Karlsruhe Institute of Technology
Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

Prof. Dr. A. Shnirman
Dr. D. Shapiro, H. Perrin

Solutions to sheet 2
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Category A

1. Rotation symmetry (10 + 5 + 5 = 20 points)

The proof of the Bloch theorem was based on the commutation of the Hamiltonian with the translation operators $T_{\mathbf{R}}$. In fact, any unitary symmetry can be expressed similarly. As an example, consider particles in a two-dimensional lattice potential which has C_n symmetry, i.e. it has an n-fold rotation symmetry ($n \in \{2, 3, 4, 6\}$).

(a) Assuming spinless particles, express the C_n symmetry in terms of a group of unitary operators (in a specific representation) that commute with the Hamiltonian.

Solution: We choose the coordinate system such that the rotation center is located at the origin (more precisely: *one possible choice* of the rotation center). Rotation symmetry is present if $H(\vec{r}) = H(U_\phi \vec{r})$, where U_ϕ is the 2×2 rotation matrix with angle $\phi = \dfrac{2\pi}{n}$. It is convenient to switch from cartesian to polar coordinates: $\vec{r} = (x, y) \to (r, \varphi)$. Then,

$$H(r, \varphi) = H\left(r, \varphi + \frac{2\pi}{n}\right).$$

This motivates the definition of the operators R_j with $j \in \mathbb{Z}_n = \{0, \ldots, n-1\}$ which act on $f(r, \varphi)$ by

$$R_j f(r, \varphi) = f\left(r, \varphi + \frac{2\pi j}{n}\right).$$

It is easily shown that $R_j^{-1} = R_{(-j) \bmod n}$. Let us prove that R_j is unitary i.e. $R_j^\dagger = R_j^{-1}$:

$$\begin{aligned} \langle \phi_1 | R_j^{-1} | \phi_2 \rangle &= \int \mathrm{d}^2\vec{r} \phi_1^*(r, \varphi) R_j^{-1} \phi_2(r, \varphi) = \int r \mathrm{d}r \mathrm{d}\varphi \phi_1^*(r, \varphi) \phi_2\left(r, \varphi - \frac{2\pi j}{n}\right) \\ &= \int r \mathrm{d}r \mathrm{d}\varphi' \phi_1^*\left(r, \varphi' + \frac{2\pi j}{n}\right)) \phi_2(r, \varphi') = \langle \phi_1 | R_j^\dagger | \phi_2 \rangle \end{aligned}$$

$\{R_j\}$ form a group: $R_i R_j = R_{(i+j) \bmod n}$ which is Abelian and R_0 is the identity operator. Furthermore, these operators commute with H:

$$R_j H(r, \varphi) \Psi(r, \varphi) = H(r, \varphi + \frac{2\pi j}{n}) \Psi(r, \varphi + \frac{2\pi j}{n}) = H(r, \varphi) R_j \Psi(r, \varphi).$$

(b) Now repeat the task with spin-$\frac{1}{2}$ particles.

Solution: Recall that a 360-degree rotation of a spin-$\frac{1}{2}$ particle yields a minus sign in the wave function. Therefore, $[H, R_j] = 0$ cannot be a sufficient description of the symmetry. We have to include the spin rotation (more generally: any internal degrees of freedom) in the symmetry operator. In spin space, a rotation by $2\pi/n$ around the z axis is performed with the operator

$$\hat{r} = \exp\left(i\frac{\pi}{n}\sigma_z\right) = \cos\frac{\pi}{n} + i\sigma_z \sin\frac{\pi}{n}$$

with the Pauli matrix σ_z (Prove this if you don't know it!). The symmetry condition for the Hamiltonian can then be expressed as

$$\hat{r}^\dagger H(U_\phi \vec{r})\hat{r} = H(\vec{r})$$

with the rotation matrix U_ϕ, or, using $R = R_1$, with the commutator

$$[\hat{r}R, H] = 0\,.$$

Note how

$$\hat{r}^n = \exp(i\pi\sigma_z) = \cos\pi = -1\,,$$

such that our rotation operator $\hat{r}R$ will generate the required sign in one full rotation.

(c) Can you label the eigenstates of the Hamiltonian with a rotation eigenvalue c_n and the crystal momentum $\mathbf{k}$ at the same time?

Solution: This is only possible when the different symmetries commute mutually. Translation and rotation do, in general, not commute. Therefore, we can usually not use c_n and $\mathbf{k}$ simultaneously as quantum numbers.

However, certain points of the first Brillouin zone (BZ) are invariant under rotation, i.e., they map onto themselves up to a reciprocal lattice vector. For instance, the simple square lattice has C_4 symmetry. The reciprocal lattice is also the square lattice. Hence, the first Brillouin zone is quadratic with $k_x, k_y \in \{-\pi/a, \pi/a\}$. One corner of the Brillouin zone, e.g., $\mathbf{K} = (\pi/a, \pi/a)$, is mapped onto another corner under $\frac{\pi}{2}$ rotation, namely $\mathbf{K}' = (-\pi/a, \pi/a)$. On the other hand, all corners are equivalent: $\mathbf{K}' - \mathbf{K} = -\frac{2\pi}{a}\hat{e}_x$, which is a reciprocal lattice vector.

At such special points, all $\psi_{K,n}$ are also eigenstates of R_j and can be assigned a well-defined eigenvalue c_n.

Category B

2. Bloch wavefunctions (10 + 5 + 10 + 5 = 30 points)

Consider an infinitely extended one-dimensional system of electrons in a potential of periodically occurring delta functions. The Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U\sum_{n=-\infty}^{\infty}\delta(x + na) \tag{1}$$

with a constant U. This is a simple version of the Kronig-Penney model. It allows us to study the properties of Bloch states ψ_k exactly.

(a) Let $U > 0$. Derive the Bloch wavefunctions and an implicit form of the dispersion relation $E(k)$ by solving the Schrödinger equation. Start with one unit cell, then use the Bloch theorem.

Solution: Within one unit cell, e.g. $x \in (0, a)$, the potential is zero and the Schrödinger equation is trivially solved by plane waves

$$\phi_K(x) = Ae^{iKx} + Be^{-iKx}$$

where $K > 0$. The energy of this state is $E = \hbar^2 K^2/(2m)$.

We know from the Bloch theorem that the general solutions for $x \in \mathbb{R}$ have the form

$$\psi_k(x) = u_k(x)e^{ikx}$$

with a lattice-periodic function $u_k(x)$. It follows that $\psi_k(x - a) = e^{-ika}\psi_k(x)$. Because $\psi_k(x) = \phi_K(x)$ on the interval $(0, a)$ for some (yet undetermined) parameters K, A, B, we conclude that

$$\psi_k(x + na) = \phi_K(x)e^{ikna}.$$

Now we have to ensure the correct behavior of ψ_k at the boundaries of the unit cells. On the one hand, continuity of ψ_k demands that

$$\lim_{x\to 0, x>0} \phi_K(x) - e^{-ika} \lim_{x\to a, x<a} \phi_K(x) = 0\,,$$

whereas the derivative of the wavefunction has a finite step at the δ peaks of the potential,

$$\lim_{x\to 0, x>0} \frac{\partial\phi_K(x)}{\partial x} - e^{-ika} \lim_{x\to a, x<a} \frac{\partial\phi_K(x)}{\partial x} = \frac{2m}{\hbar^2} U\psi(0)\,.$$

From these two conditions we obtain the two equations

$$\begin{aligned} A + B - e^{-ika}\left(Ae^{iKa} + Be^{-iKa}\right) &= 0 \\ A - B - e^{-ika}\left(Ae^{iKa} - Be^{-iKa}\right) &= \frac{2mU}{i\hbar^2 K}(A + B)\,. \end{aligned}$$

This linear system for the coefficients A and B only has a solution if we demand that K satisfies

$$\cos(Ka) + \frac{mU}{\hbar^2 K}\sin(Ka) = \cos(ka).$$

If we express K in terms of the energy E, $K(E) = \frac{1}{\hbar}\sqrt{2mE}$, this equation defines implicitly the dispersion relation $E(k)$. If K is chosen such that this condition is met for a given crystal momentum k, we can determine the ratio of A and B in the wavefunction ϕ_K and thereby obtain the exact form of the Bloch state ψ_k for $x \in \mathbb{R}$:

$$\begin{aligned} \psi_k(x) &= e^{ikx} C_k e^{-ik(x-na)} \left[\left(e^{ika} - e^{-iKa}\right) e^{iK(x-na)} - \left(e^{ika} - e^{iKa}\right) e^{-iK(x-na)}\right] \\ &=: e^{ikx} u_k(x)\,, \end{aligned}$$

where $n = n(x)$ is chosen such that $x - na \in (0, a)$ and C_k is a constant which finally has to be calculated such that ψ_k is normalized:

$$\begin{aligned} 1 &\stackrel{!}{=} \frac{1}{a}\int_0^a dx\, u_k^*(x)u_k(x) \\ &= |C_k|^2 \left[\left|e^{ika} - e^{-iKa}\right|^2 + \left|e^{ika} - e^{iKa}\right|^2 - \frac{\sin(2Ka)}{Ka}\right] \\ &= |C_k|^2 \left[4\left(1 - \cos(ka)\cos(Ka)\right) - \frac{\sin(2Ka)}{Ka}\right] \\ \Rightarrow |C_k| &= \left[4\left(1 - \cos(ka)\cos(Ka)\right) - \frac{\sin(2Ka)}{Ka}\right]^{-1/2} \end{aligned}$$

The phase of C_k is arbitrary.

(b) Show explicitly that the group velocity in this system is zero at the zone boundaries in reciprocal space.

Solution: The group velocity follows directly from the dispersion relation

$$v_g(k) = \frac{\partial}{\partial k}E(k)\,.$$

We will calculate v_g^{-1}, because we only know the inverse function in the form $k(E) = \arccos F(K)$:

$$\frac{1}{v_g} = \frac{\partial}{\partial E}k(E) = \left(\frac{\partial K}{\partial E}\right)\frac{\partial}{\partial K}k(K) = -\frac{\sqrt{m}}{\hbar\sqrt{2E}}\frac{1}{\sqrt{1-F(K)^2}}\frac{\partial F(K)}{\partial K}$$

where

$$\frac{\partial F(K)}{\partial K} = \frac{amU}{i\hbar^2 K}\cos(Ka) - \left[a + \frac{mU}{i\hbar^2K^2}\right]\sin(Ka)\,.$$

At the zone boundary, $ka = \pm\pi + 2\pi n \;\Rightarrow\; F(K) = -1$. This causes a divergence of $(1-F^2)^{-1/2}$, hence $v_g(ka = \pm\pi) = 0$. Note, though, that the divergence is canceled by $\partial_K F(K)$ if we set $U = 0$.

(c) Use the dispersion relation from (a) to state a condition for which energies are allowed in this system. In between these bands, energy gaps occur. Derive the approximate size of the gap between the energetically lowest bands for both the limit of very weak U and the limit of very strong U.

Solution: The condition for the energies which are possible in this system simply follows from $|\cos ka| \leq 1$ in the dispersion relation:

$$\left|\cos(Ka) + \frac{mU}{\hbar^2 K}\sin(Ka)\right| \leq 1. \qquad (*)$$

or

$$\left|\cos\left(\frac{a}{\hbar}\sqrt{2mE}\right) + \frac{\sqrt{m}U}{\hbar\sqrt{2E}}\sin\left(\frac{a}{\hbar}\sqrt{2mE}\right)\right| \leq 1\,.$$

Equality holds exactly at the edges of the energy bands. It is easily seen that $K_n a = n\pi$ always solves the equation, where $n \in \mathbb{N}$ is the index of the band in the reduced zone scheme. Note how K_n alternatingly corresponds to $k = 0$ (zone center) or $k = \pm\pi/a$ (zone boundary). If K_n is increased slightly, the left side of

$(*)$ becomes larger than one. Thus, $E(K_n)$ is the energy of the *upper* band edge of the n-th band. The lower band edge can only be approximated.

For large U, we expect narrow bands and large gaps (at low energies, at $E \to \infty$ one will, of course, always recover (quasi-)free particles). Therefore, we linearize the relation within the band for $K = K_n - \kappa$ ($\kappa > 0$) to estimate the position of the lower band edge,

$$\left| 1 - \frac{mU}{\hbar^2 K_n} \kappa a \right| \leq 1 \,,$$

and the other edge follows from

$$\frac{mU}{\hbar^2 K_n} \kappa a = 2 \qquad \Rightarrow \quad \kappa = \frac{2\pi n \hbar^2}{a^2 m U} \,.$$

We obtain the gap between the bands n and $n+1$ to leading order in U^{-1}:

$$\begin{aligned} E(K_{n+1} - \kappa_{n+1}) - E(K_n) &= \frac{\hbar^2 \pi^2 (n+1)^2}{2ma^2} \left(1 - \frac{4\hbar^2}{amU} \right) - \frac{n^2 \hbar^2 \pi^2}{2ma^2} \\ &= \frac{\hbar^2 \pi^2 (2n+1)}{2ma^2} - \frac{2\hbar^4 \pi^2 (n+1)^2}{m^2 a^3 U} \end{aligned}$$

For small U, we expect small gaps therefore an expansion of $(*)$ around K_n will capture the lower edge of the next band:

$$1 - \frac{1}{2}(\kappa a)^2 + \frac{amU}{\hbar^2 n\pi} \kappa a = 1$$

$$\kappa = \frac{2mU}{\hbar^2 n \pi}$$

and the gap is

$$E(K_n + \kappa_n) - E(K_n) = \frac{\hbar^2}{2m} (2K_n \kappa) + \mathcal{O}\left(\kappa^2\right) = 2\frac{U}{a} \,.$$

(d) Now let $U < 0$. Obtain the (implicit) dispersion relation for states with $E < 0$.

Solution: The Schrödinger equation is solved exactly as in (a), but for $E < 0$ we have to insert an imaginary wave number K in the ansatz ϕ_K, corresponding to evanescent wavefunctions. The same steps as before lead to the implicit dispersion relation

$$\frac{mU}{i\hbar^2 K} \sinh(iKa) + \cosh(iKa) = \cos(ka)$$