According to W. De Heer, the Mintmire, Dunlap and White [23] paper *Are Fullerene tubules metallic?* which took care of chiral rotations for nanotubes by a tight-binding calculation, played a key role in physicists' understanding of line groups.

8.2.3 Time reversal symmetry

Consequences of time-reversal symmetry on line groups are discussed by Božović [6]; In the case when the Hamiltonian is invariant under time reversal [14], the symmetry group is enlarged: $L + \theta L$. It is interesting to learn if the degeneracy of the levels is doubled or not.

Johnston [19] *Group theory in solid state physics* is one of the many reviews that discusses Wigner's time-reversal theorems for a many-electron system, including the character tests for time-reversal degeneracy, the double space groups, and the time-reversal theorems (first discussed by Herring [14] in *Effect of time-reversal symmetry on energy bands of crystals*).

8.3 Elastodynamic equilibria of 2D solids

Artificial lattices are often introduced to formulate classical field theories (described by partial differential equations) and quantum field theories (described by path integrals) as finite-dimensional problems, either for theoretical reasons (QM in a periodic box), or in order to port them to computers. For example, lattice QCD approximates Quantum Chromodynamics by a 4-dimensional cubic crystal. What follows is a simple example of such formulation of a classical field theory, taken from Mehran Kardar's MIT course, Lecture 23.

Consider a perfect two-dimensional solid at $T = 0$. The equilibrium configuration of atoms forms a lattice,

$$\boldsymbol{r}_0(m, n) = m\boldsymbol{e}_1 + n\boldsymbol{e}_2 \,,$$

where $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ are basis vectors, $a = |\boldsymbol{e}_j|$ is the lattice spacing, and $\{m, n\}$ are integers. At finite temperatures, the atoms fluctuate away from their equilibrium position, moving to

$$\boldsymbol{r}(m,n) = \boldsymbol{r}_0(m,n) + \boldsymbol{u}(m,n)\,,$$

As the low temperature distortions do not vary substantially over nearby atoms, one can define a coarse-grained distortion field $\boldsymbol{u}(\boldsymbol{x})$, where $\boldsymbol{x} = (x_1, x_2)$ is treated as continuous, with an implicit short distance cutoff of the lattice spacing a. Due to translational symmetry, the elastic energy depends only on the strain matrix,

$$u_{ij}(\boldsymbol{x}) = \tfrac{1}{2}\left(\partial_i u_j + \partial_j u_i\right)\,.$$

Kardar picks the triangular lattice, as its elastic energy is isotropic (i.e., invariant under lattice rotations, see Landau and Lifshitz [22]). In terms of the Lamé coefficients λ and μ,

$$\begin{aligned}\beta H &= \frac{1}{2}\int d^2\boldsymbol{x}\,(2\mu\, u_{ij}u_{ij} + \lambda\, u_{ii}u_{jj}) \\ &= -\frac{1}{2}\int d^2\boldsymbol{x}\, u_i[2\mu\,\Box\,\delta_{ij} + (\mu+\lambda)\,\partial_i\partial_j]\, u_j\,. \end{aligned} \tag{8.2}$$

(here we have assumed either infinite or doubly periodic lattice, so no boundary terms from integration by parts), with the equations of motion something like (FIX!)

$$\partial_t^2 u_i = [2\mu\,\Box\,\delta_{ij} + (\mu+\lambda)\,\partial_i\partial_j]\, u_j\,. \tag{8.3}$$

(Note that Kardar keeps time continuous, but discretizes space. In numerical computations time is discretized as well.) The symmetry of a square lattice permits an additional term proportional to $\partial_x^2 u_x^2 + \partial_y^2 u_y^2$. In general, the number of independent elastic constants depends on the dimensionality and rotational symmetry of the lattice in question. In two dimensions, square lattices have three independent elastic constants, and triangular lattices are “elastically isotropic” (i.e., elastic properties are independent of direction and thus have only two [22]).

The Goldstone modes associated with the broken (PC: why “broken”?) translational symmetry are *phonons*, the normal modes of vibrations. Eq. (8.3) supports two types of lattice normal modes, transverse and longitudinal.

The order parameter describing broken translational symmetry is

$$\rho_{\boldsymbol{G}}(\boldsymbol{x}) = e^{i\boldsymbol{G}\cdot\boldsymbol{r}(\boldsymbol{x})} = e^{i\boldsymbol{G}\cdot\boldsymbol{u}(\boldsymbol{x})}\,,$$

where $\boldsymbol{G}$ is any reciprocal lattice vector. Since, by definition, $\boldsymbol{G}\cdot\boldsymbol{r_0}$ is an integer multiple of 2π, $\rho_{\boldsymbol{G}} = 1$ at zero temperature. Due to the fluctuations,

$$\langle\rho_{\boldsymbol{G}}(\boldsymbol{x})\rangle = \langle e^{i\boldsymbol{G}\cdot\boldsymbol{u}(\boldsymbol{x})}\rangle$$

decreases at finite temperatures, and its correlations decay as $\langle\rho_{\boldsymbol{G}}(\boldsymbol{x})\rho^*_{\boldsymbol{G}}(\boldsymbol{0})\rangle$. This is the order parameter ChaosBook and Gaspard use in deriving formulas for deterministic diffusion. Kardar computes this in Fourier space by approximating $\boldsymbol{G}\cdot\boldsymbol{q}$ with its angular average $G^2q^2/2$, ignoring the rotationally symmetry-breaking term $\cos\boldsymbol{q}\cdot\boldsymbol{x}$, and getting only the asymptotics of the correlations right (the decay is algebraic).

The translational correlations are measured in diffraction experiments. The scattering amplitude is the Fourier transform of $\rho_{\boldsymbol{G}}$, and the scattered intensity at a wave-vector q is proportional to the structure factor. At zero temperature, the structure factor is a set of delta-functions (Bragg peaks) at the reciprocal lattice vectors.

The orientational order parameter that characterizes the broken rotational symmetry of the crystal can be defined as

$$\Psi(\boldsymbol{x}) = e^{6i\theta(\boldsymbol{x})} ,$$

where $\theta(\boldsymbol{x})$ is the angle between local lattice bonds and a reference axis. The factor of 6 accounts for the equivalence of the 6 possible C_{3v} orientations of the triangular lattice. (Kardar says the appropriate choice for a square lattice is $\exp(4i\theta(\boldsymbol{x}))$ - shouldn't the factor be 8, the order of C_{4v}?) The order parameter has unit magnitude at $T = 0$, and is expected to decrease due to fluctuations at finite temperature. The distortion $u(\boldsymbol{x})$ leads to a change in bond angle given by

$$\theta(\boldsymbol{x}) = -\tfrac{1}{2}\left(\partial_x u_y - \partial_y u_x\right) .$$

(This seems to be dimensionally wrong? For detailed calculations, see the above Kardar lecture notes.)

8.4 Literature, reflections

Predrag The story of quantum scattering off crystals, I believe, starts with the Bouckaert, Smoluchowski and Wigner (1936) paper [5].

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 8.2 (figs. 8.8 and 8.12 in Joshi [20]). 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 8.2 (a). The tetrahedron ΓXMR, 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.

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

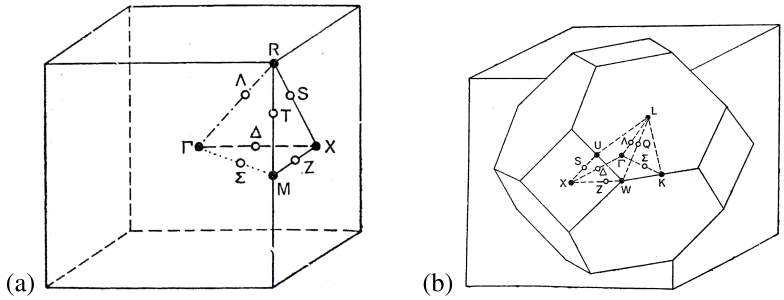

Figure 8.2: (a) The special points and the lines of symmetry in the first Brillouin zone of a simple cubic lattice define its fundamental domain, the tetrahedron ΓXMR. (b) Just not to get any ideas that this is easy: the fundamental domain for the first Brillouin zone of a bcc lattice. (From Joshi [20].)

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 [16] 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 [17] paper (but not the Hestenes and Holt [18] follow up). 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 [10] discussion of planar tilings, please do report back to me.

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 [4, 26] 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 [30] 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 (Wallace [30] 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 [2] - I have extracted above history of graphene from De Heer's notes (the "con man" is my own angle on what went down with this particular Nobel prize).

Predrag Martin Mourigal found the Presqu'île Giens, May 2009 *Contribution of Symmetries in Condensed Matter* Summer School very useful. Villain [29] *Symmetry and group theory throughout physics* gives a readable overview. The overheads are here, many of them are of potential interest. Mourigal recommends

Canals and Schober [8] *Introduction to group theory*. It is very concise and precise, a bastard child of Bourbaki and Hamermesh [13]. Space groups show up only once, on p. 24: "By working with the cosets we have effectively factored out the translational part of the problem."

Ballou [1] *An introduction to the linear representations of finite groups* appears rather formal (and very erudite).

Grenier, B. and Ballou [12] *Crystallography: Symmetry groups and group representations*.
The word crystal stems from Greek 'krustallas' and means "solidified by the cold."

Schober [27] *Symmetry characterization of electrons and lattice excitations* gives an eminently readable discussion of space groups.

Rodríguez-Carvajal and Bourée [25] *Symmetry and magnetic structures*

Schweizer [28] *Conjugation and co-representation analysis of magnetic structures* deals with black, white and gray groups that Martin tries not to deal with, so all Mourigal groups are gray.

Villain discusses graphene in the Appendix A of *Symmetry and group theory throughout physics* [29].

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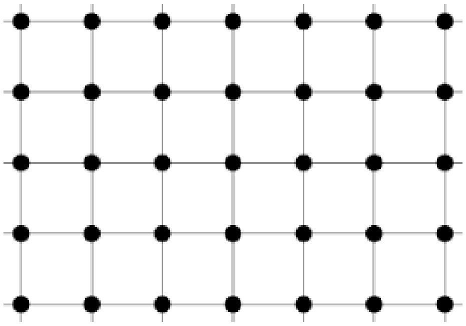

Figure 8.3: Square lattice of atoms

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 8.3.

(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.

(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.