Karlsruhe Institute of Technology
Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

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Solutions to sheet 1
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Category A

1. Reciprocal lattice (3 + 5 + 5 + 5 + 2 = 20 points)

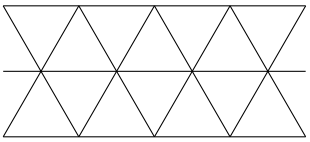
(a) Let L be a D-dimensional Bravais lattice and L' its reciprocal lattice. Show that $(L')'$ is identical to L.

Solution: Let $\vec{a}_i$, $\vec{b}_i$, and $\vec{c}_i$ (with $i \in \{1, \dots, D\}$) denote the lattice basis vectors of L, L', and $(L')'$, respectively. Given that L' is the reciprocal lattice of L, and $(L')'$ the reciprocal lattice of L', we know that

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij} \qquad \text{and} \qquad \vec{b}_i \cdot \vec{c}_j = 2\pi\delta_{ij}\,.$$

Consequently, $(\vec{a}_i - \vec{c}_i)\cdot\vec{b}_j = 0$ for any i, j. This can only be true if $\vec{a}_i = \vec{c}_i$ for any i, because the vectors $\vec{b}_j$ form a complete D-dimensional basis. Thus, we have shown that the lattices L and $(L')'$ are identical.

(b) Construct explicitly the reciprocal lattice of the displayed hexagonal (also called triangular) Bravais lattice. Each vertex represents an atom.



Solution: In cartesian coordinates, the lattice vectors of the hexagonal lattice (not to be confused with the honeycomb lattice) are

$$\vec{a}_1 = \begin{pmatrix} a \\ 0 \end{pmatrix} \qquad \text{and} \qquad \vec{a}_2 = \frac{1}{2}\begin{pmatrix} a \\ \sqrt{3}a \end{pmatrix},$$

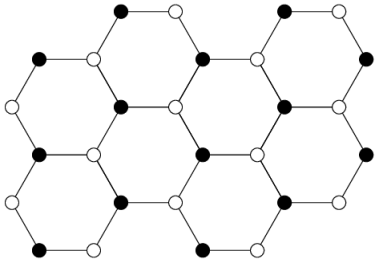
where a is the lattice constant. The basis vectors of the reciprocal lattice are

$$\left[\vec{b}_1, \vec{b}_2\right]^{\mathrm{T}} = 2\pi\left[\vec{a}_1, \vec{a}_2\right]^{-1} = 2\pi \begin{pmatrix} a & \frac{1}{2}a \\ 0 & \frac{1}{2}\sqrt{3}a \end{pmatrix}^{-1} = \frac{2\pi}{a}\begin{pmatrix} 1 & -\frac{1}{\sqrt{3}} \\ 0 & \frac{2}{\sqrt{3}} \end{pmatrix}$$

$$\Rightarrow \quad \vec{b}_1 = \frac{4\pi}{\sqrt{3}a}\begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix}, \qquad \vec{b}_2 = \frac{4\pi}{\sqrt{3}a}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

This is again a hexagonal lattice, but rotated by $\frac{\pi}{6}$ with respect to the original one.

(c) Construct the reciprocal lattice of the honeycomb lattice



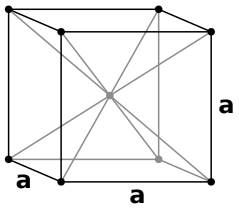
Solution: A primitive unit cell of the honeycomb lattice is

$$\vec{a}_1 = \frac{a}{2}\begin{pmatrix} 3 \\ \sqrt{3} \end{pmatrix} \qquad \text{and} \qquad \vec{a}_2 = \frac{a}{2}\begin{pmatrix} 3 \\ -\sqrt{3} \end{pmatrix},$$

$$\left[\vec{b}_1, \vec{b}_2\right]^{\mathrm{T}} = 2\pi \left[\vec{a}_1, \vec{a}_2\right]^{-1} = 2\pi \begin{pmatrix} \frac{3a}{2} & \frac{3a}{2} \\ \frac{a\sqrt{3}}{2} & -\frac{a\sqrt{3}}{2} \end{pmatrix}^{-1} = \frac{2\pi}{3a}\begin{pmatrix} 1 & \sqrt{3} \\ 1 & -\sqrt{3} \end{pmatrix}$$

$$\Rightarrow \quad \vec{b}_1 = \frac{2\pi}{3a}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \qquad \vec{b}_2 = \frac{2\pi}{3a}\begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix}$$

(d) Now we turn to three dimensions: Construct the reciprocal lattice of the body-centered cubic (bcc) Bravais lattice.



Solution: A primitive unit cell of the bcc lattice is given by the vectors

$$\vec{a}_1 = \frac{1}{2}\begin{pmatrix} a \\ a \\ -a \end{pmatrix}, \quad \vec{a}_2 = \frac{1}{2}\begin{pmatrix} a \\ -a \\ a \end{pmatrix}, \quad \vec{a}_3 = \frac{1}{2}\begin{pmatrix} -a \\ a \\ a \end{pmatrix}.$$

We find the vectors of the reciprocal lattice by matrix inversion:

$$\left[\vec{b}_1, \vec{b}_2, \vec{b}_3\right]^{\mathrm{T}} = 2\pi \left[\vec{a}_1, \vec{a}_2, \vec{a}_3\right]^{-1} = \frac{4\pi}{a}\begin{pmatrix} 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \end{pmatrix}^{\text{-1}} = \frac{2\pi}{a}\begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

$$\Rightarrow \quad \vec{b}_1 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \vec{b}_2 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \vec{b}_3 = \frac{2\pi}{a}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

(e) Deduce, without any calculations, the reciprocal lattice of the face-centered cubic (fcc) lattice.

Solution: The reciprocal lattice of the body-centered cubic lattice corresponds to the face-centered cubic (fcc) lattice. From question (a), we know that the reciprocal lattice of the reciprocal lattice is the original lattice itself. Then we deduce, that the reciprocal lattice of the face-centered cubic lattice is the body-centered cubic lattice:

$$\vec{a}_1 = \frac{a}{2}\begin{pmatrix}1\\1\\0\end{pmatrix}, \quad \vec{a}_2 = \frac{a}{2}\begin{pmatrix}1\\0\\1\end{pmatrix}, \quad \vec{a}_3 = \frac{a}{2}\begin{pmatrix}0\\1\\1\end{pmatrix}$$

$$\Rightarrow \quad \vec{b}_1 = \frac{2\pi}{a}\begin{pmatrix}1\\1\\-1\end{pmatrix}, \quad \vec{b}_2 = \frac{2\pi}{a}\begin{pmatrix}1\\-1\\1\end{pmatrix}, \quad \vec{b}_3 = \frac{2\pi}{a}\begin{pmatrix}-1\\1\\1\end{pmatrix}$$

Category B

2. Born-Oppenheimer approximation (5 + 10 + 15 = 30 points)

(a) Explain in words what the Born-Oppenheimer approximation is and why it is important when dealing with the full solid-state Hamiltonian.

Solution: The Born-Oppenheimer approximation exploits that heavy particles move much slower than light particles. Therefore, the problem of light masses can be solved assuming that the heavy masses are static. The heavy masses can be treated within the effective potential formed by the averaged fast dynamics of light particles. The approximation is useful to decouple electron and ion dynamics in solid-state physics, because electrons are much lighter than ions.

(b) Consider the quantized version of the following one-dimensional system: a mass M is attached to the point $x = 0$ by a spring of constant k_1. A second mass m is attached to the first mass by a spring of constant k_2. The Hamiltonian of this system is

$$H = \frac{p_1^2}{2M} + \frac{p_2^2}{2m} + \frac{1}{2}k_1 x_1^2 + \frac{1}{2}k_2 \left(x_1 - x_2\right)^2,$$

with quantum operators $p_{1,2}, x_{1,2}$. Calculate the eigenenergies using the Born-Oppenheimer approximation, assuming that $m \ll M$ (you may think of an electron bound to an ion which oscillates around its crystal position).

Solution: The Hamiltonian is given by Eq. (2b), where now p_1, x_1 and p_2, x_2 are pairs of operators with canonical commutation relations. We can write it as

$$H = H_M + H_m + H_{M\leftrightarrow m}$$

with

$$H_M = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x_1^2} + \frac{1}{2}\left(k_1 + k_2\right)x_1^2,$$

$$H_m = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + \frac{1}{2}k_2 x_2^2,$$

$$H_{M\leftrightarrow m} = -k_2 x_1 x_2.$$

Within the Born-Oppenheimer approximation, we first neglect the dynamics of the large mass M to evaluate the eigenenergies ϵ of the small mass m, i.e., we discard

H_M and solve $H_m + H_{M\leftrightarrow m}$. The coordinate x_1 becomes a numerical parameter (not an operator) in the effective Hamiltonian for m. We find that

$$H_m + H_{M\leftrightarrow m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \tilde{x}_2^2} + \frac{1}{2}k_2\tilde{x}_2^2 + V(x_1)\,,$$

where we have introduced $\tilde{x}_2 = x_2 - x_1$ and the potential $V(x_1) = -\frac{1}{2}k_2x_1^2$, which is independent of x_2 and therefore a constant with respect to the dynamics of m. The first two terms above form a harmonic oscillator. Using the standard ladder operators $a_m, a_m^\dagger$ for this harmonic oscillator, we can write

$$H_m + H_{M\leftrightarrow m} = \hbar\omega_m\left(a_m^\dagger a_m + \frac{1}{2}\right) + V(x_1)$$

with the frequency

$$\omega_m = \sqrt{\frac{k_2}{m}}\,.$$

Now, we return to the dynamics of M, where we have to include the effective potential $V(x_1)$. Thus, we have to solve the Hamiltonian

$$H_M + V(x_1) = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x_1^2} + \frac{1}{2}k_1x_1^2\,,$$

which in this very simple system is again just an harmonic oscillator. We can write it with ladder operators $a_M, a_M^\dagger$ as

$$H_M + V(x_1) = \hbar\omega_M\left(a_M^\dagger a_M + \frac{1}{2}\right)$$

with the frequency

$$\omega_M = \sqrt{\frac{k_1}{M}}\,.$$

The eigenenergies of the full Hamiltonian are

$$\epsilon_{n_M,n_m} = \hbar\omega_M\left(n_M + \frac{1}{2}\right) + \hbar\omega_m\left(n_m + \frac{1}{2}\right)$$

within the Born-Oppenheimer approximation (with eigenvalues n_μ of $a_\mu^\dagger a_\mu$).

(c) Now calculate the eigenenergies exactly, which is still possible in this simple case. Verify that you get the same result as in (b) if you take the limit $m \ll M$.
Hint: You may follow the steps below.

1. *Substitute* $\tilde{x}_1 = (m_1/m_2)^{1/4}x_1$ *and* $\tilde{x}_2 = (m_2/m_1)^{1/4}x_2$.
2. *Transform to* $(X_1, X_2)^T = R_\alpha(\tilde{x}_1, \tilde{x}_2)^T$, *where* R_α *is a* 2×2 *rotation matrix with angle* α
3. *Determine* α *such that* X_1 *and* X_2 *decouple.*
4. $\cos(\arctan x) = 1/\sqrt{1+x^2}$, $\sin(\arctan x) = x/\sqrt{1+x^2}$.

Solution: Simply shifting the coordinate $\tilde{x}_2 = x_2 - x_1$ does not help if x_1, p_1 are operators: this would introduce a new term that couples the momentum operators p_1 and p_2. The goal of the steps described in the hint is to find a transformation that removes the mixing terms in both position and momentum.

1. The substitution leads to

$$H = -\frac{\hbar^2}{2\sqrt{Mm}}\left(\frac{\partial^2}{\partial\tilde{x}_1^2}+\frac{\partial^2}{\partial\tilde{x}_2^2}\right)+\sqrt{\frac{m}{M}}\frac{k_1+k_2}{2}\tilde{x}_1^2+\sqrt{\frac{M}{m}}\frac{k_2}{2}\tilde{x}_2^2-k_2\tilde{x}_1\tilde{x}_2$$

where the momentum terms now have equal coefficients.

2. Explicitly, the transformation reads

$$X_1=\tilde{x}_1\cos\alpha+\tilde{x}_2\sin\alpha,\qquad X_2=-\tilde{x}_1\sin\alpha+\tilde{x}_2\cos\alpha.$$

We obtain

$$\begin{aligned}H &= -\frac{\hbar^2}{2\sqrt{Mm}}\left(\frac{\partial^2}{\partial X_1^2}+\frac{\partial^2}{\partial X_2^2}\right)\\ &\quad+\frac{1}{2}\sqrt{Mm}\left[\left(\frac{1}{2}\left(\omega_1^2+\omega_2^2\right)+\frac{1}{2}\left(\omega_1^2-\omega_2^2\right)\cos(2\alpha)-\omega_{12}^2\sin(2\alpha)\right)X_1^2\right.\\ &\qquad+\left(\frac{1}{2}\left(\omega_1^2+\omega_2^2\right)-\frac{1}{2}\left(\omega_1^2-\omega_2^2\right)\cos(2\alpha)+\omega_{12}^2\sin(2\alpha)\right)X_2^2\\ &\qquad\left.+\left(\left(\omega_2^2-\omega_1^2\right)\sin(2\alpha)-2\omega_{12}^2\cos(2\alpha)\right)X_1X_2\right]\end{aligned}$$

with

$$\omega_1=\sqrt{\frac{k_1+k_2}{M}},\qquad \omega_2=\sqrt{\frac{k_2}{m}},\qquad \omega_{12}=\sqrt{\frac{k_2}{\sqrt{Mm}}},$$

and we used double-angle trigonometric functions for convenience. Note how $\left(\frac{\partial^2}{\partial\tilde{x}_1^2}+\frac{\partial^2}{\partial\tilde{x}_2^2}\right)$ is invariant under any orthogonal transformation. Thus, no mixing is generated in the momentum terms.

3. To remove the term $\propto X_1X_2$, we set

$$2\alpha=\arctan\frac{2\omega_{12}^2}{\omega_2^2-\omega_1^2}\,.$$

Thus,

$$\cos(2\alpha)=\frac{|\omega_1^2-\omega_2^2|}{\sqrt{(\omega_1^2-\omega_2^2)^2+4\omega_{12}^4}}\,,$$
$$\sin(2\alpha)=\frac{2\omega_{12}^2}{\sqrt{(\omega_1^2-\omega_2^2)^2+4\omega_{12}^4}}\,.$$

Without the mixing term, the Hamiltonian is just the sum of two harmonic oscillators, and the eigenfrequencies of the two oscillators can be read off from the coefficient of either X_1^2 or X_2^2 (both give the same two solutions, depending on the sign of $\omega_1^2-\omega_2^2$):

$$\begin{aligned}\omega_{a,b}^2 &= \frac{1}{2}\left(\omega_1^2+\omega_2^2\right)\pm\frac{1}{2}\frac{(\omega_1^2-\omega_2^2)^2}{\sqrt{(\omega_1^2-\omega_2^2)^2+4\omega_{12}^4}}\pm\frac{2\omega_{12}^4}{\sqrt{(\omega_1^2-\omega_2^2)^2+4\omega_{12}^4}}\\ &= \frac{1}{2}\left[\omega_1^2+\omega_2^2\pm\sqrt{(\omega_1^2-\omega_2^2)^2+4\omega_{12}^4}\right]\\ &= \frac{1}{2}\left[\frac{k_1+k_2}{M}+\frac{k_2}{m}\pm\sqrt{\left(\frac{k_1+k_2}{M}-\frac{k_2}{m}\right)^2+4\frac{k_2^2}{Mm}}\right]\end{aligned}$$

It is easy to check that $\omega_{M,m}$ from (b) are recovered in the limit $m \ll M$, when k_2/M is negligible compared to k_2/m.
The exact eigenenergies are

$$\epsilon_{n_a,n_b} = \hbar\omega_a \left(n_a + \frac{1}{2}\right) + \hbar\omega_b \left(n_b + \frac{1}{2}\right).$$