Collective modes in Condensed Matter Physics

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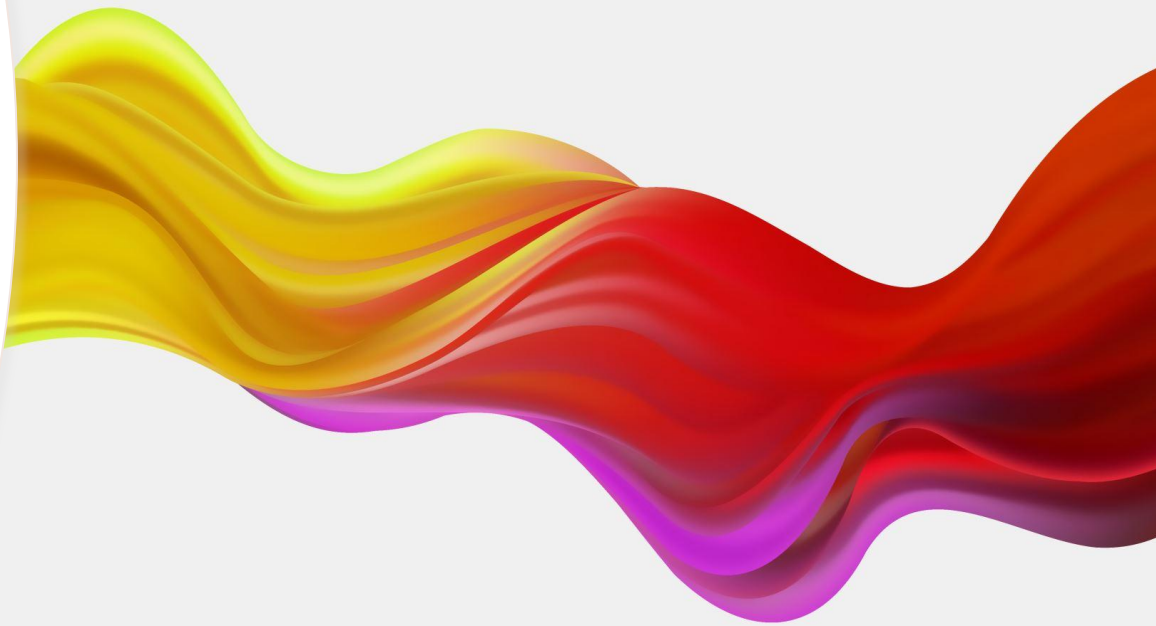
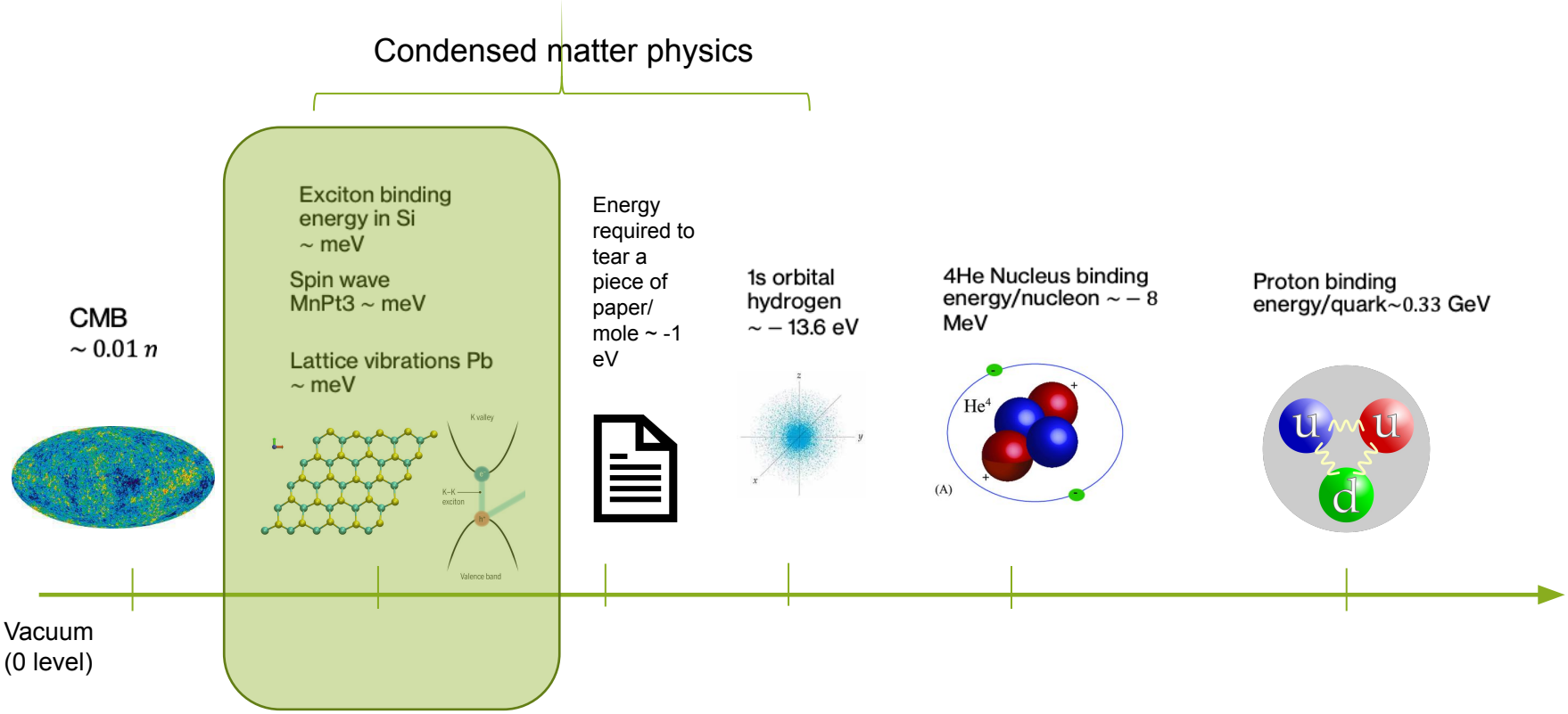


Full disclosure

- A lot of intro topics.
- Slides are just a rough skeleton. Will most probably have to expand on it.
- I'll Try to keep it jargon free. But if I do use some, just ask!
- Some calculations "left for the reader". Not a lot …. hopefully

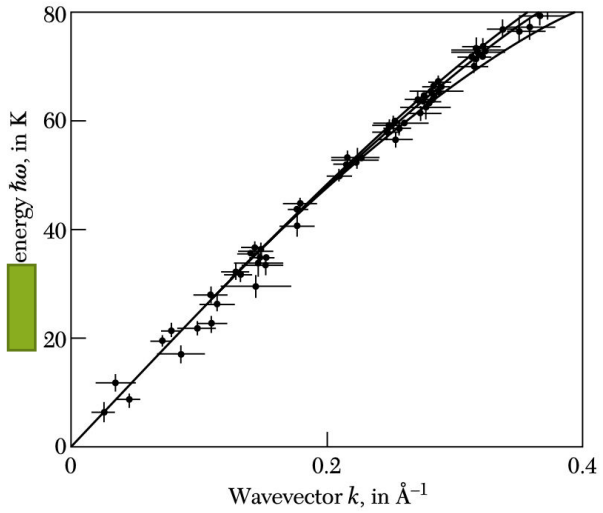
Energy scales of the universe



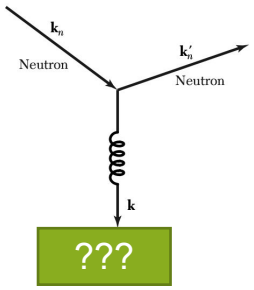
Some lab results- Inelastic neutron scattering

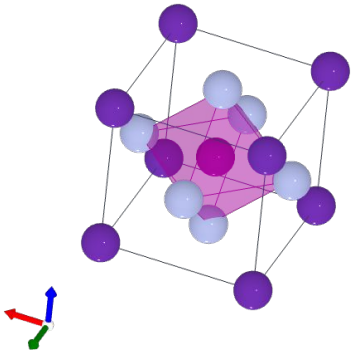
Reference momenta: Colour red $k = 0.001\ A^{o-1}$

Microwave $k = 0.0006\ A^{o-1}$



RbMnF3 inelastic neutron scattering





Purple: Rb+

Magenta:Mn

Blueish: F

Theory of everything condensed matter physics

At this energy scale non-relativistic quantum mechanics is used to describe the physics

Many body Schrodinger equation N_e electrons and N_n nuclei:

$$\hat{H}(\{\mathbf{r}_i\},\{\mathbf{R}_I\}) = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_I \frac{\hbar^2}{2M_I}\nabla_I^2 + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|} + \frac{1}{2}\sum_{I\neq J}\frac{e^2}{4\pi\epsilon_0}\frac{Z_I Z_J}{|\mathbf{R}_I-\mathbf{R}_J|} - \sum_{i,I}\frac{e^2}{4\pi\epsilon_0}\frac{Z_I}{|\mathbf{R}_I-\mathbf{r}_i|}$$

KE e^- | KE $ion\ cores$ | Coulomb repulsion electrons | Coulomb interaction ions | e^- − ion coulomb interaction

Very complicated. Cannot be solved directly, moreover initial conditions impossible to get

Need some simplifications

1) Ions much heavier than electrons ⇒ Treat classically (as parameters $\{R_I\}$) and still.

Constant

$$\hat{H}(\{\mathbf{r}_i\},\{\mathbf{R}_I\}) - \frac{1}{2}\sum_{I\neq J}\frac{e^2}{4\pi\epsilon_0}\frac{Z_I Z_J}{|\mathbf{R}_I-\mathbf{R}_J|} = -\sum_i\left(\frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_I \frac{e^2}{4\pi\epsilon_0}\frac{Z_I}{|\mathbf{R}_I-\mathbf{r}_i|}\right) + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}$$

$$\tilde{H}(\{\mathbf{r}_i\},\{\mathbf{R}_I\}) = \sum_i\left(\frac{\hbar^2}{2m_e}\nabla_i^2 - V_n(\mathbf{r}_i)\right) + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}$$

Effect of nuclear potential on i'th electron

Single particle

Two particle interaction

Gone from complicated mess to (still but) less complicated mess

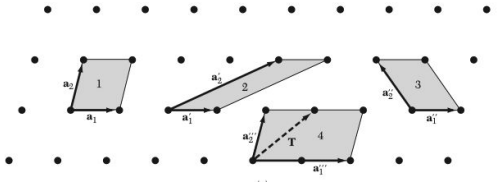
Next simplification (subtle): Remove effect of coulomb repulsion and solve the problem

(my opinion) Most of condensed matter physics is finding the essence of the coulomb interaction + permutation symmetry of the electron. Conductors-Insulators-Magnets-Superconductors-ferroelectrics-Chern insulators- …….

Solid state theory- Lattices

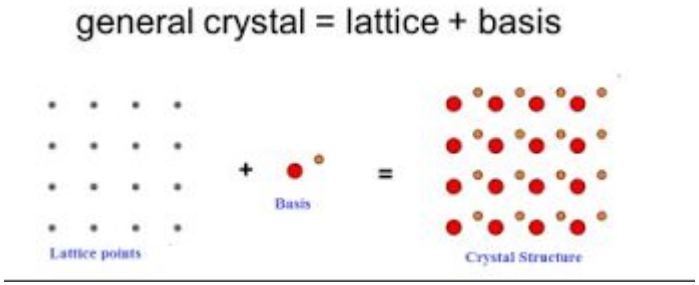
Lattice: a periodic array of points

2D $\{\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 | n_1, n_2 \in \mathrm{Z}\}$



At each point you can attach an atom (or atoms)

Called a basis



Mass of electron ≪ Mass of ions

⇒ We can just consider the ions as still and just think of the electrons (decoupled)

↔ Electron in a static periodic potential

Reciprocal lattice

Define a new set of vectors: $e^{i\mathbf{G}\cdot\mathbf{R}} = 1$

$$\{\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 | m_1, m_2 \in \mathrm{Z}\} \qquad \mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

(hence the name – Reciprocal/dual)

G is also periodic

Usefulness:

A function periodic in R can be expanded in G (Fourier exponential series):

$$f(\boldsymbol{x}+\boldsymbol{R}) = f(\boldsymbol{x}) \Rightarrow f(\boldsymbol{x}) = \sum_{\boldsymbol{G}} f_{\boldsymbol{G}} e^{-i\,\boldsymbol{G}\cdot\boldsymbol{x}}$$

Electron in a periodic potential-Bloch's theorem

$H(x) = \frac{\hbar^2}{2m}\nabla^2 + V(x), \qquad V(x+R) = V(R)$

Solve in periodic boundary conditions e.g 1D
$\psi(x+L) = \psi(x)$

Bloch's theorem: Eigenstates in a crystal are of the form $\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$

Cell periodic part: $u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}+\mathbf{R})$

For translation operators T_j, $[H, T_j] = 0$

Eigenfunctions of H are also Eigenfunctions of T_j

$$T_j\ \psi = \lambda_j \psi;$$
$$\psi(\vec{r} + \vec{a}_j) = \lambda_j \psi(\vec{r});$$
$$\psi(\vec{r} + n\vec{a}_j) = T_j^n \psi = \lambda_j^n \psi.$$

With periodic boundary conditions

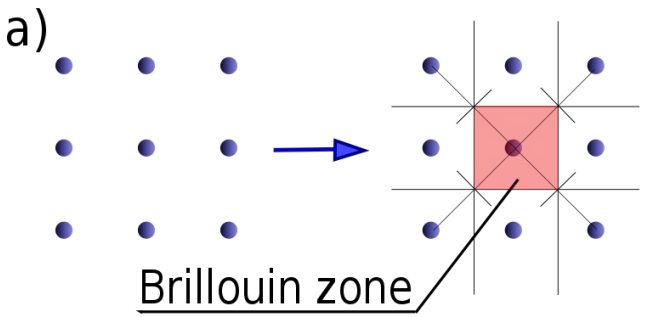
$$\psi(\vec{r} + M\vec{a}_j) = \psi(\vec{r}),$$

$$\lambda_j^M = 1.$$

Along with $T_R T_{R'} = T_{R+R'}$

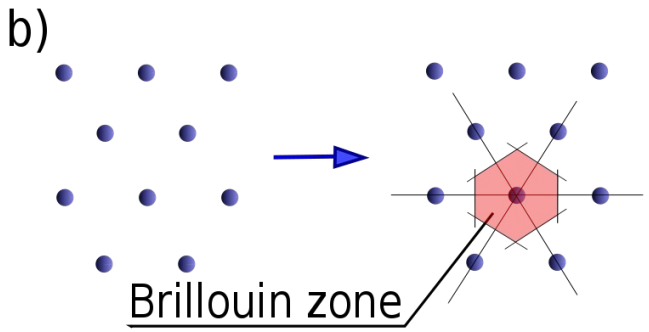
$$\Rightarrow \quad \lambda_j = e^{i\vec{k}\cdot\vec{a}_j}$$

Notice that eigenvalues $e^{i\,(k+G)\cdot a_j} = e^{ik\cdot a_j}$ $k \in$ "Brillouin Zone"



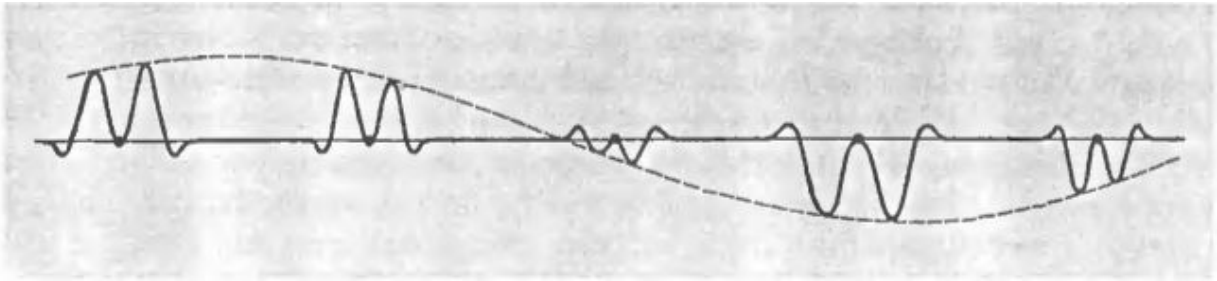
The most general form of an eigenfunction (that gives eigenvalue λ_j) is:

$$\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$



The Brillouin zone parameterizes the electron eigenstates in a crystal

$$\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

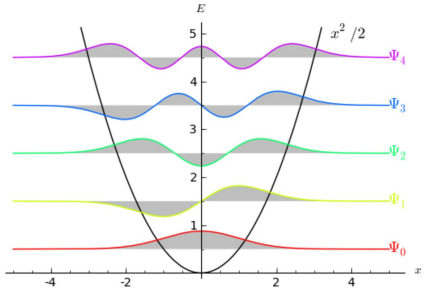


Planewave x cell periodic part

Heads up: Remember second quantization. Like that of the harmonic oscillator

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$
$$a|n\rangle = \sqrt{n}|n-1\rangle$$

$a^\dagger$ “Creates a particle” of the harmonic oscillator



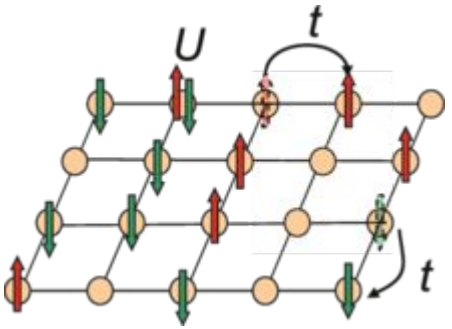
Hubbard Hamiltonian for square lattice

Toy model designed to capture essence of magnetic effects due to the coulomb interaction

[redacted]

Hopping term (kinetic energy decrease on delocalization).

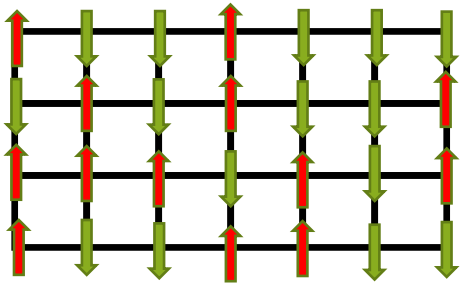
Coulomb repulsion cost to sit on the same site



When we have N sites and N electrons in the system

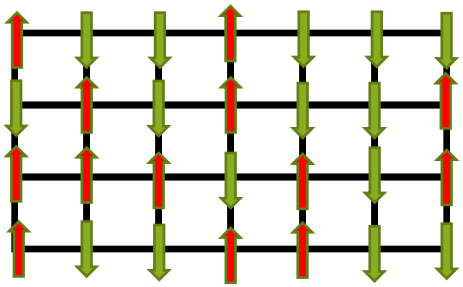
Called ‘half filling’

(each site can support two particles)



[redacted]

1. Let $t = 0$. Ground state: electrons occupy one site (either spin). E = 0



There is a massive degeneracy $g = 2^N$

No magnetic ordering preferred

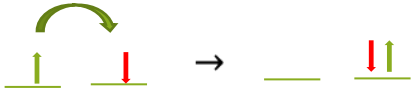
2. Include hopping as a perturbation (is any spin direction preferred?) (U>>t)

[redacted]

$T = T_+ + T_-$

Hopping that decreases number of doubly occupied sites by 1

Hopping that increases number of doubly occupied sites by 1



Let [redacted] S is unitary!

$[V, T_\pm] = \pm U T_\pm \quad \Rightarrow \quad \tilde{H} = V + \frac{1}{U}[T_+, T_-] + O(t^3)$

Ground state at half filling: no doubly occupied sites, so for all states $V|\Psi\rangle = 0 \quad T_-|\Psi\rangle = 0$

Effective Hamiltonian at half filling is $\tilde{H} = -\frac{1}{U} T_- T_+$

For pair of sites i and j

$$\tilde{H}|\uparrow\uparrow\rangle = \tilde{H}|\downarrow\downarrow\rangle = 0.$$

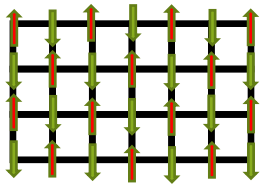
$$\langle\uparrow\downarrow|\tilde{H}|\uparrow\downarrow\rangle = \langle\downarrow\uparrow|\tilde{H}|\downarrow\uparrow\rangle = +2\frac{t^2}{U},$$

$$\langle\uparrow\downarrow|\tilde{H}|\downarrow\uparrow\rangle = \langle\downarrow\uparrow|\tilde{H}|\uparrow\downarrow\rangle = -2\frac{t^2}{U}.$$

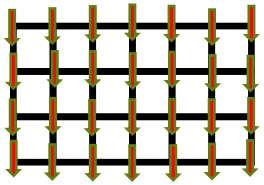
So, [redacted]

Ground state = (think classically)

- $J > 0$: Spins alternating in direction (antiferromagnet)



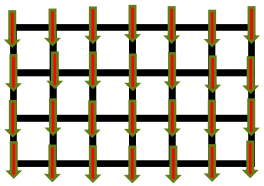
- $J < 0$: All spins pointing in one direction (ferromagnet)



What are the low lying excitations of the antiferromagnet?

Holstein-Primakoff approach (map to bosons)

Will do for ferromagnet and in analogy with Antiferromagnet



(for all down spins)

Philosophy: Large S expansion. Take spin to be large. Get exact solution. Hope if corrections are not big enough to not be observed in experiment

Let spin be S At each site s_z quantum # can be $m \in \{-S, -S+1, \ldots, S-1, S\}$

Note:

$$S_+|m\rangle = \sqrt{S(S+1) - m(m+1)}|m+1\rangle$$

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

Look very similar. In fact we can have a mapping $|n\rangle \Leftrightarrow |m = -S + n\rangle$

With $S_{z,i} = -S + a_i^\dagger a_i$ Boson number operator

Similarly (suppress site index):

[redacted]

$$= a^\dagger \sqrt{2S - a^\dagger a} | - S + n + 1 \rangle$$

So, $S_+ = 2S a^\dagger \sqrt{1 - \frac{a^\dagger a}{2S}}$ $\qquad S_+^\dagger = S_- = 2S \sqrt{1 - \frac{a^\dagger a}{2S}}\ a$ $\qquad S_{z,i} = -S + a^\dagger a$

Now writing Hamiltonian (Large S): [redacted]

[redacted]

[redacted]

$$\tilde{H} = 4JS \sum_i a_i^\dagger a_i + JS \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i)$$

Fourier transform

$$a_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in BZ} e^{i\mathbf{k}\cdot\mathbf{R}_i} a_{\mathbf{k}}$$

[redacted]

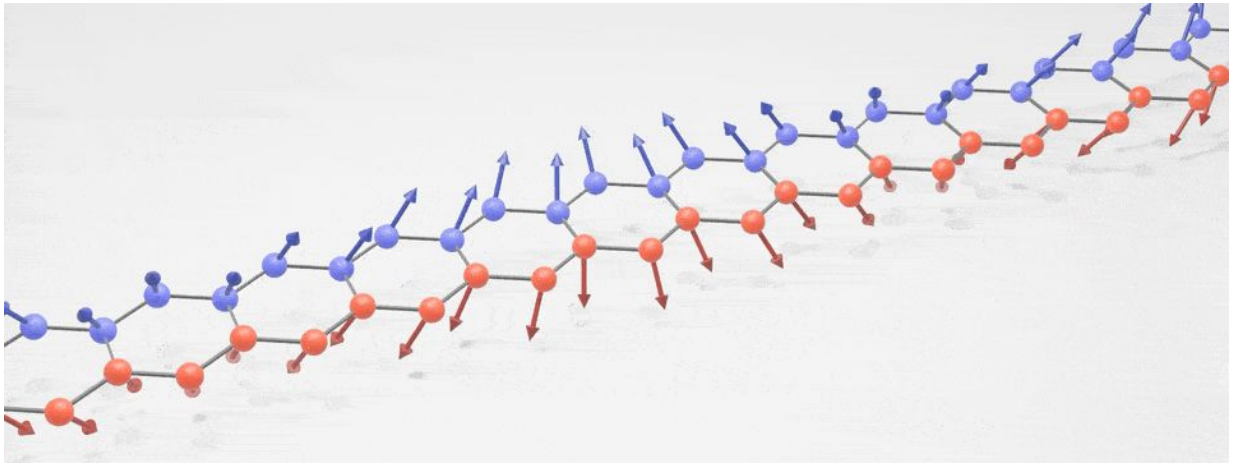
$E_{\mathbf{k}} \propto k^2$ as $k \to 0$

Almost similar treatment for but with some subtleties for antiferromagnets. It Gives:

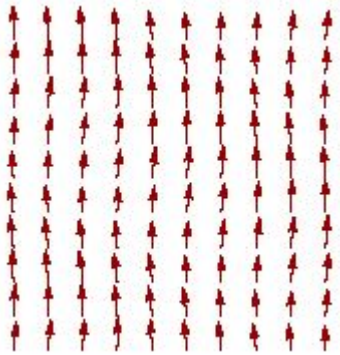
[redacted]

What is the rough image of this?

(Best animation I could find)

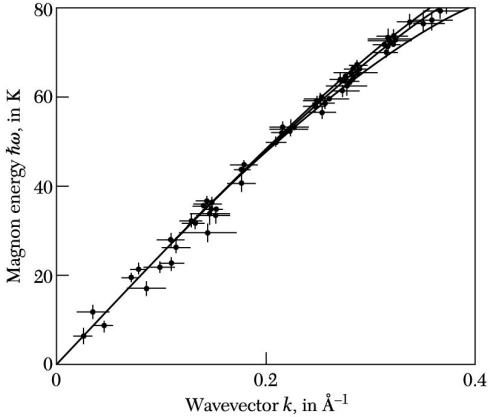


Ferromagnet



Collective motion- hence the title of the talk

[redacted] *



That’s all folks!

Tight binding and the Hubbard model

More intuitive way to look at a crystal

Hydrogen atom chain

N hydrogen atoms with all electrons in the 1s orbital

When the lattice constant ~ infinite, Eigenvalues of Hamiltonian = E_{1s} (N degenerate)
Eigenfunctions just one 1s orbital at each site (infinitely far away).

As we bring electrons closer.

1. Wavefunctions overlap slightly
2. Electrons at one site can “hop” from one site to the next.