Physics 7: The Hubbard model

Probably the simplest model of *itinerant* correlated electrons is the Hubbard model: Each atom is presumed to have a single relevant degree of freedom with room for two electrons, one 'up' and one 'down' electron. There are *chemical bonds* between neighbouring atoms (see 'Phys2') with a matrix element, t, which can be intuitively interpreted as the electrons hopping from atom to neighbouring atom. The other main energetic contribution is the *short-range* Coulomb repulsion with a matrix element, U, which contributes when two electrons sit on the same atom. The electrons are assumed only to interact when they sit on the same atom, as if the longer-range Coulomb interactions do not exist: In fact, the longer-range interactions are assumed *screened*, ie small collective 'sloshings' of intermediate electrons counteract the effects. This screening assumption is only valid in 'uniform' metallic states, and the model often predicts an *inconsistent* 'phase separated' style of solution of no physical significance. One might interpret the model in terms of electrons hopping from atom to atom, avoiding electrons of opposite spin due to the penalty of U from doubly occupying atoms, but this ignores the *strongest* 'force' in the problem: *Fermi statistics*. Electrons of the same spin must be anti-symmetric under exchange, and this prohibits double occupancy (known as Pauli exclusion and analogous to $U = \infty$) and provides many more restrictions in higher dimensions. So, in fact, electrons hop around strongly avoiding electrons of the same spin and more weakly avoiding electrons of the opposite spin.

The first task is to *mathematically* formulate this model in a usable form. The basic idea is to use operators, $c^\dagger_{i\sigma}$ ($c_{i\sigma}$), which create (annihilate) electrons of spin σ ($\uparrow$ or $\downarrow$) on site i. A particular state:

corresponds to:

$$c^\dagger_{1\uparrow} c^\dagger_{3\uparrow} c^\dagger_{3\downarrow} c^\dagger_{4\uparrow} \mid 0 >$$

where $\mid 0 >$ is known as the *vacuum* and corresponds to the state with no electrons present. Using these operators the Hubbard model is quite easy to formulate:

$$H = -t \sum_{<ii'>\sigma} c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i c^\dagger_{i\sigma} c^\dagger_{i\bar{\sigma}} c_{i\bar{\sigma}} c_{i\sigma}$$

where $\bar{\sigma}$ is the opposite spin to σ. The first term hops electrons from site i' to site i and the second term annihilates a *pair* of electrons on site i and then replaces them again. In order to ensure that the interactions only contribute when electrons actually move or exist, we need to impose that, $c_{i\sigma} \mid 0 >= 0$, and hence only an electron which is present may be annihilated. The Fermi-statistics is much more subtle to formulate, and is effected by imposing *anticommutation relations* on the operators:

$$\begin{aligned}
c^\dagger_{i\sigma} c^\dagger_{i'\sigma'} + c^\dagger_{i'\sigma'} c^\dagger_{i\sigma} &\equiv \{c^\dagger_{i\sigma}, c^\dagger_{i'\sigma'}\} = 0 \\
c_{i\sigma} c_{i'\sigma'} + c_{i'\sigma'} c_{i\sigma} &\equiv \{c_{i\sigma}, c_{i'\sigma'}\} = 0 \\
c_{i\sigma} c^\dagger_{i'\sigma'} + c^\dagger_{i'\sigma'} c_{i\sigma} &\equiv \{c_{i\sigma}, c^\dagger_{i'\sigma'}\} = \delta_{ii'}\delta_{\sigma\sigma'}
\end{aligned}$$

and this ensures antisymmetry when any two electrons are exchanged in a valid state.

There are two natural limits to the Hubbard model:

(1) $U = 0$: The 'non-interacting' limit.

Unitary transformations conserve commutation relations:

$$c^\dagger_{n\sigma} = \sum_i U^*_{ni} c^\dagger_{i\sigma} \qquad \sum_i U_{ni} U^*_{n'i} = \delta_{nn'}$$

constitutes a unitary transformation, and then:

$$\{c_{n\sigma}, c^\dagger_{n'\sigma'}\} = \sum_{ii'} U_{ni} U^*_{n'i'} \{c_{i\sigma}, c^\dagger_{i'\sigma'}\} = \sum_{ii'} U_{ni} U^*_{n'i'} \delta_{ii'} \delta_{\sigma\sigma'} = \sum_i U_{in} U^*_{in'} \delta_{\sigma\sigma'} = \delta_{nn'} \delta_{\sigma\sigma'}$$

and so the hopping contribution can be *diagonalised* without interfering with the Fermi-statistics.

$$H_1 = -t \sum_{<ii'>\sigma} c^\dagger_{i\sigma} c_{i'\sigma} \equiv \sum_{ii'\sigma} c^\dagger_{i\sigma} H_{ii'} c_{i'\sigma}$$

$$\mapsto \sum_{nn'\sigma} \sum_{ii'} c^\dagger_{n\sigma} U_{ni} H_{ii'} U^*_{n'i'} c_{n'\sigma} = \sum_{nn'\sigma} \sum_i c^\dagger_{n\sigma} U_{ni} U^*_{n'i} c_{n'\sigma} \epsilon_n = \sum_{n\sigma} \epsilon_n c^\dagger_{n\sigma} c_{n\sigma}$$

provided that: $\sum_i U_{ni} H_{ii'} = \epsilon_n U_{ni'}$ and the U_{ni} are eigenvectors of the Hamiltonian matrix. As is explained in 'Phys3' and 'Phys4', Bloch's theorem diagonalises periodic symmetries, and if there is a single atom per unit cell, then:

$$c^\dagger_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}.\mathbf{R}_i} c^\dagger_{\mathbf{k}\sigma}$$

constitutes the unitary transformation and:

$$H_1 = -t \sum_{<ii'>\sigma} c^\dagger_{i\sigma} c_{i'\sigma} = -\frac{t}{N} \sum_{\mathbf{k}\mathbf{k}'\sigma} \sum_{<ii'>} e^{i\mathbf{k}.\mathbf{R}_i - i\mathbf{k}'.\mathbf{R}_{i'}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma} = -Zt \sum_{\mathbf{k}\sigma} \gamma_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

where Z is the *coordination number*, the number of nearest neighbours, and the so-called structure factor is:

$$\delta_{\mathbf{k}\mathbf{k}'} \gamma_{\mathbf{k}} = \frac{1}{ZN} \sum_{<ii'>} e^{i\mathbf{k}.\mathbf{R}_i - i\mathbf{k}'.\mathbf{R}_{i'}} = \frac{1}{N} \sum_i e^{i\mathbf{R}_i(\mathbf{k}-\mathbf{k}')} \frac{1}{Z} \sum_{<0n>} e^{i\mathbf{k}'.\mathbf{R}_n}$$

where we have used $\mathbf{R}_n = \mathbf{R}_i - \mathbf{R}_{i'}$ which depends only on the relative distances between nearest-neighbours and so, from 'Phys4':

$$\frac{1}{N} \sum_i e^{i\mathbf{R}_i(\mathbf{k}-\mathbf{k}')} = \delta_{\mathbf{k}\mathbf{k}'}$$

and hence:

$$\gamma_{\mathbf{k}} = \frac{1}{Z} \sum_{<0n>} e^{i\mathbf{k}.\mathbf{R}_n}$$

is the sum over the phases picked up in hopping to the nearest-neighbours, $\mathbf{R}_n$.

The energetics is controlled by the *density of states*:

$$\rho(\gamma) = \frac{1}{N}\sum_{\mathbf{k}} \delta(\gamma - \gamma_{\mathbf{k}}) \mapsto \int_V \frac{d^d\mathbf{k}}{V}\delta(\gamma - \gamma_{\mathbf{k}})$$

in terms of which the energy is:

$$E = \sum_{\mathbf{k}\sigma}(-tZ\gamma_{\mathbf{k}})n(-tZ\gamma_{\mathbf{k}}) = \sum_{\mathbf{k}\sigma}(-tZ\gamma_{\mathbf{k}})n(-tZ\gamma_{\mathbf{k}}) \times \int_{\mathbf{R}} d\gamma\delta(\gamma - \gamma_{\mathbf{k}})$$

$$= -2tZN\int_{\mathbf{R}} d\gamma\rho(\gamma)\frac{1}{1+\exp\left[-\frac{tZ\gamma+\mu}{k_BT}\right]}$$

where we have employed the Fermi-occupation number:

$$n(\epsilon) = \frac{1}{1+\exp\left[\frac{\epsilon-\mu}{k_BT}\right]}$$

which is the probability that a state at energy ϵ is occupied at temperature T. The chemical potential, μ, is a variable whose job is to eventually provide the correct *total* number of electrons.

The analogous entropy is:

$$S = -k_B\sum_{\mathbf{k}\sigma}\left(n(-tZ\gamma_{\mathbf{k}})\log n(-tZ\gamma_{\mathbf{k}}) + [1-n(-tZ\gamma_{\mathbf{k}})]\log[1-n(-tZ\gamma_{\mathbf{k}})]\right)$$

$$= -2k_BN\int_{\mathbf{R}} d\gamma\rho(\gamma)\left(n(-tZ\gamma)\log n(-tZ\gamma)[1-n(-tZ\gamma)] + \log[1-n(-tZ\gamma)]\right)$$

which provides a complete description of the statistical physics in terms of the density of states $\rho(\gamma)$.

(2) t=0: The correlated, atomic and magnetic limit.

In this limit none of the electrons can move. The low energy states are those for which there are a minimum number of doubly occupied atoms. It is quite natural for atoms to have fixed spin directions, which constitutes *magnetism.*

In fact, all states with the same number of doubly occupied atoms are *degenerate*, and the physics of this limit is controlled by how both this positional and spin degeneracy is lifted.

There is a useful representation for the Coulomb repulsion term which *implicitely* suggests magnetism. The idea is to rerepresent combinations of operators as:

$$\hat{n}_i = \frac{1}{2}\left[c^\dagger_{i\uparrow}c_{i\uparrow} + c^\dagger_{i\downarrow}c_{i\downarrow}\right]$$

for the *number operator* yielding the average number of electrons on site i *per spin*, and:

$$\begin{aligned}
\hat{m}_i^x &= \frac{1}{2}\left[c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow}\right] \equiv \frac{1}{2}\sum_{\sigma\sigma'} c_{i\sigma}^\dagger \hat{\sigma}_{\sigma\sigma'}^x c_{i\sigma'} \\
\hat{m}_i^y &= \frac{(-i)}{2}\left[c_{i\uparrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\uparrow}\right] \equiv \frac{1}{2}\sum_{\sigma\sigma'} c_{i\sigma}^\dagger \hat{\sigma}_{\sigma\sigma'}^y c_{i\sigma'} \\
\hat{m}_i^z &= \frac{1}{2}\left[c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}\right] \equiv \frac{1}{2}\sum_{\sigma\sigma'} c_{i\sigma}^\dagger \hat{\sigma}_{\sigma\sigma'}^z c_{i\sigma'}
\end{aligned}$$

are the magnetic moment operators, in terms of the infamous Pauli-matrices, $\hat{\boldsymbol{\sigma}}$:

$$\hat{\sigma}^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{\sigma}^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \hat{\sigma}^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

In terms of these operators:

$$H_2 = U\sum_i c_{i\sigma}^\dagger c_{i\bar{\sigma}}^\dagger c_{i\bar{\sigma}} c_{i\sigma} = U\sum_i [\hat{n}_i\hat{n}_i - \hat{m}_i^x\hat{m}_i^x] = U\sum_i [\hat{n}_i\hat{n}_i - \hat{m}_i^y\hat{m}_i^y] = U\sum_i [\hat{n}_i\hat{n}_i - \hat{m}_i^z\hat{m}_i^z]$$

$$= U\sum_i [\hat{n}_i\hat{n}_i - (\hat{\mathbf{r}}.\hat{\mathbf{m}}_i)(\hat{\mathbf{r}}.\hat{\mathbf{m}}_i)]$$

for any *unit* vector $\hat{\mathbf{r}}$. These results are easy to prove using the commutation relations. A useful result is:

$$\hat{m}_i^\alpha \hat{m}_i^\beta = \delta^{\alpha\beta}\hat{n}_i[1-\hat{n}_i] + \frac{1}{2}i\epsilon^{\alpha\beta\gamma}\hat{m}_i^\gamma$$

central in quantum spin physics. These representations for H_2, show that the build-up of charge is energetically unfavourable, but a frozen magnetic moment is energetically favourable, since a moment appears to *gain* energy comparitively, whatever the direction.

The existence, or not, of this magnetism is a central problem in understanding the Hubbard model.