LABORATORY NOTEBOOK

Phases & Dynamics of Interacting Quantum Particles

ETH

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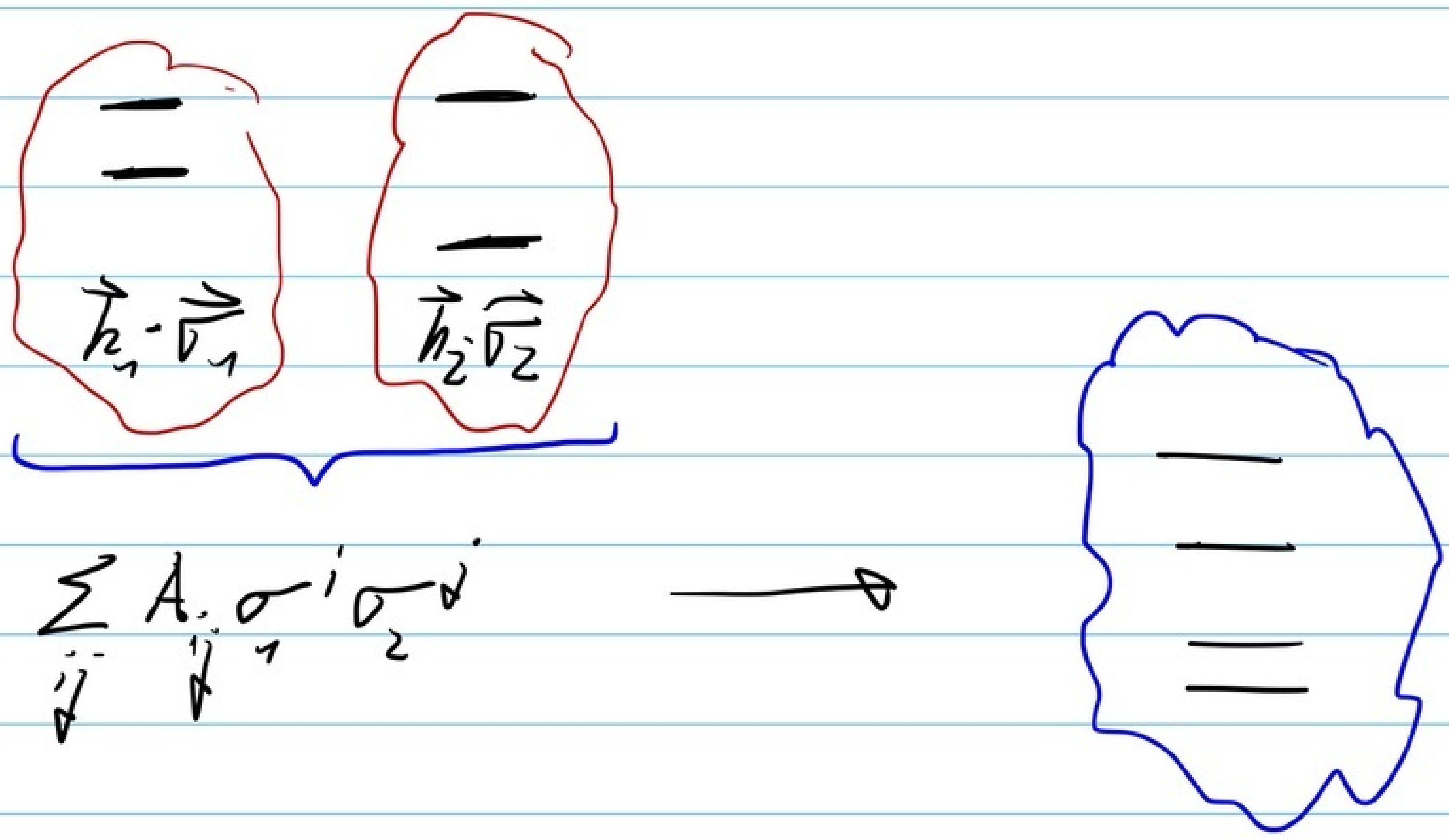
0. Overview

This course deals with the physics that arises when many particles that interact strongly with each other are brought together in solids or engineered quantum systems. Why is it interesting to deal with such a setup?

Imagine two quantum particles, let's take two 2-level systems and let them interact strongly:



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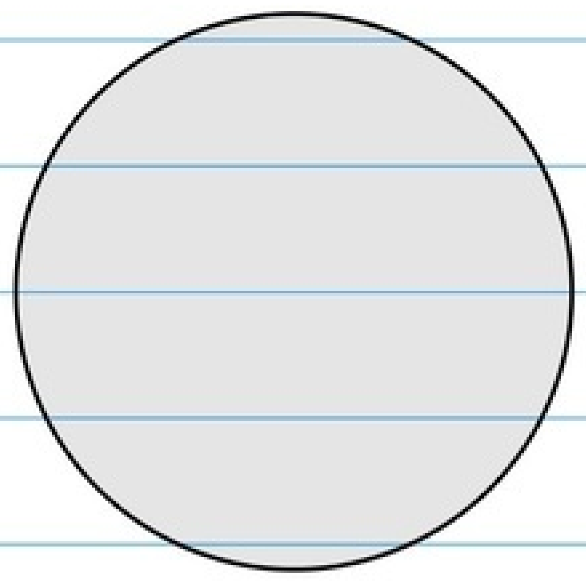
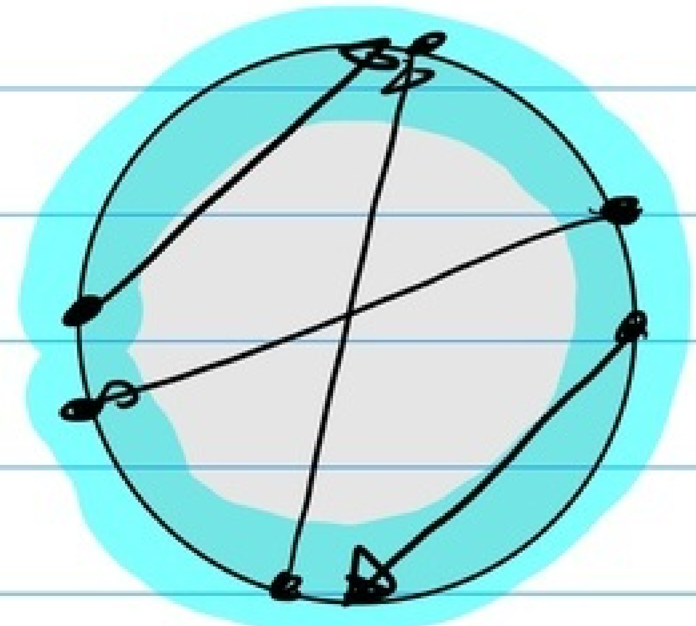
Even for $|A_{ij}| \gg |h_i|$, all I get is "just" another set of levels. Nothing profoundly new arose. If we now take many particles, but let them interact only weakly we get also nothing qualitatively new:

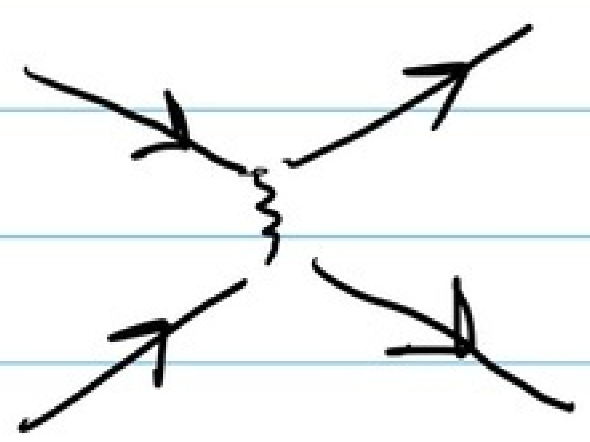


Fermi surface of non-interacting electrons



bare electrons turn into Landau quasi-particles

$\Downarrow$



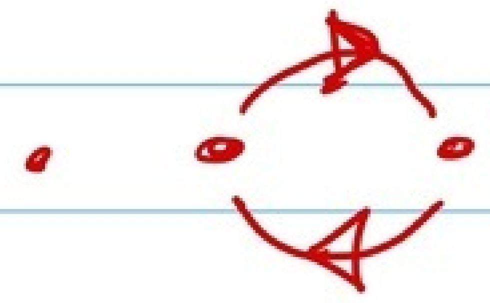
extremely successful in describing a huge number of metals

$\Rightarrow$ But: The really challenging and interesting physics emerges when the perturbation theory fails.

When does this happen?

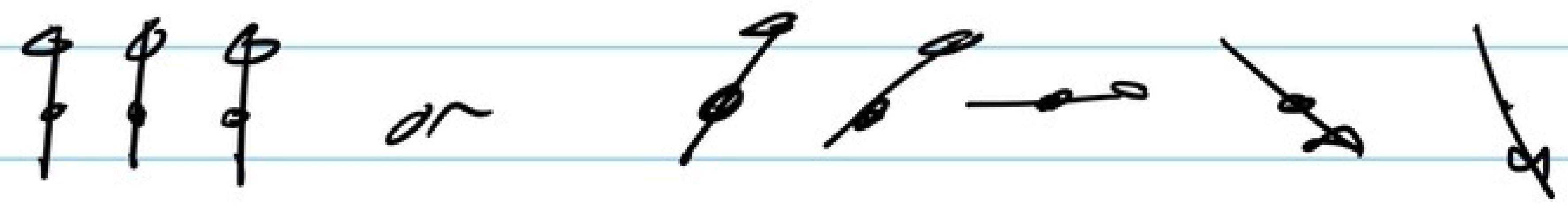
A.) Fractional Quantum Hall effect

Input:
- Electrons with charge e
- $V(\vec{r}-\vec{r}') = \frac{e^2}{|\vec{r}-\vec{r}'|}$
- strong B-field

Output:
- excitations with $e^* = \frac{e}{3}$
-  their exchange is not like for Fermions or Bosons

B.) Spin Liquids

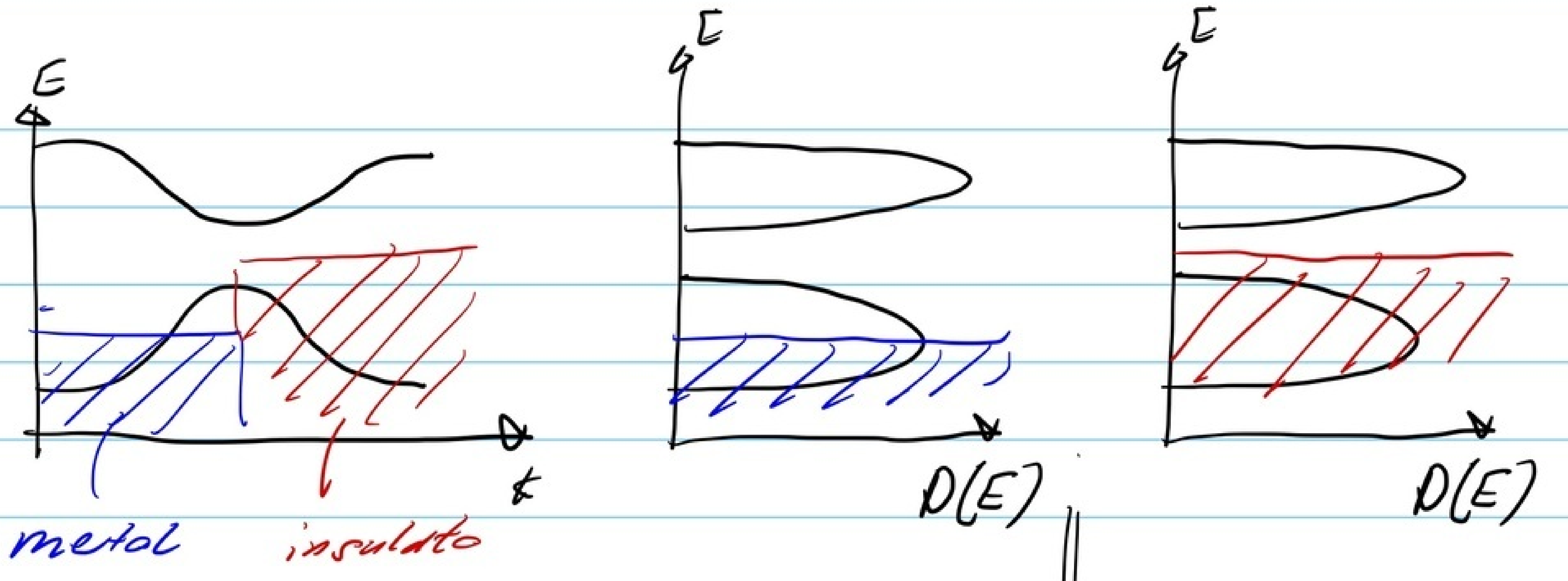
Normally, if we take a set of magnetic moments, they order at low temperature



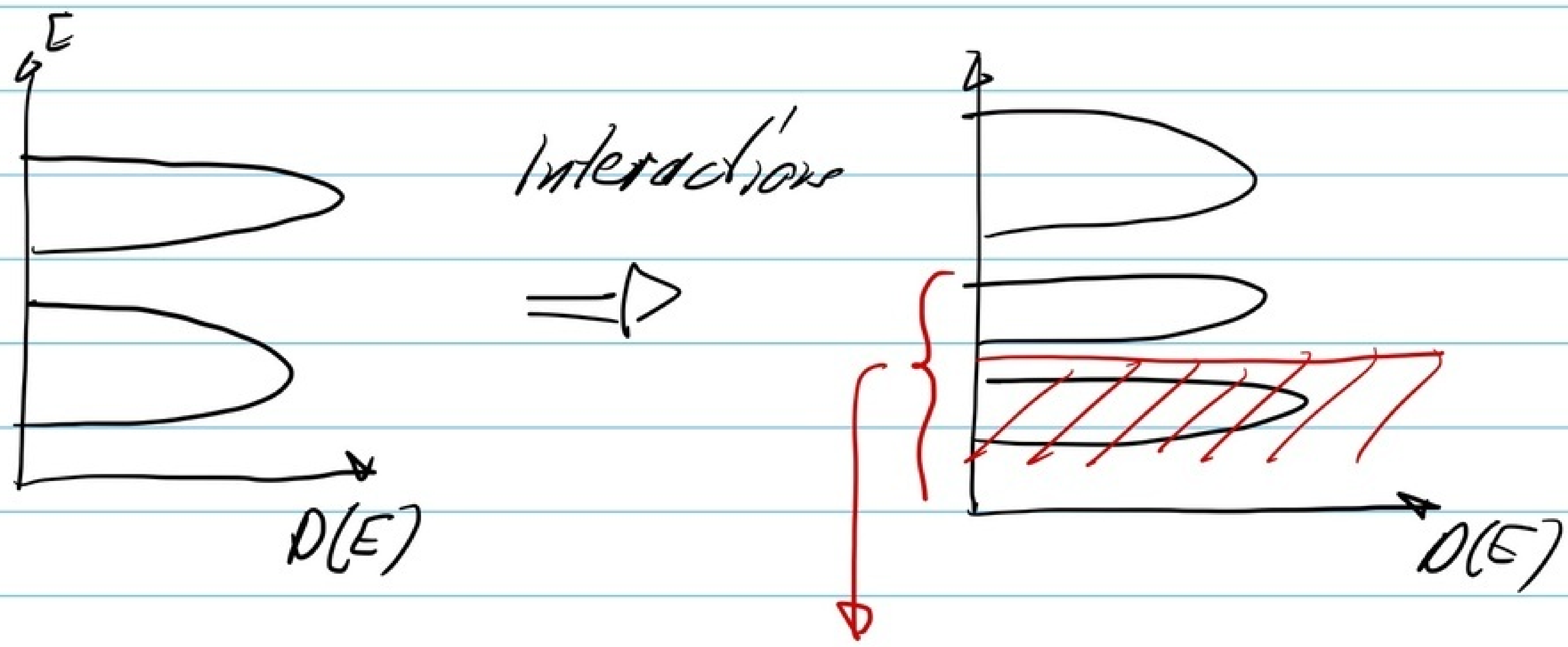
but in some systems $\langle \vec{M} \rangle = 0$ all the way down to $T=0$. Moreover, the elementary excitations in these systems tend to be "strange". E.g., they may behave as Fermions rather than spins, or behave like the quasiparticles of the fractional quantum Hall effect.

c) Mott insulators and their descendants

We learn in band theory, that one can tell an insulator from a metal by simply checking the filling:



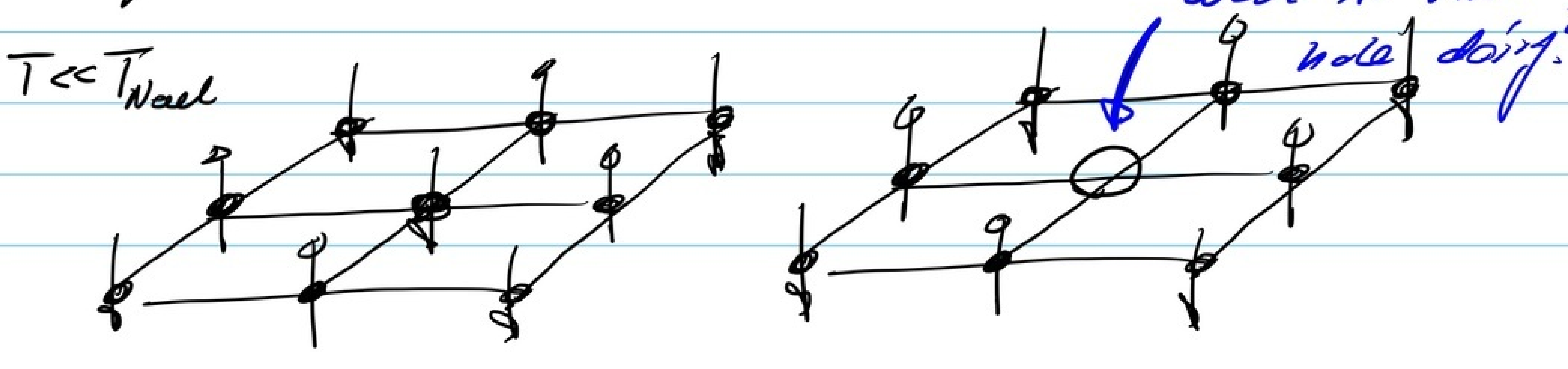
⇓ add interactions



complete change of density of states due to interactions

$\boxed{\text{Mott insulator}}$

It turns out they appear at commensurate filling of one electron per "site". ⇒



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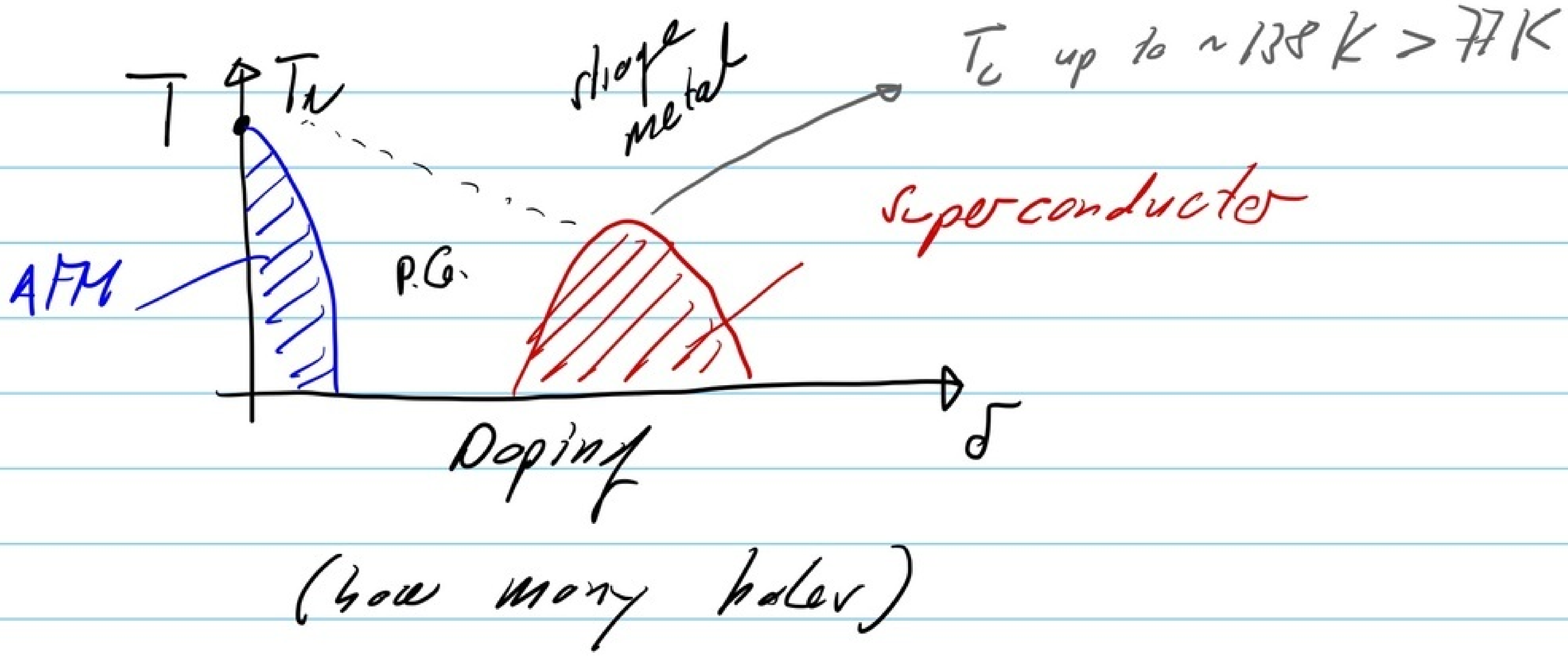
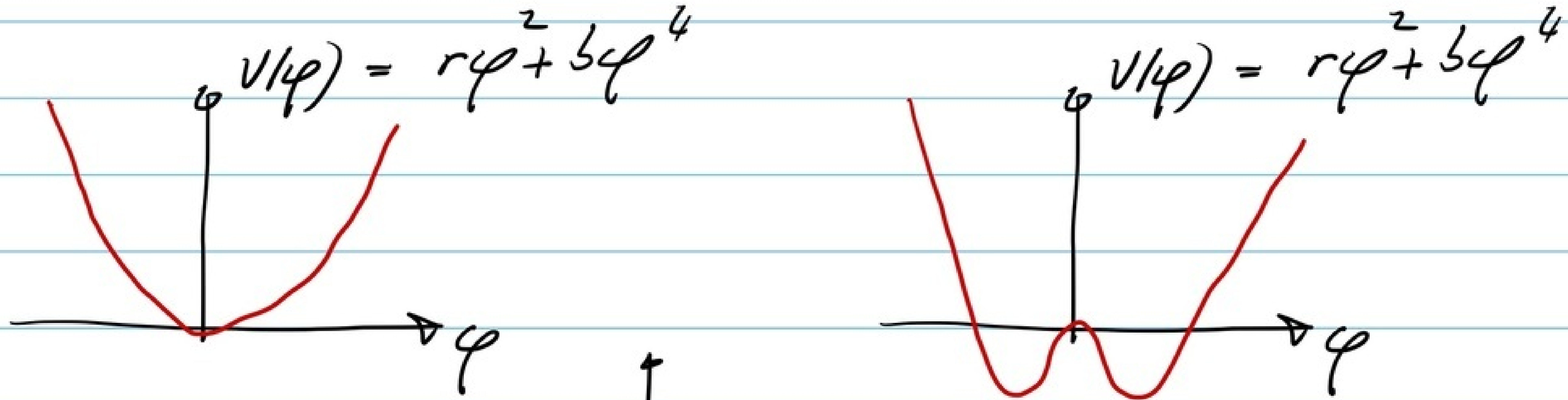
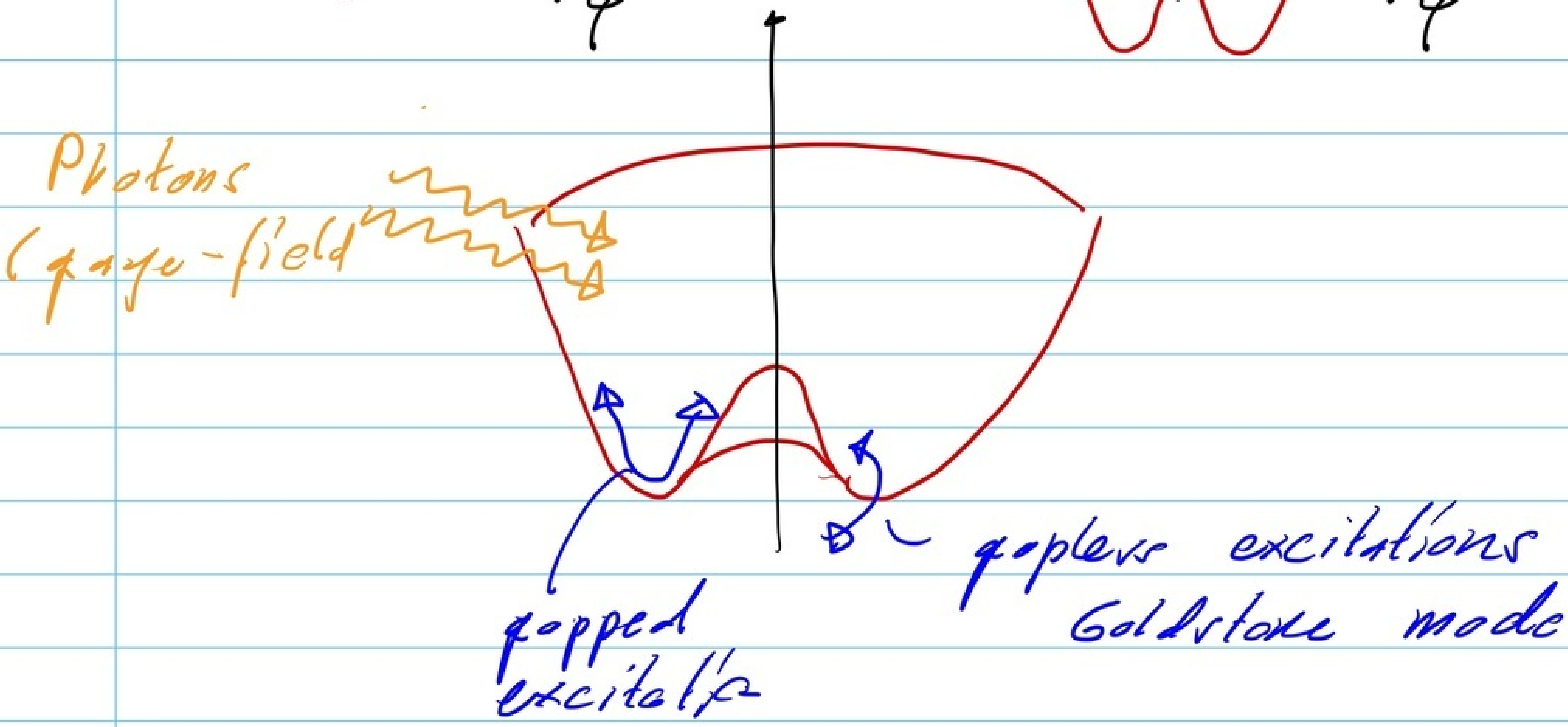


While we are at it: superconductors host fascinating physics:





The massive (gapped) excitation of a super-

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conductor endows a coupled gauge field with a mass: the Higgs mechanism! A massive photon? ⇒ the Meissner effect!

We need tools to deal with such strongly interacting phases beyond perturbation theory. ⇒ This is why you attend this course!

The goal for the next two weeks is to be able to cast the many-body Hamiltonian

$$H = \sum_{i=1}^{N} -\frac{\hbar^2 \nabla_i^2}{2m} + U(\vec{r}_i) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j)$$

together with the requirement on the wave-function:

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$$\psi(\vec{r}_1, \dots, \vec{r}_i, \dots, \vec{r}_j, \dots \vec{r}_N) =$$
$$(-1)^\eta \psi(\vec{r}_1, \dots, \vec{r}_j, \dots, \vec{r}_i, \dots \vec{r}_N)$$

with $\eta = \begin{cases} 0 & \text{Bosons} \\ 1 & \text{Fermions} \end{cases}$

into a model as simple as

$$H = -t \sum_{\langle ij \rangle} \hat{c}^{+}_{i\sigma} \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

1. Bloch theory

We start with the single-particle problem in a periodic potential

$$U(\vec{r}) = U(\vec{r} + \vec{R}_{\vec{n}})$$

with $\vec{R}_{\vec{n}} = n_i \vec{a}_i$, $n_i \in \mathbb{Z}$ and $\vec{a}_i$ the lattice vectors. The Bloch theorem states that all eigenfunctions can be

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written as

$$\psi_{nk}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{nk}(\vec{r}) \qquad (2)$$

with

$$u_{nk}(\vec{r}) = u_{nk}(\vec{r} + \vec{R}_{\vec{n}})$$

Eq. (2) is equivalent to the statement

$$\psi_{nk}(\vec{r} + \vec{R}_{\vec{n}}) = e^{i\vec{k}\vec{R}_{\vec{n}}} \psi_{nk}(\vec{r})$$

which can be derived from the fact that translations commute

$$T_{R_{\vec{n}}} \psi_{nk}(\vec{r}) = \psi_{nk}(\vec{r} + R_{\vec{n}}),$$

$$T_{\vec{R}_{\vec{n}}} T_{\vec{R}_{\vec{m}}} = T_{\vec{R}_{\vec{m}}} T_{\vec{R}_{n}}$$

from which follows that all irreducible representations are one-dimensional. Using periodic boundary conditions $(T_{\vec{R}_{\vec{n}}})^N = \mathbb{1}$

one can infer the characters to be of the form $e^{i\vec{k}\vec{R}_{\vec{m}}}$ $\square$.

How to obtain $\psi_{nk}(\vec{r})$:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right]\psi_{nk}(\vec{r}) = \lambda_{nk}\psi_{nk}(\vec{r}) \quad (3)$$

$$\psi_{nk}(\vec{r}) = e^{i\vec{k}\vec{r}}u_{nk}(\vec{r}) = e^{i\vec{k}\vec{r}}\sum_{\vec{m}} u_{nk}^{\vec{m}} e^{i\vec{K}_{\vec{m}}\vec{r}}$$

$$U(\vec{r}) = \sum_{\vec{m}} U_{\vec{m}} e^{i\vec{K}_{\vec{m}}\vec{r}}$$

with $\vec{K}_{\vec{m}} = m_i \vec{k}_i$ $\quad m_i \in \mathbb{Z}$ and

$$\vec{k}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$$

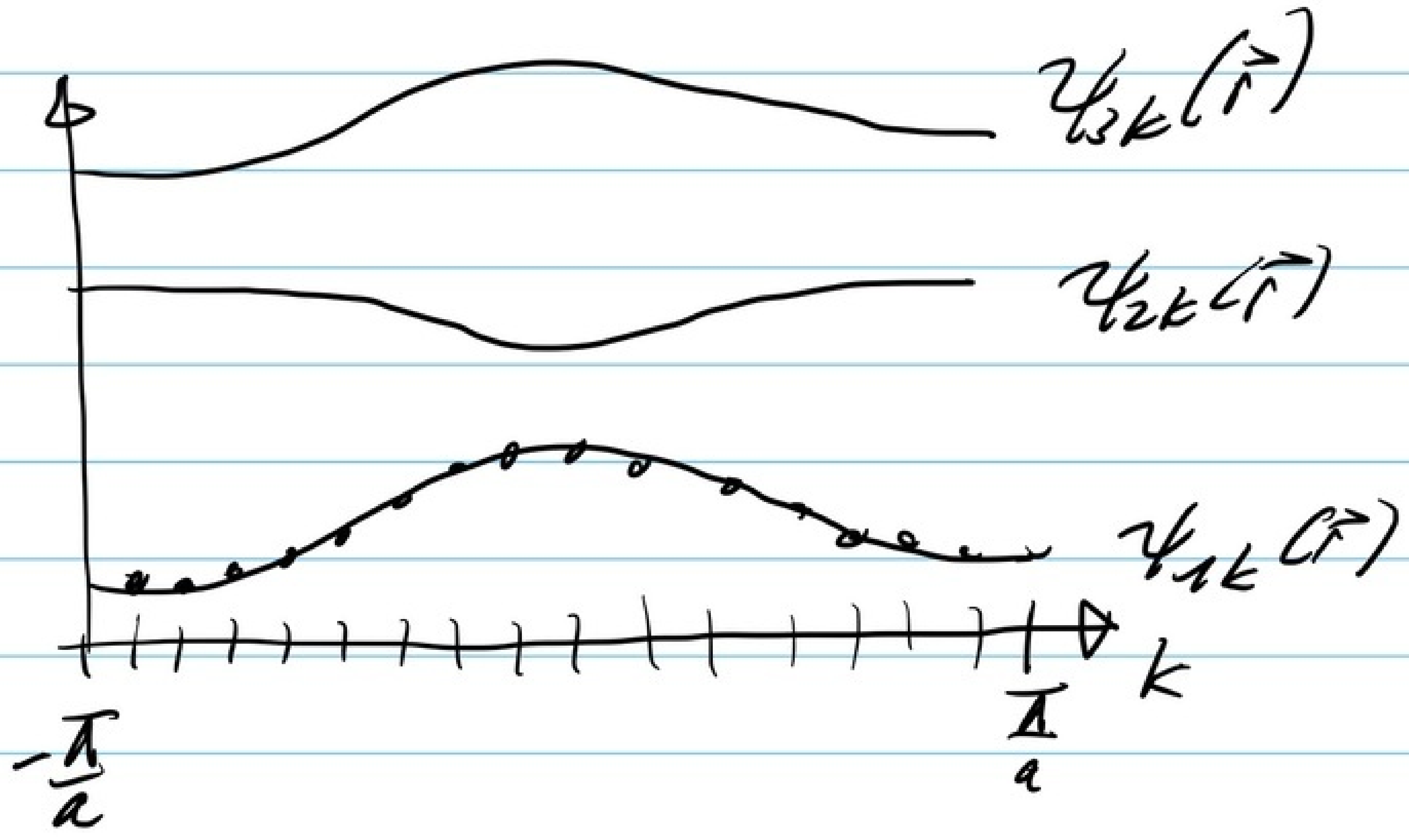
a reciprocal lattice vector.

When inserted into (3), one finds a matrix equation (here shown for one dimension) of the form

$$\mathcal{H} = \begin{pmatrix} \frac{\hbar^2}{2m}\left(k+\frac{2\pi M}{a}\right)^2 & \ddots & \ddots & & & \\ \ddots & \ddots & U_1 & U_2 & & \\ U_2 & U_1 & \frac{\hbar^2}{2m}k & U_1 & U_2 & \\ & U_2 & U_1 & \frac{\hbar^2}{2m}\left(k-\frac{2\pi}{a}\right)^2 & U_1 & \ddots \\ & & U_2 & U_1 & \ddots & \ddots \\ & & & \ddots & \ddots & \frac{\hbar^2}{2m}\left(k-\frac{2\pi M}{a}\right)^2 \end{pmatrix}$$

$$\mathcal{H}\vec{u}_{nk} = \lambda_{nk}\vec{u}_{nk} \quad \text{with} \quad \vec{u}_{nk} = \left(u_{nk}^{M}, \dots, u_{nk}^{-M}\right)$$

After solving the above Hamiltonian, we are left with the eigenvalues of the Bloch bands



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We can now choose to make a unitary transformation to another basis set of Wannier functions:

$$w_{n\vec{R}}(\vec{r}) = w_n(\vec{r}-\vec{R}_{\vec{m}}) =$$

$$= \int_{BZ} \frac{d\vec{k}}{V_{BZ}} \psi_{nk}(\vec{r}) e^{-i\vec{k}\vec{R}_{\vec{m}}}$$

$$= \int_{BZ} \frac{d\vec{k}}{V_{BZ}} u_{nk}(\vec{r}) e^{-ik(\vec{R}_m - \vec{r})}.$$

As this is a unitary transformation we have that

$$\langle w_{n\vec{R}_{\vec{m}}} | w_{m\vec{R}_{\vec{s}}} \rangle = \int_{\mathbb{R}^d} d\vec{r}\; w^*_{n\vec{R}_{\vec{m}}}(\vec{r}) w_{m\vec{R}_{\vec{s}}}(\vec{r})$$

$$= \delta_{\vec{m},\vec{s}}\, \delta_{nm}$$

This is all good, however, there is an issue. All that we did, is to combine all $\Psi_{nk}(\vec{r})$'s with a specific phase factor $e^{i\vec{k}\vec{R}_m}$. But what was the phase relation between the $\Psi_{nk}(\vec{r})$'s for different $\vec{k}$'s to begin with?

This problem becomes apparent, when we numerically diagonalize the matrix $\mathcal{H}$ on a computer: there is no relation between the obtained eigenvectors of different diagonalizations for different k's!

A first publication addressing this issue is by Walter Kohn [W. Kohn, Phys. Rev. <u>115</u> 809 (1959)]. He dealt with one dimensional, isolated bands and stated the following facts:

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- The Wannier functions can be made real
- $w_{nR_m}(\vec{r}) = \pm w_{nR_m}(-\vec{r})$
- $w_{nR_m}(\vec{r}) \sim \exp(-r/h_n)$

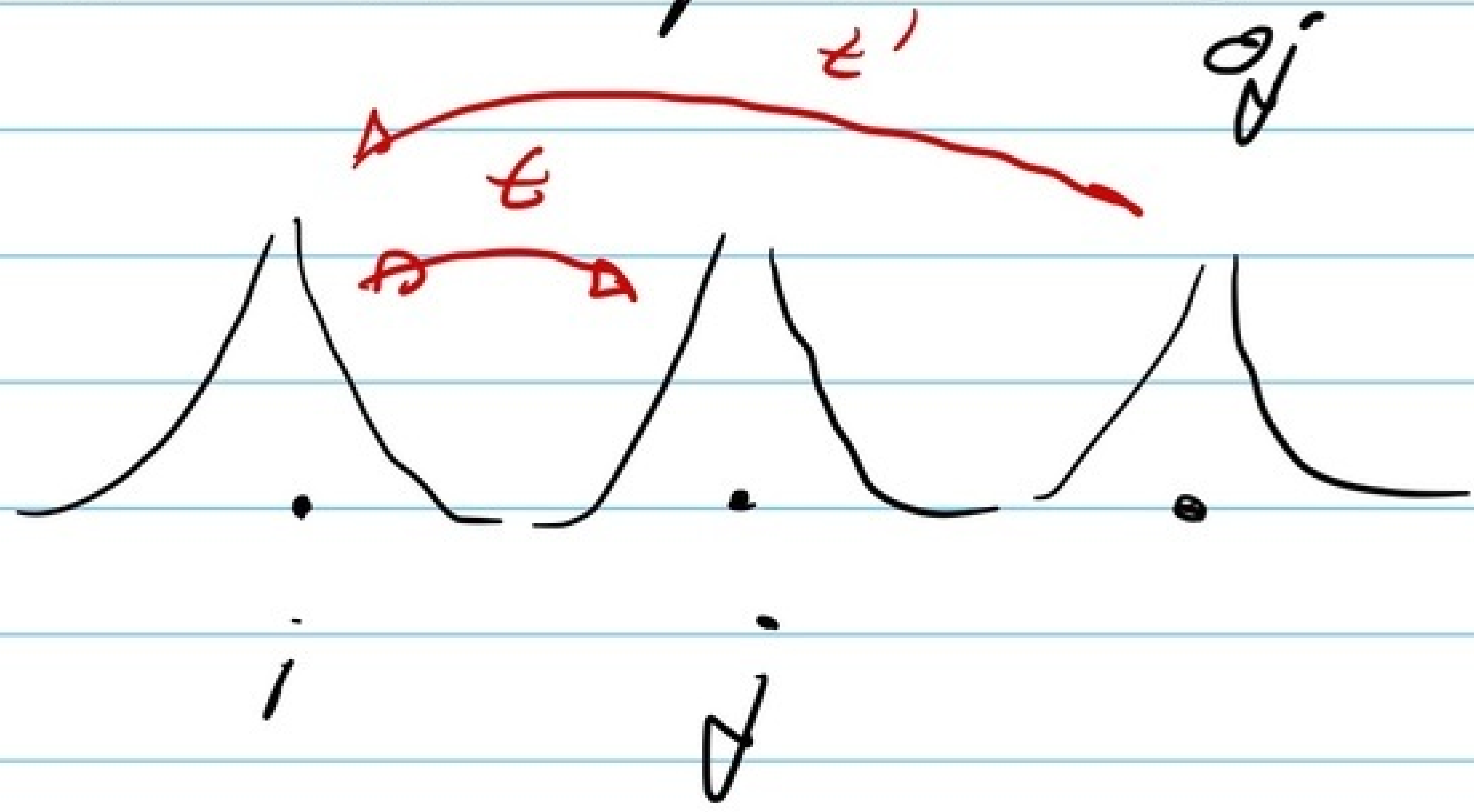
Especially the last property is extremely useful for the following reason:

We can express the Hamiltonian in this basis

$$t_{ij}^{nm} = \langle w_{nR_i} | -\frac{\hbar^2 \nabla^2}{2m} + U(\vec{r}) | w_{mR_j} \rangle$$

$$= \delta_{nm} \int_{\mathbb{R}} d\vec{r}\, w^*_{nR_i}(\vec{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + U(\vec{r}) \right] w_{nR_j}(\vec{r})$$

and we find $t_{0j} \ll t_{01} \quad \forall j > 1$



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But when do the three properties hold?

Kohn's condition is

$$\boxed{\psi_{nk}(\vec{r}=0) \text{ is a smooth function } (C^\infty) \text{ of } k}$$

Remember that the Fourier transform of an s-times differentiable function falls off at least as $\frac{1}{r^s}$.

Therefore one needs to find an optimal gauge

$$\psi_{nk}(r) \rightarrow \psi'_{nk}(r) = e^{i\delta(k)} \psi_{nk}(r)$$

with $\delta(k)$ such that $\psi'_{nk}(\vec{r})$ is a smooth function of k.

In numerical simulations of one-

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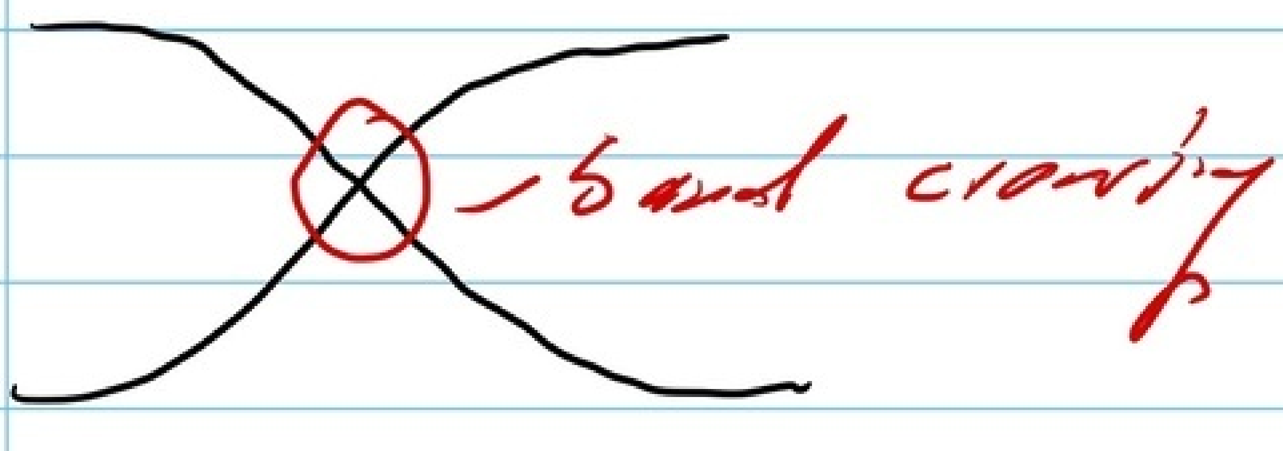
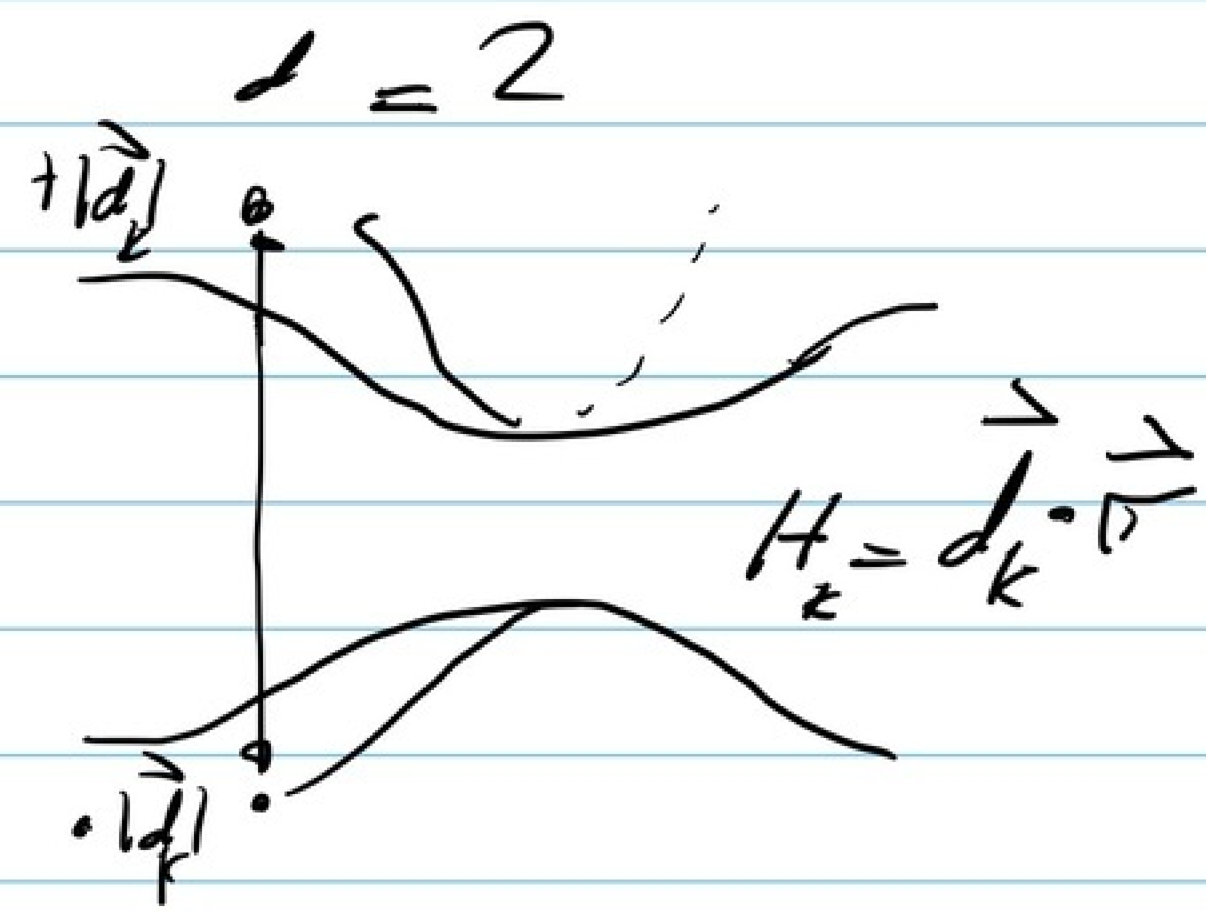
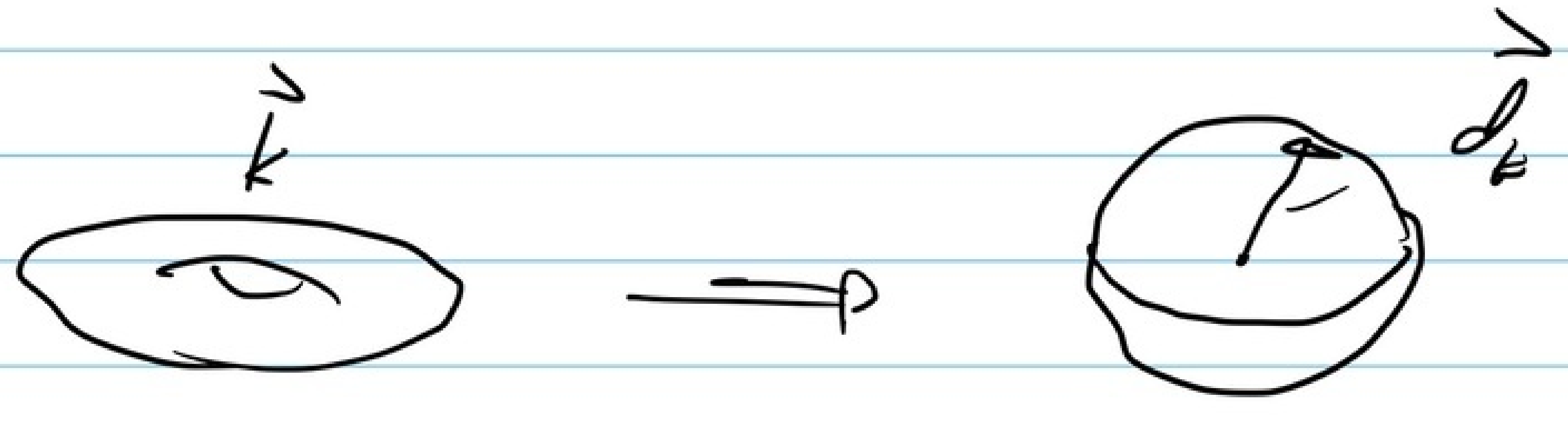
dimensional systems one typically gets back real eigenvector $\vec{u}_{nk}$. by choosing sign(u^{0}_{nk}) to be the same for all k, one achieves a smooth gauge. Note that $\vartheta(k) \in \{0, \pi\}$ and hence $\vartheta(k)$ itself is not smooth at all!

There are several reasons that may prevent a smooth gauge. Two are listed here







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If $\vec{d}_k$ wraps the whole sphere, we know that there cannot be a smooth gauge. (We have a Chern number)

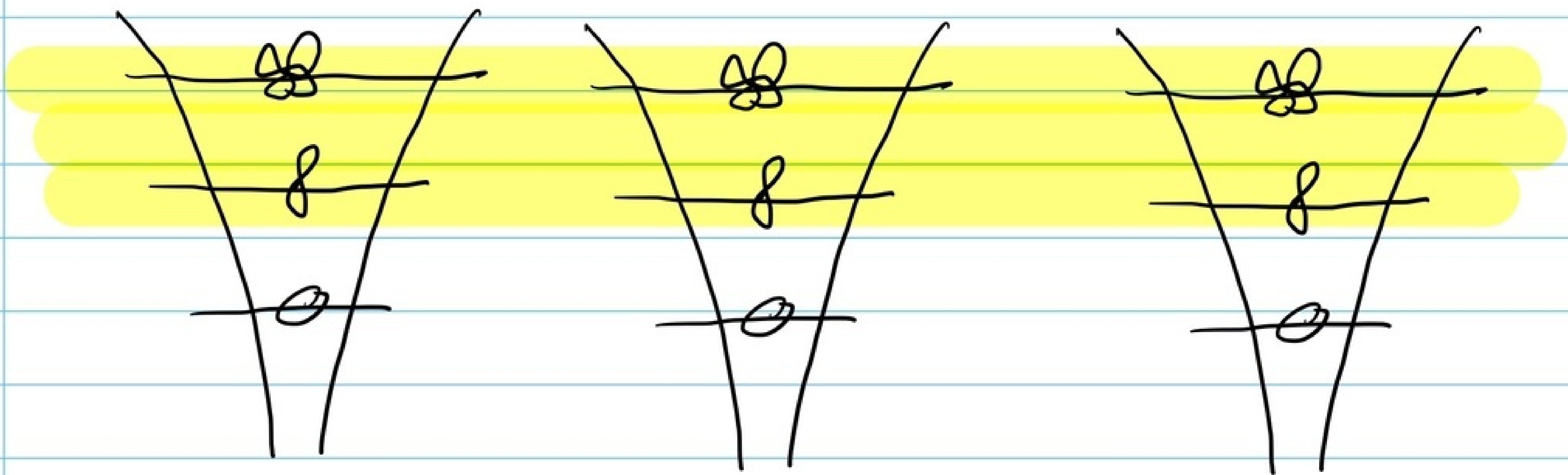
Even if we do not find exponentially localized Wannier functions for <u>one</u> band, we may still construct these for several bands. We now mix

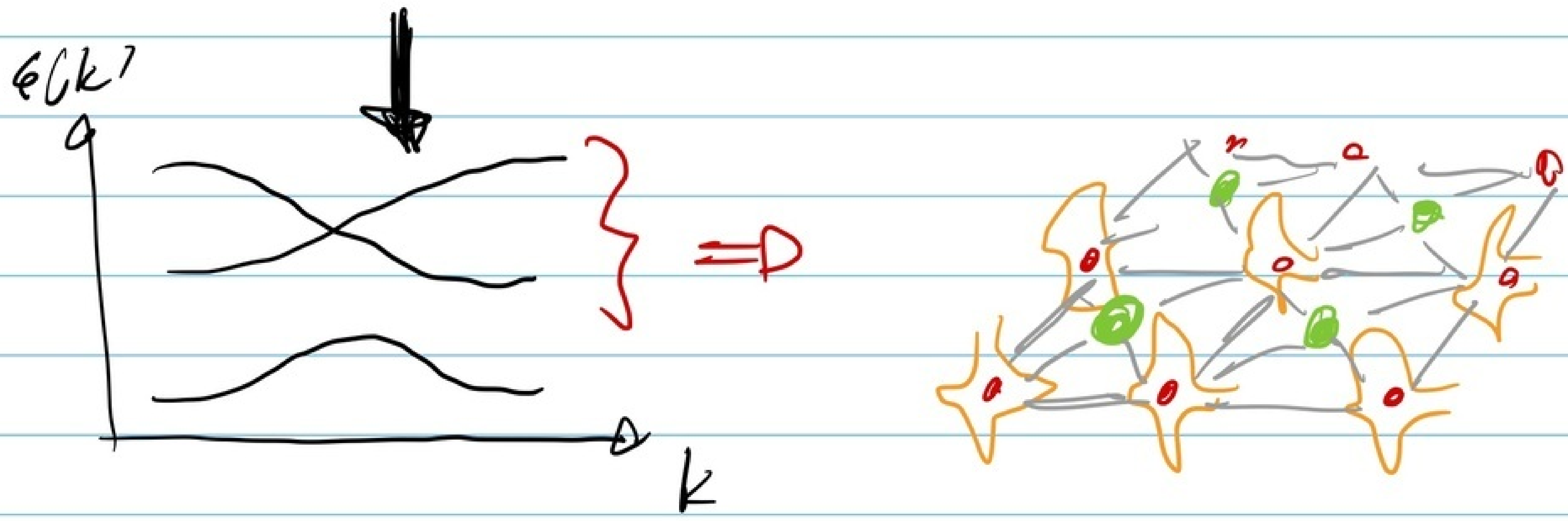
$$\psi_{nk} \rightarrow \psi'_{nk} = \sum_m U^k_{mn} \psi_{mk}$$

with U^k_{mn} a unitary matrix. If we combine two bands, we will get hoppings between different "orbitals"

$$t^{nm}_{ij} = \langle w_{in} | -\frac{\hbar \nabla^2}{2m} + U(\vec{r}) | w_{jm} \rangle$$

Note that there may not be the orbitals of the electrons at the ions





One question remains: How to choose U_{mn}^{k} to optimally localize the Wannier functions. [Marzari-Vanderbilt, PRB <u>56</u>, 12847 (1997)]: minimize the functional

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$$\Omega = \sum_{n \text{ considered}} \left[\langle r^2 \rangle_n - \langle \vec{r}_n \rangle^2 \right]$$

$$= \Omega_I + \tilde{\Omega} \leftarrow \text{positive definite.}$$

$\downarrow$

gauge invariant

$\downarrow$

related to topology

2. Second quantization

A natural symmetry of all many-particle Hamiltonians is the invariance under the exchange of identical particles:

$$H(1, 2, \dots i, \dots, j, \dots N) = H(1, 2, \dots, j, \dots i, \dots, N).$$