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# STRONGLY CORRELATED SYSTEMS IN 2D : ANALYTICAL AND NUMERICAL APPROACHES

Lecture Notes TP IV

NOTE

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# Part I

## ANALYTICAL

# 1 ANTIFERROMAGNETISM

## 1.1 MOTT TRANSITION

Consider a system with N Na atoms, at $T = 0$. The electronic configuration of the Na atoms is [Ne]$3s^1$. The Hamiltonian contains a term

$$\mathcal{H}_{\text{band}} = \varepsilon_{3s} \sum_{j\sigma} n_{j\sigma} - t_{3s} \sum_{\langle jl \rangle} \sum_{\sigma} [c^{\dagger}_{j\sigma} c_{l\sigma} + c^{\dagger}_{l\sigma} c_{j\sigma}] \tag{1.1}$$

with $n_{j\sigma} = c^{\dagger}_{j\sigma} c_{j\sigma}$ and $t_{3s} > 0$. The band structure of this system is given in Figure 1.1. Only the 3s band is half-filled, thus Na is expected to be metal according to band theory, for any lattice constants, since even the 3s band in narrowing as one increases $a$, it remains half-filled. This leads to an absurdity since for a large $a$, $e^-$ would remain on site.

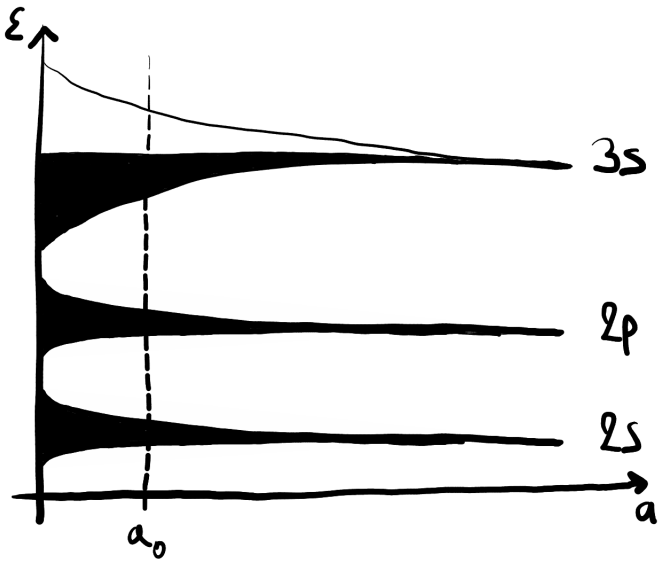


*Figure* 1.1 – Tight-binding band structure of Na.

For electrical conduction, $e^-$ should propagate through the lattice inducing charge fluctuations, as shown on Figure 1.2. Each $e^-$ in a 3s band has energy $\varepsilon_{3s}$. If two share the same atomic shell, a repulsion appears leading to the Coulomb energy

$$U_{3s} = \int d\mathbf{r}_1 d\mathbf{r}_2 \, |\phi(\mathbf{r}_1)|^2 \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} |\phi(\mathbf{r}_2)|^2 \tag{1.2}$$

This process usually costs a lot of energy so it does not want to happen. This suppresses charge fluctuations that are necessary for metallic conduction, leading to a metallic-insulator transition for $a$ above some critical value.

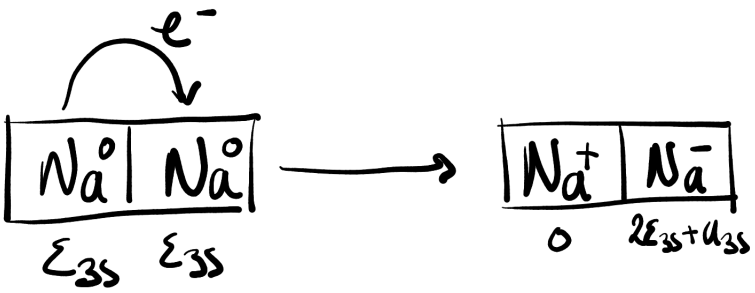


*Figure* 1.2 – Charge fluctuation showing an $e^-$ hopping to form an higher energetic doubly-occupied site.

The total Hamiltonian is thus $\mathcal{H} = \mathcal{H}_{\text{band}} + \mathcal{H}_{\text{Coulomb}}$ with

$$\mathcal{H}_{\text{Coulomb}} = U_{3s} \sum_j n_{j\uparrow} n_{j\downarrow} \tag{1.3}$$

The kinetic term $\mathcal{H}_{\text{band}}$ can be written making use of the Bloch operators

$$\mathcal{H}_{\text{band}} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \tag{1.4}$$

whose ground state is the metallic Fermi sea corresponding to the uncorrelated ground state

$$|\text{FS}\rangle = \prod_k^{\varepsilon_k < \varepsilon_{3s}} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} |0\rangle \tag{1.5}$$

remembering that $c^\dagger_{k\sigma} = \frac{1}{\sqrt{N}} \sum_j e^{ik\cdot j} c^\dagger_{j\sigma}$. This leads the the expectation value

$$\frac{1}{N} \langle \text{FS}|\mathcal{H}_{3s}|\text{FS}\rangle = \varepsilon_{3s} - \alpha t_{3s} + \frac{U_{3s}}{4} \tag{1.6}$$

Therefore, increasing $a$ makes $t_{3s}$ fall exponentially, leading to $U_{3s}/t_{3s}$ passing through the critical value $4\alpha$, indicating that the Coulomb energy cost of charge fluctuation exceeds the kinetic energy gain for occupying the lower half of a band. Hence the formation of the band — an itinerant ground state — is no longer favorable, leading to a localization of each $e^-$ alone on a single site. To sum up, if $U_{3s}/t_{3s} < 4\alpha$, the uncorrelated $|\text{FS}\rangle$ is the ground state, and if $U_{3s}/t_{3s} > 4\alpha$, the system is an array of neutral Na atoms. The transition is shown on Figure 1.3.

Thereby, the insulating system is highly correlated, since the $e^-$ avoid themselves a lot to minimize the Coulomb interaction. Also, $|\text{FS}\rangle$ is not unique since $2^N$-fold degeneracy in the limit $U_{3s}/t_{3s} \to \infty$ and should be lifted for any finite value. Finally, Mott insulator just described turn out to be antiferromagnets, especially in the large-U limit where writing its Heisenberg Hamiltonian makes this explicit.

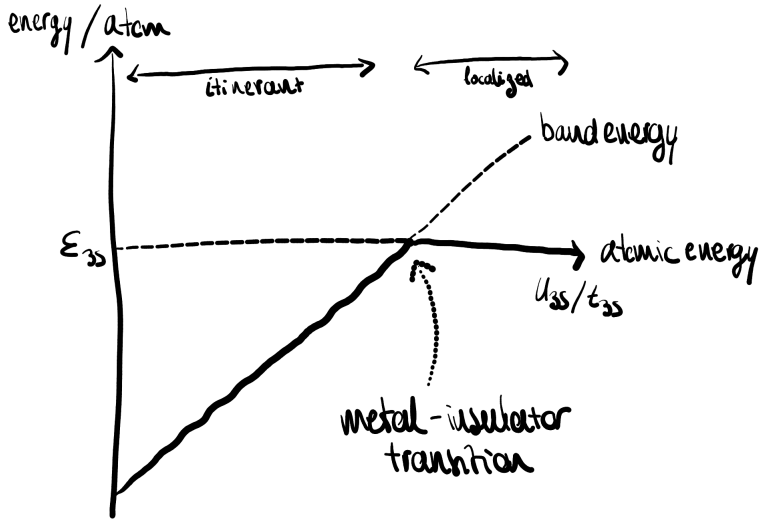


*Figure* 1.3 – Naive Mott transition showing the metal-insulator transition for the Na system.

## 1.2 MEAN FIELD APPROXIMATION

Magnetic order arises from the inequivalence between the number of up- and down-spins. For this to be understood introduce the $z$-component of the spin at site $\mathbf{j}$ as

$$\langle S_j^z \rangle = \frac{\langle n_{j\uparrow} \rangle - \langle n_{j\downarrow} \rangle}{2} \tag{1.7}$$

Hence, a magnetically ordered state has $\langle S_j^z \rangle \neq 0$ either $\forall \mathbf{j}$ or $\forall \mathbf{j} \in \mathcal{A}$ where $\mathcal{A}$ describes a sublattice of the sites. Since Hubbard Hamiltonian

$$\mathcal{H} = -t \sum_{\langle jl \rangle} \sum_{\sigma} [c_{j\sigma}^\dagger c_{l\sigma} + c_{l\sigma}^\dagger c_{j\sigma}] + U \sum_j n_{j\uparrow} n_{j\downarrow} \tag{1.8}$$

has spin-rotational invariance, finding a magnetically ordered ground states underlies a symmetry-breaking. Now, express

$$\begin{aligned} n_{j\uparrow} n_{j\downarrow} &= [n_{j\uparrow} - \langle n_{j\uparrow} \rangle + \langle n_{j\uparrow} \rangle][n_{j\downarrow} - \langle n_{j\downarrow} \rangle + \langle n_{j\downarrow} \rangle] \\ &= [n_{j\uparrow} - \langle n_{j\uparrow} \rangle] \langle n_{j\uparrow} \rangle + [n_{j\downarrow} - \langle n_{j\downarrow} \rangle] \langle n_{j\downarrow} \rangle \\ &+ \langle n_{j\uparrow} \rangle \langle n_{j\downarrow} \rangle + [n_{j\uparrow} - \langle n_{j\uparrow} \rangle][n_{j\downarrow} - \langle n_{j\downarrow} \rangle] \end{aligned} \tag{1.9}$$

Mean field approximation consists in considering the fluctuations of the spins around their mean value as negligible, hence neglect the last term, leading to

$$n_{j\uparrow} n_{j\downarrow} \sim n_{j\uparrow} \langle n_{j\uparrow} \rangle + n_{j\downarrow} \langle n_{j\downarrow} \rangle - \langle n_{j\uparrow} \rangle \langle n_{j\downarrow} \rangle \tag{1.10}$$

and thus writing $n_j = n_{j\uparrow} + n_{j\downarrow}$ gives

$$2 n_{j\uparrow} n_{j\downarrow} \sim n_j \langle n_j \rangle - 4 S_j^z \langle S_j^z \rangle - \frac{\langle n_j \rangle^2}{2} + 2 \langle S_j^z \rangle^2 \tag{1.11}$$

However, the Hubbard Hamiltonian being isotropic, one has to be careful to not prefer one particular orientation of the spin and write the complete

Hartree-Fock approximation, but one is not going to seek into cumbersome derivations rather fix the $z$-axis. Finally writing this decoupled scheme, neglecting local charge deviation $\langle \delta n_j \rangle = 0$, one finds

$$U \sum_j n_{j\uparrow} n_{j\downarrow} \sim -2U \sum_j S_j \langle S_j \rangle + U \sum_j \left\langle S_j^2 \right\rangle + \frac{LUn^2}{4} \tag{1.12}$$

with $n = N/L$.

## 1.3 STONER MODEL

The goal is to find a criterion for the Hubbard model to be ferromagnetic. Into a uniform magnetic field, express

$$\mathcal{H} = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow} - \frac{g\mu_B H}{2} \sum_j [n_{j\uparrow} - n_{j\downarrow}] \tag{1.13}$$

leading to a uniform spin polarization $m$ allowing to write

$$\langle n_{j\uparrow} \rangle = \frac{n}{2} + m \quad \text{and} \quad \langle n_{j\downarrow} \rangle = \frac{n}{2} - m \tag{1.14}$$

The mean field decoupling (1.10) helping, one finds the total energy density

$$\mathcal{E}(m) = \int_B^{\mu_\uparrow} d\varepsilon\ \rho(\varepsilon)\varepsilon + \int_B^{\mu_\downarrow} d\varepsilon\ \rho(\varepsilon)\varepsilon + U\left[\frac{n^2}{2} - m^2\right] - g\mu_B H m \tag{1.15}$$

where $B$ is the bottom energy of the band as presented on Figure 1.4, and with $\mu_\sigma$ such that $n_\sigma = \int_B^{\mu_\sigma} d\varepsilon\ \rho(\varepsilon)$. Now, try to find the energy change induced by the polarization

$$\begin{aligned} \Delta\mathcal{E}(m) &= \mathcal{E}(m) - \mathcal{E}(0) \\ &= \int_{\mu_0}^{\mu_\uparrow} d\varepsilon\ \rho(\varepsilon)\varepsilon - \int_{\mu_0}^{\mu_\downarrow} d\varepsilon\ \rho(\varepsilon)\varepsilon - Um^2 - g\mu_B H m \end{aligned} \tag{1.16}$$

with $\mu_0$ the chemical potential for $H = 0$.

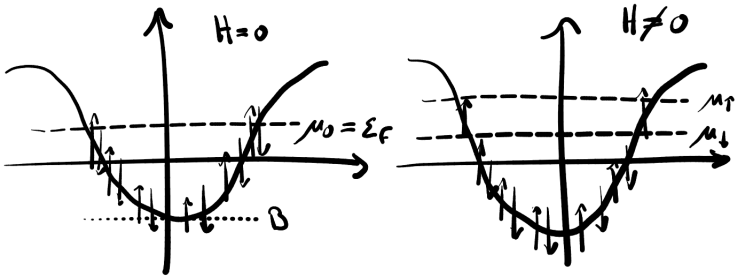


*Figure* 1.4 – Chemical potentials with and without magnetic field.

Increasing $U$ starting from 0 yields a $T = 0$ paramagnetic-ferromagnetic transition. Consider it to be of second order. Then, $m$ is continuously induced by $H$. For $H \ll 1$, one can replace $\rho(\varepsilon) \simeq \rho(\varepsilon_F)$ and at second order

$$\Delta\mathcal{E}(m) = \frac{m^2}{\rho(\varepsilon_F)} - Um^2 - g\mu_B H m \tag{1.17}$$

Further minimizing with respect to $m$ yields the susceptibility being

$$\chi = \frac{mg\mu_B}{H} = \frac{(g\mu_B)^2}{2}\frac{\rho(\varepsilon_F)}{1 - U\rho(\varepsilon_F)} \tag{1.18}$$

which diverges for the critical

$$U_{crit}\rho(\varepsilon_F) = 1 \tag{1.19}$$

This is the Stoner criterion, which implies that approaching $U_{crit}$ from below yields a divergence of $\chi$ and thus an instability of the symmetric paramagnetic ground state, falling into a ferromagnetic ordering. Finally, this means that as long as $\rho(\varepsilon_F) \neq 0$, ferromagnetism is ensured by the Stoner criterion at sufficiently large $U$. The problem is that near half-filling, the Hubbard model prefers antiferromagnetism. This leads to the generalized Stoner model.

## 1.4 GENERALIZED STONER MODEL

The instability of the Hubbard model must take the form of a divergent response to an external magnetic field with wavevector $\mathbf{q}$. The full Hamiltonian is

$$\mathcal{H} = \mathcal{H}_{band} + \mathcal{H}_U + \mathcal{H}_{field} \tag{1.20}$$

The coupling of the spins to the field is

$$\mathcal{H}_{field} = -\int d\mathbf{r}\ \mathbf{H}(\mathbf{r}) \cdot \mathbf{M}(\mathbf{r}) = -g\mu_B \int d\mathbf{r}\ \mathbf{H}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{r}) \tag{1.21}$$

where $\mathbf{M}(\mathbf{r})$ is the density of magnetic moment and $\mathbf{S}(\mathbf{r}) = \sum_j \delta(\mathbf{r} - \mathbf{r}_j)\mathbf{S}_j$ the density of spin. Go to the Fourier space as

$$\mathbf{S}(\mathbf{q}) = \int d\mathbf{r}\ e^{-i\mathbf{q}\cdot\mathbf{r}}\mathbf{S}(\mathbf{r}) = \sum_j e^{-i\mathbf{q}\cdot\mathbf{r}_j}\mathbf{S}_j \tag{1.22}$$

Looking for a period magnetic field $\mathbf{H}(\mathbf{r}) = \mathbf{H}_\mathbf{q} \cos \mathbf{q} \cdot \mathbf{r}$, and knowing the Hamiltonian is spin-rotationally invariant, choose the x-direction and find

$$\begin{aligned}
\mathcal{H}_{field} &= -g\mu_B \sum_j \mathbf{H}(\mathbf{r}_j) \cdot \mathbf{S}_j \\
&= -g\mu_B \sum_j H^x S_j^x \frac{e^{i\mathbf{q}\cdot\mathbf{r}_j} + e^{-i\mathbf{q}\cdot\mathbf{r}_j}}{2} \\
&= -\frac{g\mu_B H^x}{2}[S^x(\mathbf{q}) + S^x(-\mathbf{q})]
\end{aligned} \tag{1.23}$$

Now, writing

$$\begin{aligned}
n_{j\uparrow}n_{j\downarrow} &= c_{j\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}^\dagger c_{j\downarrow} = n_{j\uparrow} - c_{j\uparrow}^\dagger c_{j\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow} \\
&= n_{j\uparrow} - S_j^+ S_j^- \\
\text{and} \quad n_{j\uparrow}n_{j\downarrow} &= n_{j\downarrow} - S_j^- S_j^+
\end{aligned} \tag{1.24}$$

one arrives at the expression

$$\mathcal{H}_U = U \sum_j n_{j\uparrow} n_{j\downarrow} = \frac{NU}{2} - U \sum_j [(S_j^x)^2 + (S_j^y)^2] \tag{1.25}$$

Then decoupling like $(S_j^x)^2 \sim 2S_j^x \langle S_j^x \rangle - \langle S_j^x \rangle^2$ and assuming that the only non-vanishing average is due to the spin density wave induced by the external magnetic field, *ie* neglecting the $y$ component, as long as writing $\langle S_j^x \rangle = \mathcal{S} \cos \mathbf{q} \cdot \mathbf{j}$, one finds

$$\mathcal{H}_U = -U\mathcal{S}[S^x(\mathbf{q}) + S^x(-\mathbf{q})] \tag{1.26}$$

Write the term

$$\mathcal{H}' = -\left[\frac{g\mu_B H^x}{2} + U\mathcal{S}\right][S^x(\mathbf{q}) + S^x(-\mathbf{q})] \tag{1.27}$$

Treat now the spin density as $\mathcal{S} \ll 1$. Then $\mathcal{H}'$ is to be considered as a perturbation of $\mathcal{H}_{\text{band}}$ whose ground state is the Fermi sea $|FS\rangle$. Via first-order perturbation theory

$$\begin{aligned} |\psi\rangle = |FS\rangle - &\left[\frac{g\mu_B H^x}{2} + U\mathcal{S}\right] \\ &\cdot \sum_{\mathbf{p}\sigma} \left[\frac{c^\dagger_{\mathbf{p}+\mathbf{q},\sigma} c_{\mathbf{p},-\sigma}}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}}} + \frac{c^\dagger_{\mathbf{p}-\mathbf{q},\sigma} c_{\mathbf{p},-\sigma}}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}-\mathbf{q}}}\right] |FS\rangle \end{aligned} \tag{1.28}$$

having used the $S^x(\mathbf{q}) = \frac{1}{2}\sum_{\mathbf{p}\sigma} c^\dagger_{\mathbf{p}+\mathbf{q},\sigma} c_{\mathbf{p},-\sigma}$. Now computing at first order and assuming $\mathbf{q} \neq 0$

$$\begin{aligned} \frac{\langle\psi|c^\dagger_{\mathbf{p}+\mathbf{q},\sigma} c_{\mathbf{p},-\sigma}|\psi\rangle}{\frac{g\mu_B H^x}{2} + U\mathcal{S}} = -\sum_{\mathbf{k}\sigma'} \langle FS| \Bigg[ &\cancel{\frac{c^\dagger_{\mathbf{p}+\mathbf{q},\sigma} c_{\mathbf{p},-\sigma} c^\dagger_{\mathbf{k}+\mathbf{q},\sigma'} c_{\mathbf{k},-\sigma'}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}} \\ &+ \frac{c^\dagger_{\mathbf{p}+\mathbf{q},\sigma} c_{\mathbf{p},-\sigma} c^\dagger_{\mathbf{k}-\mathbf{q},\sigma'} c_{\mathbf{k},-\sigma'}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}}} \\ &+ \frac{c^\dagger_{\mathbf{k},-\sigma'} c_{\mathbf{k}+\mathbf{q},\sigma'} c^\dagger_{\mathbf{p}+\mathbf{q},\sigma} c_{\mathbf{p},-\sigma}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}} \\ &+ \cancel{\frac{c^\dagger_{\mathbf{k},-\sigma'} c_{\mathbf{k}-\mathbf{q},\sigma'} c^\dagger_{\mathbf{p}+\mathbf{q},\sigma} c_{\mathbf{p},-\sigma}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}}}} \Bigg] |FS\rangle \end{aligned} \tag{1.29}$$

where the cancellation comes from the impossibility to recover the Fermi sea without taking $\mathbf{q} = 0$. Introducing the occupying function as the Fermi-Dirac distribution at $T = 0$

$$f_{\mathbf{p}} = \Theta(\varepsilon_F - \varepsilon_{\mathbf{p}}) = \langle FS|c^\dagger_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma}|FS\rangle \tag{1.30}$$

the first non-vanishing term in (1.29) imposes $\mathbf{k} = \mathbf{p} + \mathbf{q}$ and the second one $\mathbf{k} = \mathbf{p}$. This yields, using the anti-commutation relations

$$\begin{aligned} \frac{\langle\psi|c^\dagger_{\mathbf{p}+\mathbf{q},\sigma} c_{\mathbf{p},-\sigma}|\psi\rangle}{\frac{g\mu_B H^x}{2} + U\mathcal{S}} &= -\frac{f_{\mathbf{p}}(1 - f_{\mathbf{p}+\mathbf{q}}) - f_{\mathbf{p}+\mathbf{q}}(1 - f_{\mathbf{p}})}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{q}}} \\ &= \frac{f_{\mathbf{p}} - f_{\mathbf{p}+\mathbf{q}}}{\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}}} \end{aligned} \tag{1.31}$$

Hence, introducing

$$\chi^{(0)}(\mathbf{q}) = \sum_{\mathbf{p}} \frac{f_{\mathbf{p}} - f_{\mathbf{p}+\mathbf{q}}}{\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}}} \tag{1.32}$$

one gets

$$S = \langle\psi|S^x(\mathbf{q})|\psi\rangle = \left[\frac{g\mu_B H^x}{2} + US\right]\chi^{(0)}(\mathbf{q}) \tag{1.33}$$

and rearranging the terms of the auto-coherent equation for the spin density

$$\implies S = \frac{g\mu_B H^x}{2}\frac{\chi^{(0)}(\mathbf{q})}{1 - U\chi^{(0)}(\mathbf{q})} \tag{1.34}$$

which gives the generalized $\mathbf{q}$-dependent static susceptibility

$$\chi(\mathbf{q}) = (g\mu_B)^2\frac{\chi^{(0)}(\mathbf{q})}{1 - U\chi^{(0)}(\mathbf{q})} \tag{1.35}$$

making use of (1.23) and minimizing $\langle\psi|\mathcal{H}_{\text{field}}|\psi\rangle$ with respect to $H^x$ then inserting (1.34) and recovering the magnetization density. The generalized Stoner criterion then reads

$$U^{\mathbf{q}}_{\text{crit}}\chi^{(0)}(\mathbf{q}) = 1 \tag{1.36}$$

To recover the Stoner criterion (1.19), take the $\mathbf{q} \to 0$ limit. Then

$$\begin{aligned} f_{\mathbf{p}} - f_{\mathbf{p}+\mathbf{q}} &\simeq -\frac{\partial f}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial \mathbf{p}} \cdot \mathbf{q} \\ \text{and} \quad \varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}} &\simeq \frac{\partial \varepsilon}{\partial \mathbf{p}} \cdot \mathbf{q} \end{aligned} \tag{1.37}$$

which implies

$$\chi^{(0)}(\mathbf{q}) \simeq -\int d\varepsilon\ \rho(\varepsilon)\frac{\partial f}{\partial \varepsilon} = \rho(\varepsilon_F) \tag{1.38}$$

since at $T = 0$ one has $\frac{\partial f}{\partial \varepsilon} = -\delta(\varepsilon - \varepsilon_F)$. Therefore, at arbitrary band-filling, the system becomes unstable against the formation of a spin density wave with arbitrary $\mathbf{q}$ if $U$ is large enough. Only the instability occurring at the lowest $U_{\text{crit}} = \min_{\mathbf{q}} U^{\mathbf{q}}_{\text{crit}}$ happens. This peaks out a certain $\mathbf{q}_0$ for the spin density wave, which depends on the band-filling. Increasing further $U$ beyond its critical value leads to a saturation of the amplitude of the wave, yielding sometimes a phase transition to another magnetic ordering.

Taking a D-dimensional cubic lattice, the dispersion relation reads

$$\varepsilon(\mathbf{k}) = -2t\sum_{i=1}^{D}\cos k_i \tag{1.39}$$

and it satisfies the perfect nesting condition $\varepsilon(\mathbf{k} + \mathbf{Q}) = -\varepsilon(\mathbf{k})\ \forall \mathbf{k}$, where $\mathbf{Q} = (\pi, \ldots, \pi)$ is the spanning-vector. At half-filling, $\varepsilon_F = 0$, and at $T = 0$ one has

$$\chi^{(0)}(\mathbf{Q}) = \int_0^{w/2} d\varepsilon\ \frac{\rho(\varepsilon)}{2\varepsilon} \tag{1.40}$$

with $w$ the bandwidth. Unless $\rho(\varepsilon) \to 0$ as $\varepsilon \to 0$, $\chi^{(0)}(\mathbf{Q})$ diverges logarithmically. Hence $U^{\mathbf{Q}}_{\text{crit}} = 0$ that is, for half-filled bands with the perfect nesting property, an arbitrary small $U > 0$ causes a transition to a two-sublattice antiferromagnetic state. In fact, it can be shown by approximating the Fermi-Dirac distribution correctly, one has

$$\chi^{(0)}(\mathbf{Q}, T) \sim \frac{1}{t} \ln \frac{t}{2k_B T} \quad \text{and} \quad \chi^{(0)}(0, T) \sim \frac{1}{t} \ln^2 \frac{t}{2k_B T} \tag{1.41}$$

which means that the antiferromagnetic instability is stronger than the ferromagnetic one, since for $T \to 0$, the response diverges faster for $\mathbf{q} = \mathbf{Q}$ than for $\mathbf{q} = 0$.

Finally, one can show that the antiferromagnetic state is insulating, meaning that the metal-insulator transition occurs at $U = 0$ here. This comes from writing the Hamiltonian in mean field approximation

$$\mathcal{H}_{\text{SDW}} = \mathcal{H}_{\text{band}} + U \sum_{j\sigma} n_{j\sigma} \langle n_{j,-\sigma} \rangle - U \sum_{j} \langle n_{j\uparrow} \rangle \langle n_{j\downarrow} \rangle \tag{1.42}$$

and diagonalizing it to obtain, assuming perfect nesting

$$\lambda^{\pm}(\mathbf{k}) = \frac{Un}{2} \pm \sqrt{\varepsilon_{\mathbf{k}}^2 + U^2 m^2} \tag{1.43}$$

giving a band gap of $2Um$.

# 2 FERROMAGNETISM

## 2.1 VERY WEAK ITINERANT FERROMAGNETISM

Given the lowest-order finite-temperature correction to the Pauli susceptibility $\chi^{(0)}$ whose expression is

$$\frac{\chi^{(0)}}{2\mu_B^2} \simeq \rho(\varepsilon_F) + \frac{\pi^2}{12}\left[\rho''(\varepsilon_F) - 2\frac{\rho'^2(\varepsilon_F)}{\rho(\varepsilon_F)}\right](k_B T)^2 \tag{2.1}$$

and using the generalized Stoner criterion one is able to derive the Curie temperature. One simply has to plug (2.1) into (1.19) to get

$$\frac{\pi^2 k_B^2}{6} T_C^2 = \frac{U\rho(\varepsilon_F) - 1}{\left[\frac{\rho'(\varepsilon_F)}{\rho(\varepsilon_F)}\right]^2 - \frac{\rho''(\varepsilon_F)}{\rho(\varepsilon_F)}} \tag{2.2}$$

To develop the temperature dependence of the order parameter, one assumes

$$\rho(\varepsilon) = \rho_0 - a\varepsilon^2 \quad \text{with} \quad a > 0 \tag{2.3}$$

and one also assumes that the band is half-filled. One can then derive the temperature dependence of the order parameter. For this, one can minimize the free energy $\mathcal{F} = \mathcal{E}(T) - T\mathcal{S}$. The energy in the Stoner model is given by the following

$$\mathcal{E} = \sum_\sigma \int_{-\infty}^{+\infty} d\varepsilon\ \varepsilon\rho(\varepsilon) f_\sigma(\varepsilon) + U(n^2 - m^2) - g\mu_B H m \tag{2.4}$$

where $f_\sigma$ is the Fermi distribution with the chemical potential $\mu_\sigma$ which satisfies

$$\int_{-\infty}^{+\infty} d\varepsilon\ \rho(\varepsilon) f_\sigma(\varepsilon) = n + \eta(\sigma) m \tag{2.5}$$

with

$$\eta(\sigma) = \begin{cases} 1 & \text{if } \sigma = \uparrow \\ -1 & \text{if } \sigma = \downarrow \end{cases} \tag{2.6}$$

The term $-T\mathcal{S}$ can be obtained considering the basic assumption of the Stoner theory that the entropy arises solely from the $e^-$ -hole excitations, in other terms the entropy of band $e^-$ . Using the following relation between the specific heat $C_V$ and the entropy

$$C_V = T\left(\frac{\partial \mathcal{S}}{\partial T}\right) \tag{2.7}$$

and the usual expression of the low-temperature specific heat of the spin-↑ and spin-↓ bands, one can obtain

$$-TS = -\frac{(\pi k_B T)^2}{3} \sum_\sigma \rho(\mu_{\sigma,0}) \tag{2.8}$$

with $\mu_{\sigma,0} = \mu_\sigma(T = 0)$. Therefore one eventually has

$$\begin{aligned} \mathcal{F} = &\sum_\sigma \int_{-\infty}^{+\infty} d\varepsilon \ \varepsilon \rho(\varepsilon) f_\sigma(\varepsilon) + U(n^2 - m^2) \\ &- g\mu_B H m - \frac{(\pi k_B T)^2}{3} \sum_\sigma \rho(\mu_{\sigma,0}) \end{aligned} \tag{2.9}$$

One can see that $\mathcal{F}$ depends on $m$ both explicitly and via $\mu_\sigma$. One can take the derivative of both sides of (2.5) with respect to $m$ and get, using both

$$\frac{\partial f_\sigma}{\partial \mu_\sigma} = -\frac{\partial f_\sigma}{\partial \varepsilon} \tag{2.10}$$

and the Sommerfeld expansion and one should arrive at

$$\frac{\partial \mu_\sigma}{\partial m} = \eta(\sigma) \left[ \rho(\mu_{\sigma,0}) - \frac{(\pi k_B T)^2}{3} \left( \frac{\rho'^2(\mu_{\sigma,0})}{\rho(\mu_{\sigma,0}} - \rho''(\mu_{\sigma,0}) \right) \right]^{-1} \tag{2.11}$$

One can minimize $\mathcal{F}$ with respect to $m$ proceeding analogously to the derivation of the generalized Stoner criterion; and to order $T^2$, one finds the extremum condition to be

$$(\mu_{\uparrow 0} - \mu_{\downarrow 0}) - \frac{(\pi k_B T)^2}{6} \left[ \frac{\rho'(\mu_{\uparrow 0})}{\rho(\mu_{\uparrow 0})} - \frac{\rho'(\mu_{\downarrow 0})}{\rho(\mu_{\downarrow 0})} \right] = 2Um + g\mu_B H \tag{2.12}$$

The first assumption leads to

$$\begin{aligned} \rho(\mu_{\uparrow 0}) = \rho(\mu_{\downarrow 0}) &\simeq \rho_0 - a\frac{m^2}{\rho_0^2} \\ \text{and} \qquad \rho'(\mu_{\uparrow 0}) = -\rho'(\mu_{\downarrow 0}) &\simeq -\frac{2am}{\rho_0} \end{aligned} \tag{2.13}$$

First consider the case $H = 0$. The spontaneous magnetization satisfies

$$\frac{1}{\rho_0} \left[ 1 + \frac{am^2}{\rho_0^3} \right]) + \frac{(\pi k_B T)^2}{3} \frac{a}{\rho_0^2} = U \tag{2.14}$$

At $T = 0$, this yields

$$m^2(0) = [U\rho_0 - 1] \frac{\rho_0^3}{a} \tag{2.15}$$

and requiring $m = 0$ for $T = T_C$ gives

$$\frac{\pi^2 k_B^2}{3} T_C^2 = (U\rho_0 - 1) \frac{\rho_0}{a} \tag{2.16}$$

Combining those two equations with the previous one, one obtains one of the most famous results of the Stoner model

$$\frac{m^2(T)}{m^2(0)} = 1 - \left( \frac{T}{T_C} \right)^2 \tag{2.17}$$

Eventually, allowing for the presence of $H \neq 0$, one can get the Edwards-Wohlfarth equation

$$\frac{m^2(T,H)}{m^2(0,0)} = 2\tilde{\chi}\frac{H}{m(T,H)} + 1 - \left(\frac{T}{T_C}\right)^2 \tag{2.18}$$

where

$$\tilde{\chi} = \frac{\rho_0 g \mu_B}{U\rho_0 - 1} \tag{2.19}$$

One can use the previous result to derive the paramagnetic susceptibility. In a weak external field, one can omit the $m^2$ term to obtain

$$\chi(T) = \frac{m(T,H)}{H} = \frac{2\tilde{\chi}}{\left(\frac{T}{T_C}\right)^2 - 1} \tag{2.20}$$

## 2.2 LIEB'S FERRIMAGNETISM

In this second part one discusses a result stated by Elliot Lieb and Daniel Mattis about the ordering of energy levels of interacting spin systems. The original paper of Lieb and Mattis starts with the following the Hamiltonian

$$\mathcal{H} = 2\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j \tag{2.21}$$

Consider a bipartite lattice which can be divided into two sublattices $A$ and $B$. Denote by $|A|$ and $|B|$ the number of sites in the sublattices and make one hypothesis: sublattices $A$ and $B$ are such that for all sites $i(A)$ on sublattice $A$ and $i(B)$ on sublattice $B$,

$$J_{i(A)j(A)} \leqslant g^2, \quad J_{i(B)j(B)} \leqslant g^2 \quad \text{and} \quad J_{i(A)j(B)} \geqslant g^2 \tag{2.22}$$

where $g^2$ is a positive constant. There are two cases

- there is at least one way to decompose the lattice into two sublattices that verify the above conditions (2.22): one shall show that the system is either ferrimagnetic or antiferromagnetic.
- there is none, one cannot decompose the lattice in such a way that fulfills the conditions: then the system is not necessarily ferromagnetic and only explicit solutions can determine this.

One knows that the intrisic spin of an $e^-$ is $1/2$ but to keep some generality, let the intrinsic spin be $S_i$. Define the total spins $S_A$ and $S_B$ on $A$ and $B$ sublattices as

$$S_A = \sum_{i(A)} S_{i(A)} \quad \text{and} \quad S_B = \sum_{i(B)} S_{i(B)} \tag{2.23}$$

Eventually, we define

$$\mathcal{S} = |S_A - S_B| \tag{2.24}$$

Then, the Lieb-Mattis ferrimagnetism theorem states that the ground state of $\mathcal{H}$ belongs at most to total spin $S_{tot} = \mathcal{S}$ and that for all $S_{tot} \geqslant \mathcal{S}$, one has

$$E(S_{tot} + 1) > E(S_{tot}) \tag{2.25}$$

One shall restrict the discussion to the special case $g^2 = 0$ until the end of the proof.

To sketch the proof first, recall that with the help of the total spin operator $S$ we can construct two operators that commute with the Hamiltonian, namely $\boldsymbol{S}^2$ which possesses eigenvalues $S(S+1)$, and $S_z$ which possesses eigenvalues $M$. From the general theory of angular momentum, $-S \leqslant M \leqslant S$.

It is then pretty obvious that every energy eigenvalue have a corresponding eigenstate in the $M = 0$ subspace of eigenstates; every energy level except those belonging to $S = 0$ have a corresponding eigenstate in the $M = 1$ subpsace; every energy level except those belonging to $S = 0$ and $S = 1$ has a corresponding eigenstate in the $M = 2$ subspace, and so on and so forth. Hence it follows that the inequality will be proved if one manages to show that the lowest energy in a given $M$ subspace belongs to $S = M$, since spin $S + 1$ also has a corresponding eigenstate in this precise subspace. Therefore one would indeed have $E(S) < E(S+1)$.

To detail the proof now, consider a $M$ subspace and choose the basis set formed of all distinct eigenstates of the spin values $S_i$ compatible with eigenvalues $M$. Denote each configuration in the set by $|\phi_\alpha\rangle$, where $\alpha$ is an index which runs over all members of the set. One shall provide a more precise expression of $|\phi_\alpha\rangle$ later on but before that let perform the following canonical transformation on the Hamiltonian $\mathcal{H}$

$$\begin{cases} S^x_{i(A)} & \longrightarrow & -S^x_{i(A)} \\ S^y_{i(A)} & \longrightarrow & -S^y_{i(A)} \\ S^z_{i(A)} & \longrightarrow & S^z_{i(A)} \end{cases} \tag{2.26}$$

but do not change the spins on the B-sublattice. One can check that under the action of this canonical transformation the Hamiltonian splits in two parts

$$\mathcal{H} \longrightarrow \mathcal{H}' = \mathcal{H}_0 + \mathcal{H}_1 \tag{2.27}$$

where $\mathcal{H}_0$ is the diagonal part

$$\mathcal{H}_0 = 2 \sum_i J_{ij} S^z_i S^z_j \tag{2.28}$$

and $\mathcal{H}_1$ the off-diagonal part

$$\mathcal{H}_1 = -\sum_i \left( |J_{ij}| S^+_i S^-_j + S^-_i S^+_j \right) \tag{2.29}$$

with $S^+_i$ and $S^-_i$ the spin ladder operators

$$S^\pm_i = S^x_i \pm i S^y_i \tag{2.30}$$

For a given configuration $\alpha$, $S_i^z$ has eigenvalue $m_i$. One can then choose the following expression for our state

$$|\phi_\alpha\rangle = C(S_1^+)^{S_1+m_1}(S_2^+)^{S_2+m_2}\dots(S_N^+)^{S_N+m_N}|\chi\rangle \tag{2.31}$$

where $|\chi\rangle$ is the state in which $m_i = -S_i$ such that

$$|\chi\rangle = |-S_1, -S_2, \dots, -S_N\rangle \tag{2.32}$$

and $C$ is a positive normalization constant whose expression is of no use. Using this expression, it is obvious that if one defines $K_{\beta\alpha}$ as

$$K_{\beta\alpha} = \langle\phi_\beta|\,\mathcal{H}_1\,|\phi_\alpha\rangle \tag{2.33}$$

then $K_{\beta\alpha} \leqslant 0$, which allows to write $K_{\beta\alpha} = -|K_{\beta\alpha}|$.

Denoting $|\psi\rangle$ the ground state in the $M$ subspace, which belongs to the ground-state energy $E_M$, one can write it as a linear combination of the configurations $|\phi_\alpha\rangle$ with amplitudes $c_\alpha$:

$$|\psi\rangle = \sum_\alpha c_\alpha\,|\phi_\alpha\rangle\ . \tag{2.34}$$

For the diagonal part, introduce eigenvalues $E_\alpha$:

$$\mathcal{H}_0\,|\phi_\alpha\rangle = E_\alpha\,|\phi_\alpha\rangle \tag{2.35}$$

and one can get

$$-\sum_\beta |K_{\beta\alpha}|c_\beta + E_\alpha c_\alpha = E_M c_\alpha \tag{2.36}$$

Indeed, one has

$$\mathcal{H}\,|\psi\rangle = E_M\,|\psi\rangle \tag{2.37}$$

$$\sum_\beta c_\beta \mathcal{H}\,|\phi_\beta\rangle = \sum_\beta c_\beta E_M\,|\phi_\beta\rangle \tag{2.38}$$

$$\langle\phi_\alpha|\sum_\beta c_\beta \mathcal{H}\,|\phi_\beta\rangle = \langle\phi_\alpha|\sum_\beta c_\beta E_M\,|\phi_\beta\rangle \tag{2.39}$$

$$\sum_\beta c_\beta\,\langle\phi_\alpha|\mathcal{H}\,|\phi_\beta\rangle = \sum_\beta c_\beta E_M\,\langle\phi_\alpha|\phi_\beta\rangle \tag{2.40}$$

with $\langle\phi_\alpha|\phi_\beta\rangle = \delta_{\alpha\beta}$ and

$$\begin{aligned}\langle\phi_\alpha|\,\mathcal{H}\,|\phi_\beta\rangle &= \langle\phi_\alpha|\,\mathcal{H}_0\,|\phi_\beta\rangle + \langle\phi_\alpha|\,\mathcal{H}_1\,|\phi_\beta\rangle \\ &= -|K_{\alpha\beta}| + E_\beta\delta_{\alpha\beta} = -|K_{\beta\alpha}| + E_\beta\delta_{\alpha\beta}\end{aligned} \tag{2.41}$$

one gets the expected result.

Now, let attempt to construct another state in the $S = M$ subspace. Since that was just built the ground sate, if this trial state leads to the same energy it implies that the ground state is degenerate, otherwise one should obtain a larger energy. The state

$$|\psi'\rangle = \sum_\alpha |c_\alpha|\,|\phi_\alpha\rangle \tag{2.42}$$

is a trial state with the energy $E_M$ and therefore it should verify the same equation derived before

$$-\sum_{\beta} |K_{\beta\alpha}||c_\beta| + E_\alpha|c_\alpha| = E_M|c_\alpha| \tag{2.43}$$

Notice then that it is impossible for a single state $|\phi_\alpha\rangle$ to have an energy smaller than the ground state energy. Hence one should have

$$E_\alpha - E_M > 0 \tag{2.44}$$

holding $\forall\alpha$. Which means that $|E_\alpha - E_M| = E_\alpha - E_M$. Using this, one can get two different expressions of $|(E_\alpha - E_M)c_\alpha|$. Indeed, according to (2.36)

$$|(E_\alpha - E_M)c_\alpha| = \left|\sum_{\beta} |K_{\beta\alpha}|c_\beta\right| \tag{2.45}$$

but according to (2.43)

$$|(E_\alpha - E_M)c_\alpha| = (E_\alpha - E_M)|c_\alpha| = \sum_{\beta} |K_{\beta\alpha}||c_\beta| \tag{2.46}$$

which eventually leads to

$$\left|\sum_{\beta} |K_{\beta\alpha}|c_\beta\right| = \sum_{\beta} |K_{\beta\alpha}||c_\beta| \tag{2.47}$$

This is possible if and only if

$$c_\beta \geqslant 0 \quad \forall\beta \tag{2.48}$$

In general one even has

$$c_\beta > 0 \quad \forall\beta \tag{2.49}$$

To see this is true, one only has to suppose $c_\alpha = 0$ for some $\alpha$. Then (2.43) would yield

$$\sum_{\beta} K_{\beta\alpha}|c_\beta| = 0 \tag{2.50}$$

and then one could establish that

$$c_\alpha = 0 \quad \forall\alpha \tag{2.51}$$

and this would leads to a situation where no wavefunction exists.

There is actually an exception. If the Hamiltonian is broken into sets of non-interacting spins, that means that in some bonds the interactions are zero so one forms cluster of spins; it might also happen if the interaction is varied over a period of lattice spacing. The model as one designs it does not allow the latter.

Therefore, in general, all amplitudes $c_\alpha$ are strictly positive and hence $E_M$ is non-degenerate. Indeed, it is not possible to build a state orthogonal to $|\psi\rangle$ without violating the positivity criterion just established.

Having proved the non-degeneracy on a general model, one can now consider only A-B interactions and take A-A and B-B interactions to zero being this the most interesting case. One still have to prove the inequality. In other terms

$$J_{i(A)j(A)} = J_{i(B)j(B)} = 0 \quad \text{and} \quad J_{i(A)j(B)} = J > 0 \tag{2.52}$$

The lowest energy belonging to each spin is given by $E(S)$ for $S \geqslant \mathcal{S}$, and the ground state belongs to $S = \mathcal{S}$. Indeed

$$S = S_A + S_B \Longrightarrow S^2 = S_A^2 + S_B^2 + 2S_A S_B \tag{2.53}$$

hence eventually get

$$\begin{aligned} 2S_A S_B \left|\psi\right\rangle &= \left(S^2 - S_A^2 - S_B^2\right) \left|\psi\right\rangle \\ &= \left(S(S+1) - s_A(s_A+1) - s_B(s_B+1)\right) \left|\psi\right\rangle \end{aligned} \tag{2.54}$$

which gives the energy

$$E(S) = J\left(S(S+1) - s_A(s_A+1) - s_B(s_B+1)\right) \tag{2.55}$$

This special Hamiltonian has an $S = M$ in each $M$ subspace such that $M \geqslant \mathcal{S}$. Therefore, so does $\mathcal{H}$. This completes the proof for $g^2 = 0$. The general proof, *ie* for $g^2 > 0$, would consider $\mathcal{H} - g^2\mathbf{S}^2$ instead of $\mathcal{H}$.

## 2.3 NAGAOKA'S FERROMAGNETISM

One has seen that Ferromagnetism hardly arise in a proper way. Nagaoka's ferromagnetism is an important result for ferromagnetism to have a nice and solid basis. Indeed under some conditions Nagaoka's theorem states that a whole class of Hubbard model actually describes ferromagnetic state. Which means that the ground state is a fully polarized state. One will start by presenting a weak statement of the Nagaoka theorem and afterward, introducing mathematical results and discussing some interesting geometrical conditions, will reach the full statement. One will finally show the original proof of the theorem which is more complicated but yet very interesting mathematically.

For the weak version, start with the usual Hubbard model

$$\mathcal{H} = -\sum_{\sigma} \sum_{xy} t_{xy} c_{x\sigma}^{\dagger} c_{y\sigma} + \sum_{x} U_x n_{x\uparrow} n_{x\downarrow} \tag{2.56}$$

Assume that the hopping parameters satisfy $t_{xy} = t_{yx} > 0$. Also take the $U \to \infty$ limit and finally assume a perfect half-filling profile with one hole injected in a lattice site, so that $N_e = N - 1$. Gathering all these conditions one can see that as a single hole living in a highly interacting spin cloud in the background. Nagaoka states that with this class of Hubbard model, among the ground states one correspond to the fully polarized state, thus ferromagnetic, with $S_{tot} = S_{max} = \frac{N_e}{2}$.

First of all one needs to take into account the $U \to \infty$ limit and construct an effective Hamiltonian. Toward that purpose, consider the subspace of the whole Hilbert space which consist in all the states without any doubly occupied sites. Call it $\mathbb{H}_N^{hc}$. One can easily see that for any state $|\psi\rangle \in \mathbb{H}_N^{hc}$, $\mathcal{H}_{int}|\psi\rangle = 0$. Considering the orthogonal projection $P_{hc}$ onto $\mathbb{H}_N^{hc}$, one sees that the effective Hamiltonian could be taken as

$$\mathcal{H}_{eff} = P_{hc}\mathcal{H}P_{hc} \tag{2.57}$$

which is an operator acting on $\mathbb{H}_N^{hc}$. Now need a basis to express this effective Hamiltonian and find its ground states. Build them taking into account that they have to depend on the position of the hole as well as the spin configuration of the whole lattice. Thus define

$$|\phi_{x\tilde{\sigma}}\rangle = c_{x\uparrow}\left(\prod_y c^\dagger_{y\tilde{\sigma}'_y}\right)|0\rangle = c_{x\downarrow}\left(\prod_y c^\dagger_{y\tilde{\sigma}''_y}\right)|0\rangle \tag{2.58}$$

One wants to examine the effect of $H_{eff}$ on this state. Start by applying $\sum_\sigma c^\dagger_{x\sigma}c_{z\sigma}$. Developing

$$\begin{aligned}\sum_\sigma c^\dagger_{x\sigma}c_{z\sigma}|\phi_{x\tilde{\sigma}}\rangle &= -c_{z\uparrow}\left(\prod_y c^\dagger_{y\tilde{\sigma}'_y}\right)|0\rangle - c_{z\downarrow}\left(\prod_y c^\dagger_{y\tilde{\sigma}'_y}\right)|0\rangle \\ &= -|\phi_{z\tilde{\sigma}_{z\to x}}\rangle\end{aligned} \tag{2.59}$$

where $\tilde{\sigma}_{z\to x}$ is the new spin configuration obtained by moving $\sigma_z$ to $x$. Using this result, end up with

$$\langle\phi_{y\tilde{\tau}}|H_{eff}|\phi_{x\tilde{\sigma}}\rangle = \begin{cases} -t_{xy} & \text{if } \tilde{\tau} = \tilde{\sigma}_{y\to x} \\ 0 & \text{otherwise}\end{cases} \tag{2.60}$$

One is now able to construct a ground state with respect to this basis. Therefore

$$|\phi_{GS}\rangle = \sum_x \sum_{\{\tilde{\sigma}\}} \phi(x,\tilde{\sigma})|\phi_{x\tilde{\sigma}}\rangle \tag{2.61}$$

Out of convenience, write

$$\xi_x^2 = \sum_{\{\tilde{\sigma}\}} \phi^2(x,\tilde{\sigma}) \tag{2.62}$$

so that the corresponding normalized ferromagnetic state is

$$|\phi_{FM}\rangle = \sum_x \xi_x |\phi_{x(\uparrow)}\rangle \tag{2.63}$$

where $(\uparrow)$ is the spin configuration with all spins up. Finally compare the energies of the so-built ground state and the ferromagnetic state

$$\begin{aligned}\langle\phi_{GS}|\mathcal{H}_{eff}|\phi_{GS}\rangle &= \sum_{xy}\sum_{\{\tilde{\sigma}\}\{\tilde{\tau}\}} \phi(y,\tilde{\tau})\phi(x,\tilde{\sigma})\langle\phi_{y\tilde{\tau}}|\mathcal{H}_{eff}|\phi_{x\tilde{\sigma}}\rangle \\ &= -\sum_{xy} t_{xy}\sum_{\{\tilde{\sigma}\}}\phi(y,\tilde{\sigma}_{y\to x})\phi(x,\tilde{\sigma}) \\ &\geqslant -\sum_{xy} t_{xy}\left[\sum_{\{\tilde{\sigma}\}}\phi^2(y,\tilde{\sigma}_{y\to x})\right]^{\frac{1}{2}}\left[\sum_{\{\tilde{\sigma}\}}\phi^2(x,\tilde{\sigma})\right]^{\frac{1}{2}} \\ &= \langle\phi_{FM}|\mathcal{H}_{eff}|\phi_{FM}\rangle\end{aligned} \tag{2.64}$$

Thus $|\phi_{FM}\rangle$ is also a ground state.

The extension of the Nagaoka theorem is mainly based of the Perron-Frobenius theorem, which one will state but not prove. The stronger statement enables to show that the FM state is actually the only ground state – up to trivial degeneracy.

Now, introduce the Perron-Frobenius theorem. Let $M$ be an $N \times N$ real and symmetric matrix with the following properties

- $M_{ij} < 0 \; \forall i, j$
- ll $i \neq j$ are connected by non-vanishing elements of $M$

Then the lowest eigenvalue of $M$ is non-degenerate.

One can see that the Perron-Frobenius theorem can provide the fact that the ferromagnetic ground state is indeed the only ground state. From what is already derived, one knows that the effective Hamiltonian matrix elements are negative so one needs to add the connectivity notion to the Hubbard model in order to have the final class of model that predicts exact ferromagnetism.

When it is said that every $i \neq j$ has to be connected via non-vanishing elements of the matrix $M$, it means that it exists a sequence $(i_1, i_2, \ldots, i_K)$ with $i_1 = 1$ and $i_K = j$ such that $m_{i_k, i_{k+1}} \neq 0$.

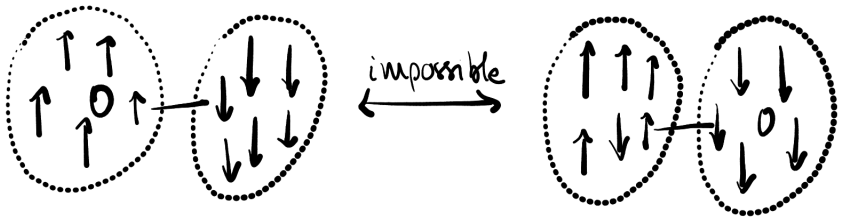


*Figure* 2.1 – Non-biconnected lattice

In the sense of Nagaoka it means that the matrix elements

$$\langle \phi_{x\tilde{\sigma}} | \mathcal{H}_{\text{eff}} | \phi_{y\tilde{\tau}} \rangle \tag{2.65}$$

has to be connected in the sense of Perron-Frobenius. Since every basis vector contains the spin configuration of the lattice, one can have a more geometrical sense of the connectivity. Indeed one can say that a Hubbard model is connected if one can pass from one configuration to another by hoppings of the hole. As a matter of fact, in 1D, very few lattices are connected. However in 2D or higher dimension, apart from a couple of examples, all lattices are connected. Figure 2.1 and Figure 2.2 are examples of 2D lattices that are clearly not connected.

The following aims at giving the idea of this proof as it is certainly interesting but now obsolete since one has the previous really solid proof. First of all, Nagaoka uses the Hamiltonian

$$\mathcal{H} = t \sum_{\langle ij \rangle} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} \tag{2.66}$$

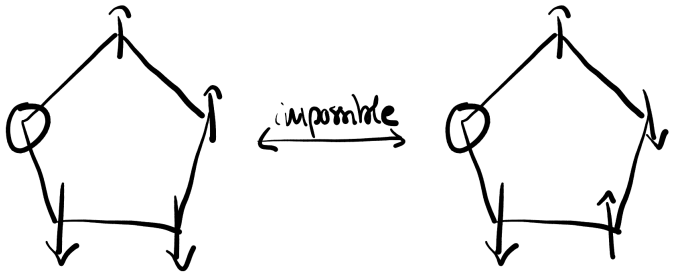


*Figure* 2.2 – Pentagon lattice

And show that the fully polarized state has $S = S_{max}$ and $E = -zt$, where $z$ is the number of nearest neighbors. The idea of the theorem proof will be to show that no energies are possible below $-zt$ and that no ground state with $S < S_{max}$ exists either.
Define the notion of superlattice which is the set $\{i_{\alpha_i}\}_{i,\alpha}$ for which each element corresponds to one site in one lattice configuration. Define a scalar product given by

$$(j_{\beta_j}|i_{\alpha_i})_\omega = \langle \psi_{j\beta_j}| \frac{1}{w - H} |\psi_{i\alpha_i}\rangle \tag{2.67}$$

where $\omega$ is any complex number. The poles of $(i_{\alpha_i}|i_{\alpha_i})_\omega$ define the eigenvalues of $\mathcal{H}$ that lie on the real axis. After some calculation one ends up with

$$(i_{\alpha_i}|i_{\alpha_i})_\omega^{-1} = \omega[1 - f(\omega)] \tag{2.68}$$

with

$$f(\omega) = \sum_{p=2}^{\infty} \frac{A_p}{z^p} \left(\frac{-zt}{\omega}\right)^p \tag{2.69}$$

After analyzing this series, one deduces that it is absolutely convergent for $\omega < -zt$. Thus for $\omega < -zt$, $(i_{\alpha_i}|i_{\alpha_i})_\omega$ is well defined and so has no pole. Hence, no energy below $-zt$ is allowed.

## 2.4 THE RING-EXCHANGE MECHANISM

Now, one is going to focus one special type of lattice, from which will be deduced some properties of quasi-equivalent physical systems.

To the end, consider the 3-site toy model given in Figure 2.3. Its Hubbard Hamiltonian can be easily written as

$$\begin{aligned}\mathcal{H}_3 = {} & t_2 \sum_\sigma [c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}] + U \sum_{i=1,2} n_{i\uparrow} n_{i\downarrow} \\ & + t_1 \sum_\sigma [c_{1\sigma}^\dagger c_{3\sigma} + c_{2\sigma}^\dagger c_{3\sigma} + c_{3\sigma}^\dagger c_{1\sigma} + c_{3\sigma}^\dagger c_{2\sigma}] \\ & + U_3 n_{3\uparrow} n_{3\downarrow} + \varepsilon_3 \sum_\sigma n_{3\sigma}\end{aligned} \tag{2.70}$$

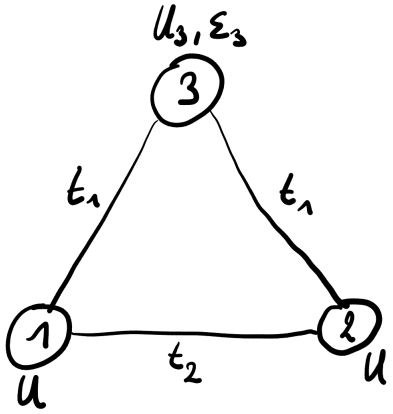


*Figure* 2.3 – Three-site toy model.

The system is considered to be ferromagnetic if its ground state is a triplet, while non-magnetic if it is a singlet. The interest of this three-site toy model is that, for a wide range of parameters, there is a triplet ground state and its ferromagnetism is quite the same as for the Tasaki's 1D chain model shown on Figure 2.4.

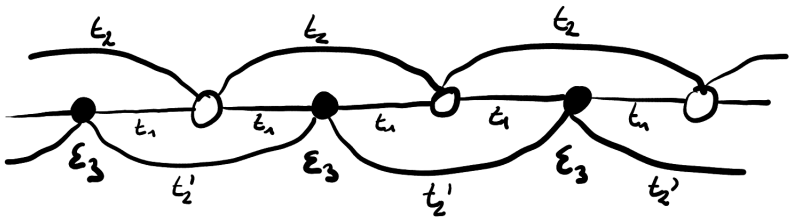


*Figure* 2.4 – Tasaki's 1D chain.

Starting with the case of $1e^-$ which shall be useful later, one can note that the system only has a symmetry with respect to the axis passing through site 3. From this and even without involving group representations theory, one observes that the antisymmetric state

$$|\psi_o\rangle = \frac{1}{\sqrt{2}}[|1\rangle - |2\rangle] \tag{2.71}$$

does not mix with $|3\rangle$. Casting the states in their fermionic form

$$|i\rangle = c^\dagger_{i\sigma}|0\rangle \tag{2.72}$$

labelling $|0\rangle$ the vacuum, one finds the action of the Hamiltonian on $|\psi_o\rangle$ as

$$\begin{aligned}
\mathcal{H}_3\sqrt{2}\,|\psi_o\rangle &= t_2[c^\dagger_{2\sigma}c_{1\sigma}c^\dagger_{1\sigma} - c^\dagger_{1\sigma}c_{2\sigma}c^\dagger_{2\sigma}]\,|0\rangle \\
&\quad + t_1[c^\dagger_{3\sigma}c_{1\sigma}c^\dagger_{1\sigma} - c^\dagger_{3\sigma}c_{2\sigma}c^\dagger_{2\sigma}]\,|0\rangle \\
&= t_2[c^\dagger_{2\sigma}(1 - \cancel{c^\dagger_{1\sigma}c_{1\sigma}}) - c^\dagger_{1\sigma}(1 - \cancel{c^\dagger_{2\sigma}c_{2\sigma}})]\,|0\rangle \\
&\quad + t_1[c^\dagger_{3\sigma}(\cancel{1} - \cancel{c^\dagger_{1\sigma}c_{1\sigma}}) - c^\dagger_{3\sigma}(\cancel{1} - \cancel{c^\dagger_{2\sigma}c_{2\sigma}})]\,|0\rangle \\
&= t_2[|2\rangle - |1\rangle] = -t_2\sqrt{2}\,|\psi_o\rangle
\end{aligned} \tag{2.73}$$

Hence denote $\lambda_0 = -t_2$ its eigenvalue. Performing the same computations for the symmetric state

$$|\psi_e\rangle = \frac{1}{\sqrt{2}}[|1\rangle + |2\rangle] \tag{2.74}$$

that now mixes with $|3\rangle$ as

$$\begin{aligned} \mathcal{H}_3 |\psi_e\rangle &= t_2 |\psi_e\rangle + t_1\sqrt{2}|3\rangle \\ \mathcal{H}_3 |3\rangle &= t_1\sqrt{2}|\psi_e\rangle + \varepsilon_3 |3\rangle \end{aligned} \tag{2.75}$$

Diagonalizing $\mathcal{H}_3$ in the subspace spanned by $\{|\psi_o\rangle, |3\rangle\}$ yields

$$0 = (t_2 - \lambda)(\varepsilon_3 - \lambda) - 2t_1^2 = \lambda^2 - \lambda(t_2 + \varepsilon_3) + t_2\varepsilon_3 - 2t_1^2 \tag{2.76}$$

and then the eigenenergies for the triplet states

$$\lambda_e^{\pm} = \frac{t_2 + \varepsilon_3 \pm \sqrt{(t_2 - \varepsilon_3)^2 + 8t_1^2}}{2} \tag{2.77}$$

Note that one does not care about the sign of $t_1$ since appearing squared. Hence, fix $t_1 > 0$ which can be justified by changing the sign of $t_1$ being equivalent to the canonical transformation $c_{3\sigma}^\dagger \to -c_{3\sigma}^\dagger$, $c_{3\sigma} \to -c_{3\sigma}$.

The case with $2e^-$ is more interesting. Begin with the system for which doubly-occupied sites are forbidden, that is $U = U_3 = \infty$. Use the following notation in the $S^z = 0$ subspace, *eg*

$$|\uparrow\downarrow 0\rangle = c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle \tag{2.78}$$

There are 6 states in total. To find the ground states, it is useful to note that the exchange of 2 spins can be viewed as an exchange in a ring with the hole hopping through the sites as in Figure 2.5, since doubly-occupied sites are impossible.

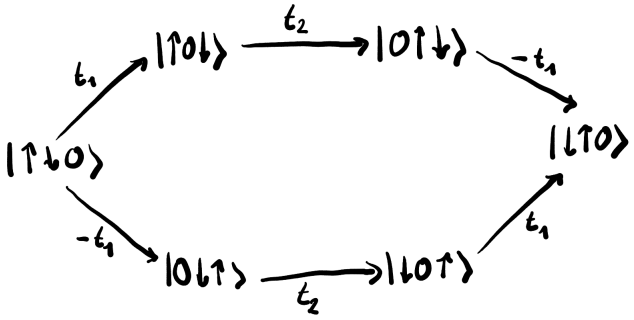


*Figure* 2.5 – Ring exchange mechanism.

It is important to note the sign of the matrix elements since they impose some constraints on the states possible. Using the argument, coming from the Perron-Frobenius theorem, that the sign between 2 states is the opposite of the one of the corresponding matrix element to lower the energy at each hopping process, one finds for $t_2 < 0$

$$|\psi_{GS}\rangle_{t_2<0} = \underbrace{\frac{1}{\sqrt{2}}[|\uparrow\downarrow 0\rangle - |\downarrow\uparrow 0\rangle]}_{|\alpha\rangle} + \underbrace{\frac{\alpha}{2}[|0\downarrow\uparrow\rangle - |0\uparrow\downarrow\rangle + |\downarrow 0\uparrow\rangle - |\uparrow 0\downarrow\rangle]}_{\alpha|\beta\rangle} \tag{2.79}$$

which is made of 3 singlets, thus is a singlet. For $t_2 > 0$

$$|\psi_{GS}\rangle_{t_2>0} = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\, 0\rangle + |\downarrow\uparrow\, 0\rangle] + \frac{\beta}{2}[|0\,\downarrow\uparrow\rangle + |0\,\uparrow\downarrow\rangle - |\downarrow\, 0\,\uparrow\rangle - |\uparrow\, 0\,\downarrow\rangle] \quad (2.80)$$

and this is a triplet. Therefore, one found that the system is ferromagnetic when $U = \infty$ and $t_2 > 0$. It is important to note that for $U = 0$, the ground state is a singlet, thus non-magnetic. This implies that there must exists a phase transition at a finite $U$.

To find the phase boundary, one has to find the energies of the singlet and triplet states and compare them. For the triplet, spins must be parallel then one must take the 2 lowest-energy single $e^-$ states, hence using the previously found eigenenergies

$$\varepsilon_t = \lambda_o + \lambda_e^- = \frac{\varepsilon_3 - t_2 - \sqrt{(t_2 - \varepsilon_3)^2 + 8t_1^2}}{2} \quad (2.81)$$

Then, for the singlet, find the action of $\mathcal{H}_3$ on the singlet pairs, introducing $|\gamma_{12}\rangle = \frac{1}{\sqrt{2}}[c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger + c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger]\,|0\rangle$ and $|\gamma_3\rangle = c_{3\uparrow}^\dagger c_{3\downarrow}^\dagger\,|0\rangle$,

$$\begin{aligned}
\mathcal{H}_3\,|\alpha\rangle &= t_1\sqrt{2}\,|\beta\rangle + 2t_2\,|\gamma_{12}\rangle \\
\mathcal{H}_3\,|\beta\rangle &= t_1\sqrt{2}\,|\alpha\rangle + (t_2 + \varepsilon_3)\,|\beta\rangle + t_1\sqrt{2}\,|\gamma_{12}\rangle + 2t_1\,|\gamma_3\rangle \\
\mathcal{H}_3\,|\gamma_{12}\rangle &= 2t_2\,|\alpha\rangle + t_1\sqrt{2}\,|\beta\rangle + U\,|\gamma_{12}\rangle \\
\mathcal{H}_3\,|\gamma_3\rangle &= 2t_1\,|\beta\rangle + (2\varepsilon_3 + U_3)\,|\gamma_3\rangle
\end{aligned} \quad (2.82)$$

Again, using $U = U_3 = \infty$, diagonalize in the subspace $\{|\alpha\rangle, |\beta\rangle\}$ and find

$$\varepsilon_s = \frac{\varepsilon_3 + t_2 - \sqrt{(t_2 + \varepsilon_3)^2 + 8t_1^2}}{2} \quad (2.83)$$

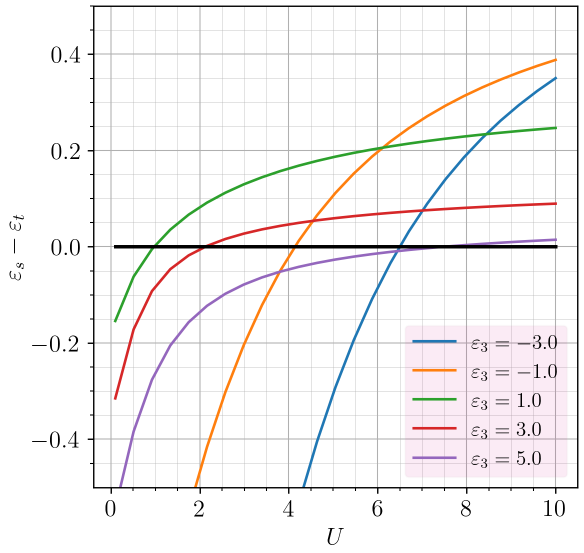


*Figure* 2.6 – Energy difference $\varepsilon_s - \varepsilon_t$ for as a function of $U$ for different values of $\varepsilon_3$.

It is possible although boring to check that $\varepsilon_t < \varepsilon_s$ for $t_2 > 0$, confirming the previous argument. For the full problem, numerical solution gives

finite-U transitions, appearing for smaller U when $\varepsilon_3$ increases, as shown on Figure 2.6. However, $\varepsilon_3$ must stay negative, since when is becomes positive, increasing it seems to make the transition occur at a larger U, as shown on Figure 2.7. This indicates a dependence in the sign and value of $\varepsilon_3$ in the effective Hamiltonian.

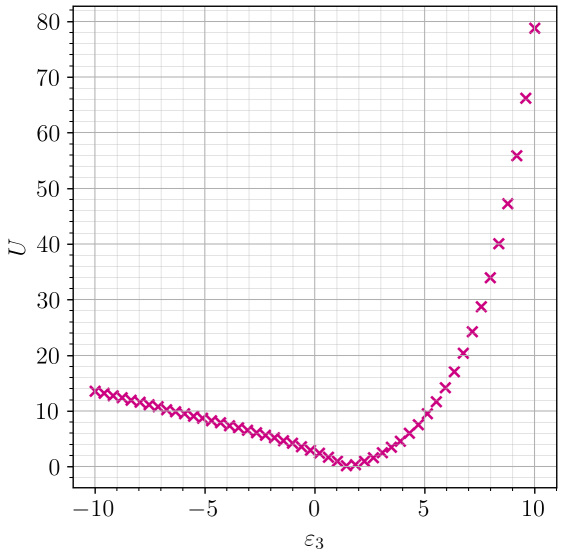


*Figure* 2.7 – Values of U for which the transition occurs as a function of $\varepsilon_3$.

Now, consider the finite case $U > \varepsilon_3 \gg t_1, t_2$, $U_3 = \infty$. The eigenvalue problem can be solved in $\{|\alpha\rangle, |\beta\rangle, |\gamma_{12}\rangle\}$, and expanding in $t_1, t_2$ gives the effective Hamiltonian

$$\mathcal{H}_{\text{eff}} \simeq \underbrace{\left[\frac{4t_2^2}{U} - \frac{4t_2 t_1^2}{\varepsilon_3^2}\right]}_{J} \mathbf{S}_1 \cdot \mathbf{S}_2 \tag{2.84}$$

with J thus coupling constant being defined here as the difference $\varepsilon_t - \varepsilon_s$ up to high orders. The third order term is precisely the ring exchange presented above. And once again, for $U = \infty$ and $t_2 > 0$, the system is ferromagnetic, and for finite U there is a competition between ferromagnetic and antiferromagnetic states.

## 2.5 THE FLAT-BAND FERROMAGNETISM

The flat-band is a version of the Hubbard model that exhibits ferromagnetism. To understand how, introduce d-dimensional $L \times L$ hypercubic lattice with $a = 1$, and another one in the middle of each bond. A $d = 2$ representation is given in Figure 2.8, where u sites do not give any $e^-$ to the system.

Now introduce the fermionic operators corresponding to the single-$e^-$ states around p and u as

$$a_{p\sigma} = c_{p\sigma} - \nu \sum_{u \text{ n.n. to } p} c_{u\sigma} \quad \text{and} \quad b_{u\sigma} = c_{u\sigma} + \nu \sum_{p \text{ n.n. to } u} c_{p\sigma} \tag{2.85}$$

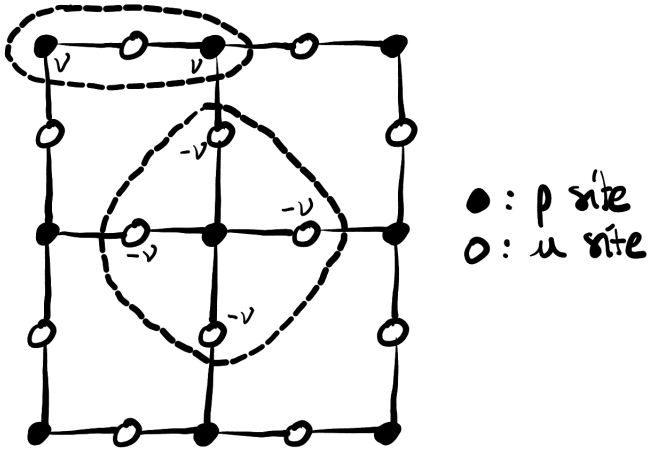


*Figure* 2.8 – Hypercubic lattice in $d = 2$.

Then write the Hamiltonian as

$$\mathcal{H} = \mathcal{H}_{\text{hop}} + \mathcal{H}_{\text{int}} = t \sum_{u,\sigma} b^{\dagger}_{u\sigma} b_{u\sigma} + U \sum_{j} n_{j\uparrow} n_{j\downarrow} \tag{2.86}$$

With this particular form, the hopping term interestingly exhibits the same structure as the 3-site toy model for $d = 1$, since hopping between all n.n. is possible as well as between p sites separated by distance 1. From this, Tasaki's flat-band ferromagnetism follows.

Consider the Hubbard model given in (2.86) with $N = L^d$ $e^-$ , $t, \nu, U > 0$. Then the ground states have $S_{\text{tot}} = \frac{N}{2}$ and are unique apart from the $(2S_{\text{tot}} + 1)$-fold degeneracy.

One is not proving this theorem but shall construct the ground states of this system when half-filled — remember that u sites do not contribute with any $e^-$ . From the orthogonality between u- and p-single-$e^-$ states, one finds $\{b_{u\sigma}, a^{\dagger}_{p\sigma}\} = 0$ — since $\{c_{\sigma}(\psi), c^{\dagger}_{\sigma'}(\psi')\} = \langle \psi | \psi' \rangle \, \delta_{\sigma\sigma'}$ — which implies $[b^{\dagger}_{u\sigma} b_{u\sigma}, a^{\dagger}_{p\sigma}] = 0$. One encourages the reader to check these relations. Therefore

$$\mathcal{H} |\psi^{\uparrow}_{\alpha}\rangle = 0 \quad \text{with} \quad |psi^{\uparrow}_{\alpha}\rangle = \left[ \prod_{p} a^{\dagger}_{p\uparrow} \right] |0\rangle \tag{2.87}$$

since $\mathcal{H}_{\text{hop}}$ is a sum of $b^{\dagger}_{u\sigma} b_{u\sigma}$ and $\mathcal{H}_{\text{int}}$ counts the number of doubly-occupied sites which do not exist when everyone has the same spin. Thus $|\psi^{\uparrow}_{\alpha}\rangle$ is ferromagnetic state of energy 0. This allows to write the ground states as

$$|\psi^{(M)}_{\text{GS}}\rangle = (S^{-}_{\text{tot}})^{\frac{N}{2} - M} |\psi^{\uparrow}_{\alpha}\rangle \quad \text{with} \quad M = -N/2, -N/2 + 1, \ldots, N/2 \tag{2.88}$$

Now, remains to find the band structure and observe that the system indeed exhibits flat-band ferromagnetism. Start by rewriting the Hamiltonian (2.86) with

$$\mathcal{H}_{\text{hop}} = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} \quad \text{with} \quad t_{ij} = \begin{cases} \nu t & \text{if } i,j \text{ n.n.} \\ \nu^2 t & \text{if } i,j \text{ s.n. p sites} \\ t & \text{if } i = j = u \\ 2d\nu^2 t & \text{if } i = j = p \\ 0 & \text{otherwise} \end{cases} \tag{2.89}$$

Then solve the for the single-$e^-$ SE to have the band structure

$$\varepsilon_{\mu}(k) = \begin{cases} 0 & \mu = 1 \\ t & \mu = 2, \dots, d \\ t + 2\nu^2 t \sum_{j=1}^{d} (1 + \cos k_j) & \mu = d+1 \end{cases} \tag{2.90}$$

which is straightforward to derive *eg* in $d = 2$ as

$$\mathcal{H} = \begin{pmatrix} 2\nu^2 t \sum_{j=x,y} (1 + \cos k_j) & \nu t(1 + e^{-ik_x}) & \nu t(1 + e^{-ik_y}) \\ \nu t(1 + e^{ik_x}) & t & 0 \\ \nu t(1 + e^{ik_y}) & 0 & t \end{pmatrix} \tag{2.91}$$

which generates the band structure

$$0 = \varepsilon(t - \varepsilon) \left[ \varepsilon - t - 2\nu^2 t \sum_{j=x,y} (1 + \cos k_j) \right] \tag{2.92}$$

having used the identity $\left|\nu t(1 + e^{ik_j})\right|^2 = 2\nu^2 t^2 (1 + \cos k_j)$. Therefore $d$ bands are flat, the lowest one being non-degenerate with energy $0$ and the other $d - 1$ are degenerate with energy $t$. Thus take the lowest one, which is more interesting since it has $L^d$ states separated from the others by a gap $t > 0$. Hence, for the many $e^-$ problem without interaction $U = 0$ the zero-energy ground states are

$$\left[ \prod_{p \in \{\uparrow\}} a^{\dagger}_{p\uparrow} \right] \left[ \prod_{p \in \{\downarrow\}} a^{\dagger}_{p\downarrow} \right] |0\rangle \tag{2.93}$$

and thereby have spin $S_{\text{tot}} = 0, \frac{1}{2}, \dots, \frac{N}{2} \to$ paramagnetism. But introducing $U > 0$ lifts the degeneracy to select the full ferromagnetic ground state with highest $S_{\text{tot}} = \frac{N}{2}$ to be the only ground state, according to Tasaki's theorem aforementioned.

Finally, it is possible and interesting to relate this to the 3-site toy model since models exhibiting flat-band ferromagnetism are 3-site toy models assemblies !

# 3 SUPERCONDUCTIVITY

## 3.1 t − J MODEL

When a small hopping term $t \ll U$ is switched on, these states are mixed and the sharp atomic level broadens into the lower Hubbard subband. The motion of the $e^-$ is constrained by having to avoid the creation of doubly occupied sites. Now one wishes to describe this in detail. Here one is faced with the basic difficulty of the theory of strongly correlated systems. At the first sight, the solution may seem straightforward since there is a small parameter $t\frac{t}{U} \ll 1$, and one could attempt to treat the effect of $\mathcal{H}_{\text{band}}$ by perturbation theory. However, the task at hand is very different from that of standard perturbation theory which is set up to handle problems with a large single-electron term and a weak interaction. In the present case, the zeroth order term is the interaction term $\mathcal{H}_U$, and the one-$e^-$ term $\mathcal{H}_{\text{band}}$ is the perturbation. In the standard case, the zeroth-order ground state is non-degenerate. Here, the ground state of $\mathcal{H}_U$ has a large degeneracy. Within a degenerate set of levels, even a weak perturbation has a drastic effect. It lifts the degeneracy. There is, however, a well-known way to treat consecutive orders of $\frac{t}{U}$ systematically. It can be accomplished by a suitable canonical transformation. The idea is the following. The zeroth-order eigenstates are mixed by the perturbation $\mathcal{H}_{\text{band}}$. If we knew the true eigenstates, one could do a Hilbert space rotation to that basis, and should not worry about the mixing of states anymore. This full solution is usually not available, and therefore proceed iteratively. In the first step, rotate to a basis whose states are not mixed in order $t$. In the second step, want to avoid mixing in order $t^2$, etc. While this is the general principle, one will be, in fact, content with the lowest-order result.

The Hamiltonian is

$$\mathcal{H} = -t \sum_{\langle ij \rangle} \sum_{\sigma} [c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}] + U \sum_j n_{j\uparrow} n_{j\downarrow} \tag{3.1}$$

Decompose it as

$$\mathcal{H} = \mathcal{H}_{\text{band}} + \mathcal{H}_U \quad \text{and} \quad \mathcal{H}^+_t + \mathcal{H}^-_t + \mathcal{H}^0_t \tag{3.2}$$

Here $\mathcal{H}^+_t$ is the hopping process that increases the number of doubly occupied sites by one, with the notation in terms of projectors for such process

$$P_{j,d} c^\dagger_{j\uparrow} c_{i\uparrow} P_{i\uparrow} = n_{j\uparrow} n_{j\downarrow} c^\dagger_{j\uparrow} c_{i\uparrow} n_{i\uparrow} (1 - n_{i\downarrow}) = n_{j\downarrow} c^\dagger_{j\uparrow} c_{i\uparrow} (1 - n_{i\downarrow}) \tag{3.3}$$

is written as

$$\mathcal{H}^+_t = -t \sum_{\langle ij \rangle} \sum_{\sigma} [n_{i-\sigma} c^\dagger_{i\sigma} c_{j\sigma} (1 - n_{j-\sigma}) + n_{j-\sigma} c^\dagger_{j\sigma} c_{i\sigma} (1 - n_{i-\sigma})] \tag{3.4}$$

and similarly the one that annihilates

$$\mathcal{H}_t^- = -t \sum_{\langle ij \rangle} \sum_{\sigma} [(1 - n_{i-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} n_{j-\sigma} + (1 - n_{j-\sigma}) c_{j\sigma}^\dagger c_{i\sigma} n_{i-\sigma}] \quad (3.5)$$

and the remaining that does creates or annihilates one

$$\mathcal{H}_t^0 = -t \sum_{\langle ij \rangle} \sum_{\sigma} [(1 - n_{i-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} (1 - n_{j-\sigma}) + n_{i-\sigma} c_{j\sigma}^\dagger c_{i\sigma} n_{j-\sigma} + hc] \quad (3.6)$$

Perform a canonical transformation to rotate the Hilbert space and avoid the mixing of the subbands. The effective Hamiltonian obtained is, expanding

$$\begin{aligned} \mathcal{H}_{eff} &= e^{iS} \mathcal{H} e^{-iS} = \mathcal{H} + i[S, \mathcal{H}] + \frac{i^2}{2}[S, [S, \mathcal{H}]] + \cdots \\ &= \mathcal{H}_U + \mathcal{H}_t^+ + \mathcal{H}_t^- + \mathcal{H}_t^0 + i[S, \mathcal{H}_U] + i[S, \mathcal{H}_t^+ + \mathcal{H}_t^- + \mathcal{H}_t^0] \\ &+ \frac{i^2}{2}[S, [S, \mathcal{H}_U]] + \cdots \end{aligned} \quad (3.7)$$

Find $S \sim \frac{t}{U}$ so that $i[S, \mathcal{H}_U]$ eliminates $H_t^+ + \mathcal{H}_t^-$. Hence compute

$$[\mathcal{H}_t^+, \mathcal{H}_U] = -U\mathcal{H}_t^+ \quad \text{and} \quad [\mathcal{H}_t^-, \mathcal{H}_U] = U\mathcal{H}_t^- \quad (3.8)$$

Therefore, one should use

$$S = -\frac{1}{U}(\mathcal{H}_t^+ - \mathcal{H}_t^-) \quad (3.9)$$

because

$$i[S, \mathcal{H}_U] = \frac{1}{U}[\mathcal{H}_t^+ - \mathcal{H}_t^-, \mathcal{H}_U] = -(\mathcal{H}_t^+ + \mathcal{H}_t^-) \quad (3.10)$$

which exactly cancels the pieces wanted. However, there is a new term

$$i[S, \mathcal{H}_t^+ + \mathcal{H}_t^-] = \frac{1}{U}[\mathcal{H}_t^+ - \mathcal{H}_t^-, \mathcal{H}_t^+ + \mathcal{H}_t^-] = \frac{2}{U}[\mathcal{H}_t^+, \mathcal{H}_t^-] \quad (3.11)$$

which is almost compensated with the term

$$\frac{i^2}{2}[S, [S, \mathcal{H}_U]] = \frac{i^2}{2}[S, \mathcal{H}_t^+ + \mathcal{H}_t^-] = -\frac{1}{U}[\mathcal{H}_t^+, \mathcal{H}_t^-] \quad (3.12)$$

Omitting the contribution from $i[S, \mathcal{H}_t^0]$, one finally finds

$$\mathcal{H}_{eff} = \mathcal{H}_t^0 + \mathcal{H}_U + \frac{1}{U}[\mathcal{H}_t^+, \mathcal{H}_t^-] \quad (3.13)$$

Introduce the Hubbard operators like

$$X_j^{\sigma \leftarrow 0} = c_{j\sigma}^\dagger (1 - n_{j\sigma}) \quad (3.14)$$

such that

$$X_j^{c \leftarrow f} X_j^{b \leftarrow a} = \delta_{bf} X_j^{c \leftarrow b} X_j^{b \leftarrow a} = \delta_{bf} X_j^{c \leftarrow a} \quad (3.15)$$

and therefore express

$$c^\dagger_{j\sigma} = X^{\sigma\leftarrow 0}_j + \eta(\sigma) X^{d\leftarrow -\sigma}_j \quad \text{with} \quad \eta(\sigma) \begin{cases} +1 & \sigma = \uparrow \\ -1 & \sigma = \downarrow \end{cases} \tag{3.16}$$

Hence rewrite

$$\mathcal{H}^+_t = -t \sum_{\langle ij \rangle} \sum_\sigma \eta(\sigma) [X^{d\leftarrow -\sigma}_i X^{0\leftarrow \sigma}_j + X^{d\leftarrow -\sigma}_j X^{0\leftarrow \sigma}_i] \tag{3.17}$$

as well as

$$\mathcal{H}^-_t = -t \sum_{\langle ij \rangle} \sum_\sigma \eta(\sigma) [X^{\sigma\leftarrow 0}_i X^{-\sigma\leftarrow d}_j + X^{\sigma\leftarrow 0}_j X^{-\sigma\leftarrow d}_i] \tag{3.18}$$

Now, separate the sub-Hamiltonians, to compute

$$\begin{aligned} [\mathcal{H}^+_t, \mathcal{H}^-_t] &= \sum_{\langle ij \rangle} \sum_{\langle kl \rangle} [\mathcal{H}^+_{t,ij}, \mathcal{H}^-_{t,kl}] \\ &= \sum_{\langle ij \rangle} [\mathcal{H}^+_{t,ij}, \mathcal{H}^-_{t,ij}] + \sum_{\langle ijk \rangle} [\mathcal{H}^+_{t,ij}, \mathcal{H}^-_{t,jk}] \end{aligned} \tag{3.19}$$

with, for only the hopping $i \to j$

$$\begin{aligned} \frac{1}{U} [\mathcal{H}^+_{t,ij}, \mathcal{H}^-_{t,ij}] &= -\frac{1}{U} \mathcal{H}^+_{t,ij} \mathcal{H}^+_{t,ij} \\ &= -\frac{t^2}{U} \sum_{\sigma,\sigma'} \eta(\sigma)\eta(\sigma') [X^{\sigma'\leftarrow 0}_j X^{-\sigma'\leftarrow d}_i X^{d\leftarrow -\sigma'}_i X^{0\leftarrow \sigma}_j] \\ &= -\frac{t^2}{U} \sum_\sigma X^{-\sigma\leftarrow -\sigma}_i X^{\sigma\leftarrow \sigma}_j + \frac{t^2}{U} \sum_\sigma X^{\sigma\leftarrow -\sigma}_i X^{\sigma\leftarrow -\sigma}_j \\ &= \frac{2t^2}{U} \left[ S^z_i S^z_j - \frac{n_i n_j}{4} \right] + \frac{t^2}{U} \left[ S^+_i S^-_j + S^+_j S^-_i \right] \\ &= \frac{2t^2}{U} \left[ \mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right] \end{aligned} \tag{3.20}$$

Hence, in total

$$\begin{aligned} \mathcal{H}_{\text{eff}} &= \mathcal{H}_{t-J} \\ &= -t \sum_{\langle ij \rangle} \sum_\sigma (1 - n_{i-\sigma}) c^\dagger_{i\sigma} c_{j\sigma} (1 - n_{j-\sigma}) + \text{hc} \\ &+ \frac{4t^2}{U} \sum_{\langle ij \rangle} \left[ \mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right] + 3 \text{ sites terms} \end{aligned} \tag{3.21}$$

## 3.2 MEAN-FIELD SUPERCONDUCTIVITY

Approximate the hopping term in the Hamiltonian (3.21) as

$$-t(1 - n_{i-\sigma}) c^\dagger_{i\sigma} c_{j\sigma} (1 - n_{j-\sigma}) \simeq -t\delta c^\dagger_{i\sigma} c_{j\sigma} \tag{3.22}$$

where $\delta$ is the fractional difference of $n$ from the half-filled case that was considered along the previous pages. Hence, the Hamiltonian is

$$\mathcal{H} = -t\delta \sum_{\langle ij \rangle} \sum_{\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + hc) - 2J \sum_{\langle ij \rangle} b^{\dagger}_{ij} b_{ij} \tag{3.23}$$

with the notation in valence bond singlets

$$b^{\dagger}_{ij} = c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow} - c^{\dagger}_{i\downarrow} c^{\dagger}_{j\uparrow} \tag{3.24}$$

BSC theory is quite good, but sometimes fails. In particular, to treat high-$T_C$ superconductivity, one uses mean-field approximation among other methods. Start in the Fourier space

$$\langle b_{ij} \rangle = \sum_{k,q} e^{ikr} e^{iq(r_i+\tau)} \underbrace{\left\langle c^{\dagger}_{k\uparrow} c^{\dagger}_{q\downarrow} - c^{\dagger}_{k\downarrow} c^{\dagger}_{q\uparrow} \right\rangle}_{\delta_{k,-q}\Delta_k} = \sum_{k} e^{-ik\tau} \Delta_k \tag{3.25}$$

that gives the Hamiltonian in the mean-field approximation

$$\mathcal{H} = -2J \sum_{\langle ij \rangle} b_{ij} \left\langle b^{\dagger}_{ij} \right\rangle + b^{\dagger}_{ij} \langle b_{ij} \rangle - \left\langle b^{\dagger}_{ij} \right\rangle \langle b_{ij} \rangle \tag{3.26}$$

The second can be expressed as, since there is no dependence on the sites $i$ and $j$, thus take the site $0$,

$$\begin{aligned}
&-2J\frac{1}{2} \sum_{i,\tau} \langle b_{0\tau} \rangle \left[ c^{\dagger}_{i\uparrow} c^{\dagger}_{i+\tau\downarrow} - c^{\dagger}_{i\downarrow} c^{\dagger}_{i+\tau\uparrow} \right] \\
&= -J \sum_{i,\tau,h,q} [\sum_{k'} e^{-ik'\tau} \Delta_{k'}] e^{ikr} e^{iq(r_i+\tau)} [c^{\dagger}_{k\uparrow} c^{\dagger}_{q\downarrow} - c^{\dagger}_{k\downarrow} c^{\dagger}_{q\uparrow}] \\
&= -2JN \sum_{\tau,k,k'} e^{i(k-k')\tau} \Delta_{k'} c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} \\
&= -4N \sum_{k,k'} V_{k,k'} \Delta_{k'} c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow}
\end{aligned} \tag{3.27}$$

with the introduction of

$$V_{k,k'} = \frac{J}{2} \sum_{\tau} e^{i(k-k')\tau} \tag{3.28}$$

The third term is expressed as

$$-2J\frac{1}{2} \sum_{i,\tau} e^{i(k-k')\tau} \Delta^{*}_{k} \Delta_{k'} = 2N \sum_{k,k'} V_{k,k'} \Delta^{*}_{k} \Delta_{k'} \tag{3.29}$$

Adding a term with chemical potential $\mu$

$$\mathcal{H}_{\mu} = \mu \sum_{i} c^{\dagger}_{i\sigma} c_{i\sigma} \tag{3.30}$$

Therefore, regroup all the term to get

$$\begin{aligned}
\mathcal{H} = &\sum_{k,\sigma} [\varepsilon_k - \mu] c^{\dagger}_{k\sigma} c_{k\sigma} - 4N \sum_{k,k'} [V_{k,k'} c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} + hc] \\
&+ 2N \sum_{k,k'} V_{k,k'} \Delta^{*}_{k} \Delta_{k'}
\end{aligned} \tag{3.31}$$

with $\varepsilon_k = -2\delta t(\cos k_x + \cos k_y)$.

Perform a Bogoliubov transformation to get

$$\mathcal{H} = \sum_{k,\sigma} E_k \left[\alpha^\dagger_{k\sigma}\alpha_{k\sigma} - \frac{1}{2}\right] + 2N\sum_{k,k'} V_{k,k'}\Delta^*_k\Delta_{k'} \tag{3.32}$$

with

$$E_k = \sqrt{(\varepsilon_k - \mu)^2 + \left|\tilde{\Delta}_k\right|^2} \quad \text{and} \quad \tilde{\Delta}_k = 4N\sum_{k'} V_{k,k'}\Delta_{k'} \tag{3.33}$$

The ground state of such model is

$$\begin{aligned} |GS\rangle &= \mathcal{P}_N \prod_k (u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{k\downarrow})\,|0\rangle \\ &= \mathcal{P}_N (b^\dagger)^N\,|0\rangle \end{aligned} \tag{3.34}$$

with

$$b^\dagger = \sum_{r,n} c^\dagger_{r\uparrow} c^\dagger_{r+n\downarrow} \tag{3.35}$$

which corresponds to a resonating valence bond state.

To derive the self-consistent equation, compute the partition function

$$\begin{aligned} Z &= \operatorname{tr} e^{-\beta\mathcal{H}} \\ &= e^{-2\beta N\sum_k \tilde{\Delta}_k\Delta^*_k} \operatorname{tr} e^{\beta\sum_{k,\sigma} E_k(\alpha^\dagger_{k\sigma}\alpha_{k\sigma} - \frac{1}{2})} \\ &= e^{-2\beta N\sum_k \tilde{\Delta}_k\Delta^*_k} \underbrace{e^{\beta\sum_{k,\sigma} E_k} \prod_k [1 + e^{-\beta E_k}]^2}_{\prod_k [e^{\frac{\beta E_k}{2}} + e^{-\frac{\beta E_k}{2}}]^2} \\ &= 4^N e^{-2\beta N\sum_k \tilde{\Delta}_k\Delta^*_k} \prod_k \cosh^2\frac{\beta E_k}{2} \end{aligned} \tag{3.36}$$

and the free energy is written

$$\begin{aligned} F &= -k_B T \ln Z \\ &= -2BT\ln 2 + 2N\sum_k \tilde{\Delta}_k\Delta^*_k - 2k_B T\sum_k \ln\cosh\frac{\beta E_k}{2} \end{aligned} \tag{3.37}$$

Thus, try to minimize the free energy

$$\begin{aligned} \frac{\partial F}{\partial\Delta^*_q} &= 0 \\ &= 2N\tilde{\Delta}_q - 2k_B T\sum_k \tanh\frac{\beta E_k}{2}\frac{\beta}{2}\frac{\partial E_k}{\partial\Delta^*_q} \\ &= 8N^2\sum_k \left[\delta_k - \sum_{k'} V_{k,k'}\Delta_{k'}\frac{\tanh\frac{\beta E_{k'}}{2}}{2E_{k'}}\right] V_{k,q} \end{aligned} \tag{3.38}$$

Therefore the self-consistent equation

$$\Delta_k = \sum_{k'} V_{k,k'}\Delta_{k'}\frac{\tanh\frac{\beta E_{k'}}{2}}{2E_{k'}} \tag{3.39}$$

which has general solution

$$\Delta_k = sc_0 + dc_2 \quad \text{with} \quad s, d \in \mathbb{C} \tag{3.40}$$

and with

$$c_0 = \cos k_x + \cos k_y \quad \text{and} \quad c_2 = \cos k_x - \cos k_y \tag{3.41}$$

representing the s- and d-waves that are cubic harmonics. Actually, the d-waves have higher $T_C$ and turn out to be useful under such considerations. Near criticality

$$\Delta = \sum_{k'} V_{k,k'} \Delta_{k'} \frac{\tanh \frac{\varepsilon_{k'} - \mu}{2k_B T_C}}{2(\varepsilon_{k'} - \mu)} \tag{3.42}$$

and the coupling constant becomes

$$\frac{1}{J} = \sum_{k'} \frac{c_i(k')}{2(\varepsilon_{k'} - \mu)} \tanh \frac{\varepsilon_{k'} - \mu}{2k_B T_C} \quad \text{with} \quad i = 0, 2 \tag{3.43}$$

At half-filling, the s- and d-wave have the same J. But close to half-filling, the d-wave solution has higher $T_C$.

At low temperatures, the free energy is

$$F = \frac{1}{J}[|s|^2 + |d|^2] - 2k_B T \sum_k \ln \cosh \frac{\beta E_k}{2} \tag{3.44}$$

and the energy

$$E_k^2 = (\varepsilon_{k'} - \mu)^2 + |s|^2 c_0^2 + |d|^2 c_2^2 + 2sd \cos\theta c_0(k) c_2(k) \tag{3.45}$$

with $\theta$ the relative phase between s and d. The energetically favorable configuration is for $\theta = \frac{\pi}{2}$. At half-filling and $T = 0$, $|s| = |d|$, one has

$$\Delta_k = \cos k_x + i \cos k_y \tag{3.46}$$

# 4 VALENCE BOND STATES

## 4.1 PARENT HAMILTONIAN

The usual procedure in approaching a problem is by taking its Hamiltonian, then do some perturbation theory to find the ground state of the system. The procedure of the parent Hamiltonian is to take a state $|\psi\rangle$ that one wants to be a ground state, from which a parent Hamiltonian will be inferred. The procedure to recover this Hamiltonian is to consider a set of operators $\{Q_\Gamma\}$ such that

$$Q_\Gamma |\psi\rangle = 0 \ \forall \Gamma \tag{4.1}$$

which would lead to the wanted Hamiltonian

$$\mathcal{H} = \sum_\Gamma Q_\Gamma \tag{4.2}$$

If one associates to $Q_\Gamma$ eigenvectors $\left|\psi_i^\Gamma\right\rangle$ forming a complete basis with eigenvalues $\lambda_i^\Gamma \geqslant 0$ – which is a correct assumption since $Q_\Gamma$ are projectors – then

$$\begin{aligned} \langle\phi|\mathcal{H}|\phi\rangle &= \sum_\Gamma \langle\phi|Q_\Gamma|\phi\rangle \\ &= \sum_\Gamma \sum_i \left\langle\phi\middle|Q_\Gamma\middle|\psi_i^\Gamma\right\rangle \left\langle\psi_i^\Gamma\middle|\phi\right\rangle \\ &= \sum_\Gamma \sum_i \lambda_i^\Gamma \left|\left\langle\psi_i^\Gamma\middle|\phi\right\rangle\right|^2 \geqslant 0 \end{aligned} \tag{4.3}$$

This means that $|\psi\rangle$ is a ground state but not if it is unique.

The parent Hamiltonian may differ from the physical model, but serves to bring a light to the relations between interactions and the ground state correlations. This concept has to be tied with the variational principle since the ground state wavefunction is not analytically known for most Heisenberg models.

## 4.2 VALENCE BOND

A valence bond state is a variational wavefunction for the antiferromagnetic Heisenberg model. This is a singlet state $|\psi_i^j\rangle$ which connects two spin-$\frac{1}{2}$ particles between sites $i$ and $j$ and thus minimizes the Heisenberg coupling. A valence bond configuration, or a dimer covering, is a tensor product of valence bond states. Examples of valence bond configurations are given in Figure 4.1 and Figure 4.2. Hence, Figure 4.1 shows a 1D configuration out of 2 possible, and Figure 4.2 a 2D one out of many. A configuration

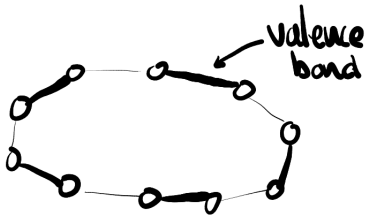


*Figure* 4.1 – Example of valence bond configuration in 1D.

has $\mathbf{S}^2_{tot} = S_{tot}(S_{tot}+1) = 0$. Also, there is in general a non-zero overlap between possible configurations.

A general valence bond state is written as

$$|\{c_\alpha\}, S\rangle = \sum_\alpha c_\alpha |\alpha\rangle \tag{4.4}$$

where $c_\alpha$ are variational parameters and $\alpha$ valence bond configuration, written as

$$|\alpha\rangle = \prod_{(ij)\in\Lambda_\alpha} [a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger]\,|0\rangle \tag{4.5}$$

with $a_i, b_i$ Schwinger bosons on site $i$ and $\Lambda_\alpha$ a particular configuration of bonds $(ij)$ on the lattice. Note that $S$ here can take any value, but one will always be able to decompose the configurations so that one can take $S = \frac{1}{2}$ in the end.

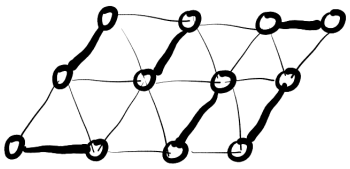

*Figure* 4.2 – Example of valence bond configuration in 2D.

The sum in (4.4) in certain cases in the large lattice limit, is made over a finite number of configurations. These cases where there are many configuration in (4.4) are denoted as resonating valence bond sates.

## 4.3 THE MAJUMDAR–GHOSH HAMILTONIAN

Consider a L unit cells 1D chain of spin-$\frac{1}{2}$ alternate pairs of sites just as in Figure 4.1. They are in a singlet state with boundary $\mathbf{S}_{L+1} = \mathbf{S}_1$

$$|d_\pm\rangle = \bigotimes_{i=1}^{L/2} \frac{1}{\sqrt{2}} \left[|\uparrow\rangle_{2i}\,|\downarrow\rangle_{2i\pm1} - |\downarrow\rangle_{2i}\,|\uparrow\rangle_{2i\pm1}\right] \tag{4.6}$$

which are the only two possible configurations. The goal is to kill these states under the action of a parent Hamiltonian. To do so, find the projector of the subspace $J = \frac{3}{2}$ so that

$$\mathcal{P}_{\frac{3}{2}}(i-1, i, i+1)\,|d_\pm\rangle = 0 \tag{4.7}$$

where one considers $\mathbf{J} = \mathbf{S}_{i-1} + \mathbf{S}_i + \mathbf{S}_{i+1}$ and thus here $J = \frac{1}{2}, \frac{3}{2}$. Since the total spin must vanish on the $z$-sector, the only possibility is to have $J = \frac{1}{2}$. The eigenvalues of $\mathbf{J}^2 = J(J+1)$ and the projectors are presented more intuitively in Table 4.1. Hence, one can think to take

| | $J(J+1)$ | $\mathcal{P}_{\frac{1}{2}}$ | $\mathcal{P}_{\frac{3}{2}}$ |
|---|---|---|---|
| $J = \frac{1}{2}$ | $\frac{3}{4}$ | 1 | 0 |
| $J = \frac{3}{2}$ | $\frac{15}{4}$ | 0 | 1 |

*Table* 4.1 – Intuitive representation of the J subspaces and their projectors.

$$\mathcal{P}_{\frac{3}{2}} \propto \mathbf{J}^2 - \frac{3}{4} \tag{4.8}$$

and noting that $\frac{15}{4} - \frac{3}{4} = 3$, one can write

$$\mathcal{P}_{\frac{3}{2}} = \frac{1}{3}\left[\mathbf{J}^2 - \frac{3}{4}\right] \tag{4.9}$$

Therefore, substitute the expression for $\mathbf{J}$ and expand to find

$$\mathcal{P}_{\frac{3}{2}} = \frac{1}{2} + \frac{2}{3}\left[\mathbf{S}_{i-1}\cdot\mathbf{S}_i + \mathbf{S}_{i-1}\cdot\mathbf{S}_{i+1} + \mathbf{S}_i\cdot\mathbf{S}_{i+1}\right] \tag{4.10}$$

enabling to find the Majumdar-Ghosh Hamiltonian

$$\begin{aligned}\mathcal{H}_{MG} &= \sum_{i=1}^{L} \mathcal{P}_{\frac{3}{2}}(i-1, i, i+1) \\ &= \frac{L}{2} + \frac{4}{3}\sum_{i=1}^{L}\left[\mathbf{S}_i\cdot\mathbf{S}_{i+1} + \frac{1}{2}\mathbf{S}_i\cdot\mathbf{S}_{i+2}\right]\end{aligned} \tag{4.11}$$

which by construction gives

$$\mathcal{H}_{MG}\,|d_\pm\rangle = 0 \tag{4.12}$$

Now take the state

$$|\phi_\pm\rangle = \frac{1}{\sqrt{2}}\left[|d_+\rangle \pm |d_-\rangle\right] \tag{4.13}$$

which is correctly normalized only for $N \to \infty$. To show this, first introduce the loop covering. This is presented on Figure 4.3, where one loop is shown. In general, a loop $\Gamma$ is set to have a length $2L(\Gamma)$ which is an even number of links. For a loop of length $2L(\Gamma)$, only Néel states contribute. There are two of them since flipping spin at each site also give the same loop. Each state has a weight $2^{-L(\Gamma)}$ from the singlet normalization. Hence, the overlap between states $|\alpha\rangle$ and $|\beta\rangle$ is

$$\langle\alpha|\beta\rangle = \prod_\Gamma 2\cdot 2^{-L(\Gamma)} = 2^{\sum_\Gamma 1} 2^{-\frac{1}{2}\sum_\Gamma 2L(\Gamma)} \tag{4.14}$$

Now, by seeing that $N = \sum_\Gamma 2L(\Gamma)$ and writing the number of loops as $p(|\alpha\rangle, |\beta\rangle)$, one gets

$$\langle\alpha|\beta\rangle = 2^{p(|\alpha\rangle,|\beta\rangle)-\frac{N}{2}} \xrightarrow{N\to\infty} 0 \tag{4.15}$$

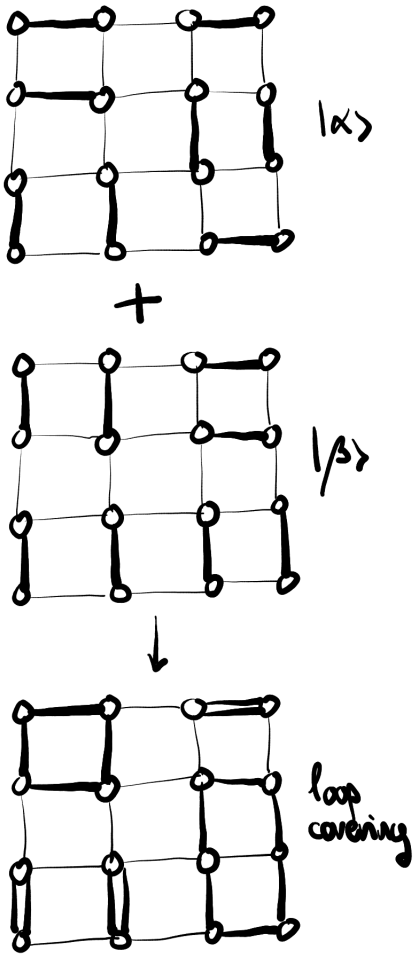


*Figure* 4.3 – Example of a loop covering by the overlap of two valence bond configurations on a 2D square spin-$\frac{1}{2}$ lattice.

For the case of Majumdar-Ghosh states, ones finds $p(|d_+\rangle, |d_-\rangle) = 1$ and thus

$$\langle d_+|d_-\rangle = 2^{1-\frac{N}{2}} \xrightarrow{N\to\infty} 0 \tag{4.16}$$

Now seek for the expectation values of the spin correlations and find in the thermodynamic limit $N \to \infty$

$$\langle \phi_\pm|\mathbf{S}_i \cdot \mathbf{S}_j|\phi_\pm\rangle = \frac{1}{2}\left[2 \cdot \frac{3}{4}\delta_{i,j} - \frac{3}{4}\delta_{|i-j|,1}\right] \tag{4.17}$$

This can be found as follows. The $\frac{1}{2}$ in front comes from the normalization of the $|\phi_\pm\rangle$. For $i = j$, one has $\mathbf{S}^2 = S(S+1) = \frac{3}{4}$ and the factor 2 comes from the 2 states $|d_\pm\rangle$ appearing in the definition of $|\phi_\pm\rangle$. For $|i-j|, 1$, only one of $|d_\pm\rangle$ contributes to gives $-\frac{3}{4}$, which can be easily computed using the definition (4.6) and the fact that

$$\mathbf{S}_i \cdot \mathbf{S}_j = S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \tag{4.18}$$

with the operators acting like

$$S^z|\sigma\rangle = \sigma|\sigma\rangle, \quad S^x|\sigma\rangle = |\sigma|-\sigma\rangle, \quad S^y|\sigma\rangle = i\sigma|-\sigma\rangle \tag{4.19}$$

For instance, consider only the $z$-component

$$\begin{aligned} S_i^z S_j^z \left|d\right\rangle_+ = \cdots \otimes \frac{1}{\sqrt{2}} \left[ -\frac{1}{2} \left|\uparrow\right\rangle_{i-1} \left|\downarrow\right\rangle_i - \frac{1}{2} \left|\downarrow\right\rangle_{i-1} \left|\uparrow\right\rangle_i \right] \otimes \cdots \\ \otimes \frac{1}{\sqrt{2}} \left[ -\frac{1}{2} \left|\uparrow\right\rangle_{j-1} \left|\downarrow\right\rangle_j - \frac{1}{2} \left|\downarrow\right\rangle_{j-1} \left|\uparrow\right\rangle_j \right] \otimes \cdots \end{aligned} \tag{4.20}$$

Therefore, taking $\langle d_+|$ one finds what expected depending one the value of $i$ and $j$. Hence it is easy to see that there is no contribution when $|i-j| \geqslant 2$.

Overall, this is manifest of a short-range correlations, characteristic of spin liquids. This is sometimes called spin-Peierls system.

## 4.4 AKLT MODEL

To goal is to construct a spin-1 wavefunction which creates spin-$\frac{1}{2}$ singlets on all bounds of a chain, and is the ground state of a Hamiltonian looking like the spin-1 Heisenberg model. The chain can be decomposed into singlet pairs as in Figure 4.4, where one can go from the singlet chain to the spin-1 one by applying the symmetrization operator on two neighboring ends of valence bonds, which gives state of spin $S = 1$. But start by working in the

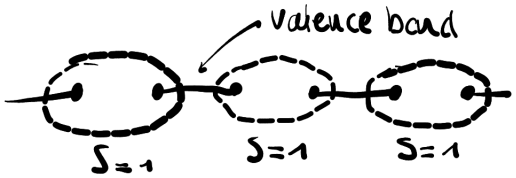


*Figure* 4.4 – Example of a decomposition of a spin-1 lattice into a product of valence bonds.

Schwinger-bosons representation

$$S^+ = a^\dagger b, \quad S^- = b^\dagger a, \quad S^z = \frac{1}{2}\left[a^\dagger a - b^\dagger b\right] \tag{4.21}$$

with each boson satisfying the SU(2) commutation relations, that is

$$[S^+, S^-] = 2S^z, \quad [S^\pm, S^z] = \pm S^\pm \tag{4.22}$$

which can be easily checked. Also, imposing the constraint

$$2S = a^\dagger a + b^\dagger b \tag{4.23}$$

one can arrive at finding

$$\mathbf{S}^2 = S(S+1) \tag{4.24}$$

Moreover, it can be shown that the state consisting of two spins-$\frac{1}{2}$ at $i$ and $j$

$$|\phi\rangle = \frac{1}{\sqrt{2}}\left[a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger\right]|0\rangle \tag{4.25}$$

is the singlet, since it is correctly normalized, that

$$S^-_{tot}\,|\phi\rangle = (S^-_i + S^-_j)\,|\phi\rangle = 0 \tag{4.26}$$

and that

$$S^z_{tot}\,|\phi\rangle = (S^z_i + S^z_j)\,|\phi\rangle = 0 \tag{4.27}$$

which can be rapidly recovered by noting that there is always 1 $a$ and 1 $b$, and that $S^z_{tot}$ is counting the number of $a$ minus the number of $b$ at both sites. Hence introduce

$$|\psi_{VBS}\rangle = 2^{-\frac{N}{2}} \prod_i \left[a^\dagger_i b^\dagger_{i+1} - b^\dagger_i a^\dagger_{i+1}\right] |0\rangle \tag{4.28}$$

which corresponds to one spin-1 per site. Indeed, the wavefunction has either a factor $a^\dagger_i a^\dagger_i$, $a^\dagger_i b^\dagger_i$ or $b^\dagger_i b^\dagger_i$, thus is an eigenstate of $a^\dagger_i a_i + b^\dagger_i b_i$ with eigenvalue 2.

Now one look for the parent Hamiltonian of which $|\psi_{VBS}\rangle$ is the ground state. Start by noticing that for a pair of spin-1

$$S \otimes S = 1 \otimes 1 = 0 \oplus 1 \oplus 2 \tag{4.29}$$

that are the subspaces of J, and that the wavefunction contains singlets, thus spin-2 is impossible. Now take again the bond spin

$$\mathbf{J}_{i,i+1} = \mathbf{S}_i + \mathbf{S}_{i+1} \tag{4.30}$$

Recalling the scheme of Table 4.1, one can find easily

$$\mathcal{P}_2 = \frac{1}{24}\mathbf{J}^2(\mathbf{J}^2 - 2) \tag{4.31}$$

since one must construct the Hamiltonian with $\mathcal{P}_2$ such that

$$\mathcal{P}_2(i, i+1)\,|\psi_{VBS}\rangle = 0 \tag{4.32}$$

Hence, noting that in this case

$$\mathbf{J}^2_{i,i+1} = 4 + 2\mathbf{S}_i \cdot \mathbf{S}_{i+1} \tag{4.33}$$

the parent AKLT Hamiltonian is found as

$$\begin{aligned} \mathcal{H}^{AKLT} &= \sum_{i=1}^{N} \mathcal{P}_2(i, i+1) \\ &= \frac{N}{3} + \frac{1}{2}\sum_{i=1}^{N}\left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2\right] \end{aligned} \tag{4.34}$$

where the constant term can often be omitted and the factor in front of the sum too. Note that the first term is the Heisenberg Hamiltonian and the second is a biquadratic interaction that can somehow be seen as a perturbation.

For the more general case with spin S, taking $M = \frac{2S}{z}$ and the 1D lattice, the valence bond solid is

$$|\psi_{VBS}\rangle = \prod_{\langle ij\rangle} \left[a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger\right]^M |0\rangle \tag{4.35}$$

The last paragraphs are obtained considering a correct normalization and $S = M = 1$. One can see that for $m = 0, 1, \ldots, \mathbf{S}_i \cdot \mathbf{S}_j$

$$\left(\mathbf{S}_i \cdot \mathbf{S}_j\right)^m = \sum_{J=0}^{2S} \left[\frac{1}{2}J(J+1) - S(S+1)\right]^m \mathcal{P}_J(i,j) \tag{4.36}$$

which can be inverted to find

$$\mathcal{P}_J(i,j) = \prod_{k=0,\ k\neq J}^{2S} \frac{2\mathbf{S}_i \cdot \mathbf{S}_j + 2S(S+1) - k(k+1)}{J(J+1) + k(k+1)} \tag{4.37}$$

As before, projecting on the subspace

$$J_{ij} > J_{max} = 2S - M \tag{4.38}$$

gives zero, so that the projector one seeks for are those. Indeed, $J^z_{max} = 2S - M$ is the maximal eigenvalue on $|\psi_{VBS}\rangle$ by counting the maximal number of $a^\dagger$ minus $b^\dagger$ in it. Since $|\psi_{VBS}\rangle$ is a singlet due to th product of singlets, it is rotationally invariant and thus if $J > J^z_{max}$, a global rotation would lead to a possible $J^z = J$ which is impossible. Thus $J^z_{max} = J_{max}$. This implies that the general parent Hamiltonian is

$$\mathcal{H}^{AKLT} = \sum_{\langle ij\rangle} \sum_{J=2S-M+1}^{2S} K_J \mathcal{P}_J(i,j) \quad \text{with} \quad K_J \geqslant 0 \tag{4.39}$$

## 4.5 SPIN CORRELATIONS

To calculate the spin correlations of the valence bond state (4.35), introduce the spin coherent states, created by applying the SU(2) rotation operator to the maximally polarized state

$$\begin{aligned} \left|\hat{\Omega}\right\rangle &= \mathcal{R}(\chi,\vartheta,\phi)\,|S,S\rangle \\ &= e^{iS^z\phi} e^{iS^y\vartheta} e^{iS^x\chi}\,|S,S\rangle \end{aligned} \tag{4.40}$$

where $\hat{\Omega} = (\cos\phi\sin\vartheta, \sin\phi\sin\vartheta, \cos\vartheta)$ is the unit vector is spherical coordinates. Thus $\chi$ is a gauge freedom. Schwinger bosons transform as

$$\begin{aligned} \begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix}' &= \mathcal{R} \begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix} \mathcal{R}^{-1} \\ &= \begin{pmatrix} u e^{i\chi/2} & v e^{i\chi/2} \\ -v^* e^{-i\chi/2} & u^* e^{-i\chi/2} \end{pmatrix} \begin{pmatrix} a^\dagger \\ b^\dagger \end{pmatrix} \end{aligned} \tag{4.41}$$

with

$$u = \cos\frac{\vartheta}{2} e^{i\phi/2} \quad \text{and} \quad v = \sin\frac{\vartheta}{2} e^{-i\phi/2} \tag{4.42}$$

found by expanding the exponential and making use of the fact that bosons here are eigenoperators of the spin ones. Then the coherent states

$$\begin{aligned}\left|\hat{\Omega}\right\rangle &= e^{iS\chi}\frac{(a^{\dagger\prime})^{2S}}{\sqrt{(2S)!}}\left|0\right\rangle \\ &= e^{iS\chi}\frac{(ua^{\dagger}+vb^{\dagger})^{2S}}{\sqrt{(2S)!}}\left|0\right\rangle \\ &= e^{iS\chi}\sqrt{(2S)!}\sum_{m}\frac{u^{S+m}v^{S-m}}{\sqrt{(S+m)!(S-m)!}}\left|S,m\right\rangle\end{aligned} \tag{4.43}$$

where in general

$$\left|S,m\right\rangle = \frac{(a^{\dagger})^{S+m}}{\sqrt{(S+m)!}}\frac{(b^{\dagger})^{S-m}}{\sqrt{(S-m)!}}\left|0\right\rangle \tag{4.44}$$

This allows to express the correlations as a classical statistical mechanics average. First

$$\begin{aligned}\left\langle\hat{\Omega}\middle|\psi_{VBS}\right\rangle &= \sqrt{(2S)!}\prod_{\langle ij\rangle}(u_i v_j - v_i u_j)^M \\ &= \sqrt{(2S)!}\prod_{\langle ij\rangle}\left(\frac{1-\hat{\Omega}_i\cdot\hat{\Omega}_j}{2}\right)^{\frac{M}{2}}\end{aligned} \tag{4.45}$$

Therefore, the spin correlations are

$$\begin{aligned}\langle\psi_{VBS}|\mathbf{S}_i\cdot\mathbf{S}_j|\psi_{VBS}\rangle = \frac{(S+1-\delta_{ij})(S+1)}{Z} \\ \cdot\int\prod_i d\hat{\Omega}_i\ \left|\left\langle\hat{\Omega}\middle|\psi_{VBS}\right\rangle\right|^2\hat{\Omega}_i\cdot\hat{\Omega}_j\end{aligned} \tag{4.46}$$

with the partition function

$$Z = \int\prod_i d\hat{\Omega}_i\ \left|\left\langle\hat{\Omega}\middle|\psi_{VBS}\right\rangle\right|^2 \tag{4.47}$$

In 1D, it is possible to compute

$$\langle\psi_{VBS}|\mathbf{S}_0\cdot\mathbf{S}_n|\psi_{VBS}\rangle = \begin{cases}(-1)^n(S+1)^2e^{-\xi(S)|n|} & n\neq 0\\ S(S+1) & n=0\end{cases} \tag{4.48}$$

with

$$\xi(S) = \ln\left(1+\frac{2}{S}\right) \tag{4.49}$$

This means that there is no long-range order. Thus, due to short-range order, the valence bonds states in 1D and 2D describe quantum spin liquids, by Mermin-Wagner theorem. In 3D, for $M$ large enough, it can be expected that the classical Hamiltonian produces long-range antiferromagnetic order, even giving rotationally invariant states.

# 5 KITAEV MODEL

## 5.1 MODEL

Consider a spin-$\frac{1}{2}$ honeycomb lattice as shown of Figure 5.1. Separate it into two sublattices, even and odd. Links between vertices are divided into $x$, $y$ and $z$ one. The Hamiltonian is then written as

$$\mathcal{H} = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z \tag{5.1}$$

with Pauli matrices. Introduce a special notation

$$K_{jk} = \begin{cases} \sigma_j^x \sigma_k^x & \text{if } (jk) \text{ is a } x\text{-link} \\ \sigma_j^x \sigma_k^y & \text{if } (jk) \text{ is a } y\text{-link} \\ \sigma_j^x \sigma_k^z & \text{if } (jk) \text{ is a } z\text{-link} \end{cases} \tag{5.2}$$

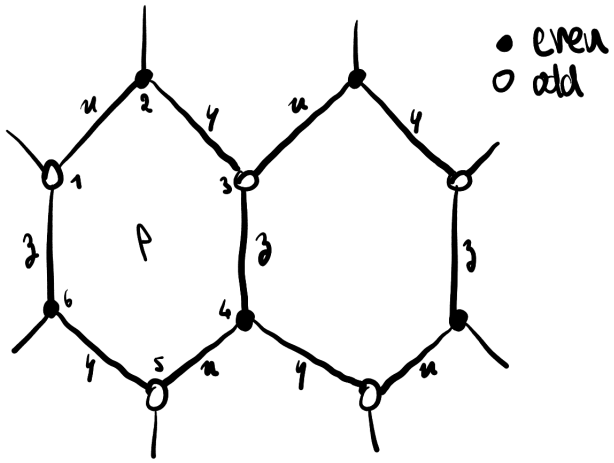


*Figure* 5.1 – Representation of the Honeycomb lattice with the specific notation for the Kitaev model.

Introduce also operators associated to lattice plaquettes $p$

$$\begin{aligned} W_p &= \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z \\ &= -\sigma_1^z \sigma_2^z \sigma_2^x \sigma_3^x \sigma_4^x \sigma_4^y \sigma_5^y \sigma_5^z \sigma_6^z \sigma_6^y \sigma_1^y \\ &= K_{12} K_{23} K_{34} K_{45} K_{56} K_{61} \end{aligned} \tag{5.3}$$

with labeling as in Figure 5.2. It is obvious that

$$[W_{p_1}, W_{p_2}] = 0 \quad \forall p_1 \neq p_2 \tag{5.4}$$

and the commutation with the Hamiltonian

$$[\mathcal{H}, W_p] = 0 \quad \forall p \tag{5.5}$$

follow from the anticommutation relations of the Pauli matrices with same index, and noticing that there are two matrices from $\mathcal{H}$ that effectively anti-commute within $W_p$.

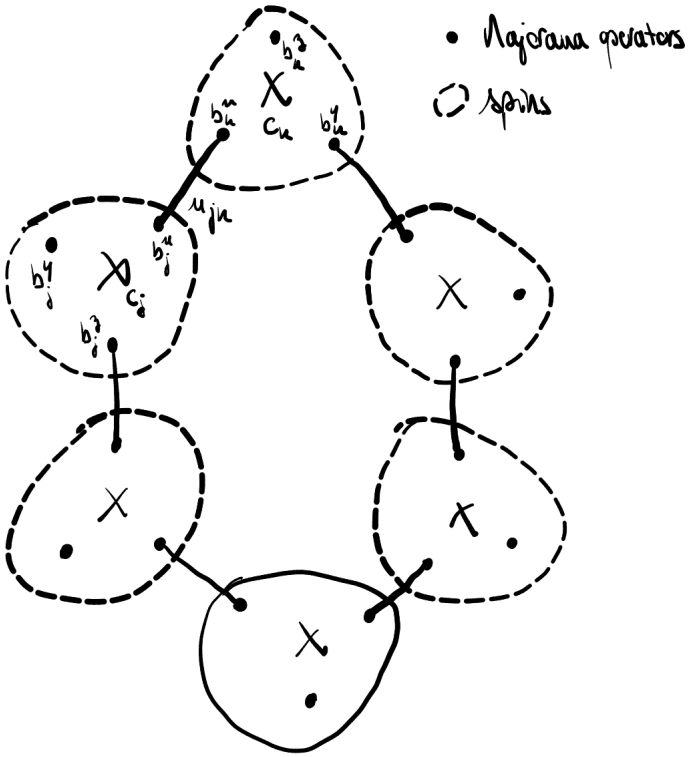


*Figure* 5.2 – Representation of the Hamiltonian of the Kitaev model on the Honeycomb lattice with Majorana operators.

To find the eigenstates of the Hamiltonian, divide the total Hilbert space $\mathcal{L}$ into sectors — eigenspaces of $W_p$ — which are invariant subspaces of $\mathcal{H}$

$$\mathcal{L} = \bigoplus_{w_1,\dots,w_m} \mathcal{L}_{w_1,\dots,w_m} \tag{5.6}$$

with $m$ the number of plaquettes and $w_p = \pm 1$ the eigenvalues of $W_p$, hence remains to solve in a particular sector $\mathcal{L}_{w_1,\dots,w_m}$. Writing as $n$ the number of vertices, there is approximately $\frac{1}{2}$ plaquette per vertex, thus $n = 2m$, and the dimension of each sector $\mathcal{L}_{w_1,\dots,w_m}$ is $2^{\frac{n}{2}}$. It can be seen that the degrees of freedom within each sector can be described by Majorana fermions, writing the restricted Hamiltonian as a quadratic form in Majorana operators.

## 5.2 SPINS AS MAJORANA OPERATORS

Usual systems are described by fermionic operators $a_k$, $k = 1, \dots, n$, also called fermionic modes. Here introduce the Majorana operators

$$c_{2k-1} = a_k + a_k^\dagger \quad \text{and} \quad c_{2k} = \frac{a_k - a_k^\dagger}{i} \tag{5.7}$$

which have the following properties. They are obviously hermitian

$$c_j^\dagger = c_j \tag{5.8}$$

They anticommute by anticommutation relations

$$\{c_j, c_l\} = 0 \quad \text{if} \quad i \neq j \tag{5.9}$$

since for $j = 2k$, remembering only one fermion per state is allowed

$$\begin{aligned} c_{2k-1}c_{2k} &= \frac{1}{i}[\cancel{a_j^2} - \cancel{(a_j^\dagger)^2} - a_j a_j^\dagger + a_j^\dagger a_j] \\ &= -\frac{1}{i}[-\cancel{a_j^2} + \cancel{(a_j^\dagger)^2} - a_j^\dagger a_j + a_j a_j^\dagger] \\ &= -c_{2k}c_{2k-1} \end{aligned} \tag{5.10}$$

and for $|j-l| \geqslant 2$ the anticommutation is straightforward. Finally, easily computed with the same remarks as before

$$c_j^2 = 1 \tag{5.11}$$

all with $j = 1, \ldots, 2n$.

Then represent a spin by two fermionic modes, thus by four Majorana operators $b^x$, $b^y$, $b^z$, $c$ instead of $c_1$, $c_2$, $c_3$, $c_4$. They act on a 4-dimensional Fock space $\widetilde{\mathcal{M}}$ when the usual Hilbert space for a spin-$\frac{1}{2}$ is 2-dimensional $\mathcal{M} \subset \widetilde{\mathcal{M}}$. With the operator

$$D = b^x b^y b^z c : \widetilde{\mathcal{M}} \to \widetilde{\mathcal{M}} \tag{5.12}$$

the restriction to $\mathcal{M}$ is defined as

$$|\xi\rangle \in \mathcal{M} \iff D\,|\xi\rangle = |\xi\rangle \tag{5.13}$$

$\widetilde{\mathcal{M}}$ is denoted as the extended subspace, and $\mathcal{M}$ the physical subspace. Hence, $D$ can be thought as a gauge transformation for the group $\mathbb{Z}_2$. The operator $D$ satisfies the hermiticity

$$\begin{aligned} D^\dagger &= c_4c_3c_2c_1 = (-1)^2 c_3c_4c_1c_2 \\ &= (-1)^6 c_1c_2c_3c_4 = D \end{aligned} \tag{5.14}$$

and the action of a projector

$$\begin{aligned} D^2 &= c_1c_2c_3c_4c_1c_2c_3c_4 = (-1)^3 c_1^2 c_2c_3c_4c_2c_3c_4 \\ &= (-1)^6 c_1^2c_2^2c_3^2c_4^2 = 1 \end{aligned} \tag{5.15}$$

where in the last equality (5.11) has been used.

The Pauli operators can then be extended to their action on the extended space $\widetilde{\sigma}^x, \widetilde{\sigma}^y, \widetilde{\sigma}^z$, still preserving the physical $\mathcal{M}$ by satisfying the same relations as $\sigma^x, \sigma^y, \sigma^z$ when restricted to $\mathcal{M}$. The extension goes as

$$\widetilde{\sigma}^\alpha = ib^\alpha c : \widetilde{\mathcal{M}} \to \widetilde{\mathcal{M}} \tag{5.16}$$

for $\alpha = x, y, z$. They indeed satisfy

$$[D, \widetilde{\sigma}^\alpha] = 0 \quad (\widetilde{\sigma}^\alpha)^\dagger = \widetilde{\sigma}^\alpha \quad (\widetilde{\sigma}^\alpha)^2 = 1 \quad \forall \alpha \tag{5.17}$$

which can be easily verified, and the relation

$$\widetilde{\sigma}^\mu \widetilde{\sigma}^\nu = \delta^{\mu\nu} + i\varepsilon^{\mu\nu\rho} D \tag{5.18}$$

which is consistent with the fact that $D|_{\mathcal{M}} = 1$ giving the expected SU(2) commutation relations for Pauli matrices on the physical $\mathcal{M}$. This can be derived as for instance, since (5.15) and (5.11)

$$\begin{aligned}\widetilde{\sigma}^x\widetilde{\sigma}^y &= i^2 b^x c b^y c = -i^2 b^x b^y D^2 \\ &= i^2 b^x b^x b^y b^y b^z c D = i\widetilde{\sigma}^z D\end{aligned} \tag{5.19}$$

Considering now many spins each described by four Majorana operators, the Hilbert space goes as

$$\widetilde{\mathcal{L}} = \bigotimes_{j=1}^{n} \widetilde{\mathcal{M}}_j \tag{5.20}$$

with the physical subspace $\mathcal{L} \subset \widetilde{\mathcal{L}}$, and the operators take the form

$$\widetilde{\sigma}_j^\alpha = i b_j^\alpha c \quad D_j = b_j^x b_j^y b_j^z c \tag{5.21}$$

and the restriction still has the same property

$$|\xi\rangle \in \mathcal{L} \iff D_j |\xi\rangle = |\xi\rangle \quad \forall j \tag{5.22}$$

All the relations derived still hold. So the spin Hamiltonian $\mathcal{H}\{\sigma_j^\alpha\}$ can be replaced by the fermionic one $\widetilde{\mathcal{H}}\{b_j^\alpha, c_j\} = \mathcal{H}\{\widetilde{\sigma}_j^\alpha\}$ restricted to the physical subspace. One can write

$$\begin{aligned}\widetilde{\mathcal{H}} = &- J_x \sum_{x\text{-links}} (i b_j^x c_j)(i b_k^x c_k) - J_y \sum_{y\text{-links}} (i b_j^y c_j)(i b_k^y c_k) \\ &- J_z \sum_{z\text{-links}} (i b_j^z c_j)(i b_k^z c_k)\end{aligned} \tag{5.23}$$

It is therefore convenient to introduce the link operators

$$\hat{u}_{jk} = i b_j^\alpha b_k^\alpha \tag{5.24}$$

and noting that the index $\alpha$ depends on the direction of the thus $\alpha = \alpha_{jk}$, rewrite

$$\widetilde{\mathcal{H}} = \frac{i}{4} \sum_{j,k} \hat{A}_{jk} c_j c_k \tag{5.25}$$

with

$$\hat{A}_{jk} = \begin{cases} 2J_{\alpha_{jk}} \hat{u}_{jk} & \text{if } j \text{ and } k \text{ form a link} \\ 0 & \text{otherwise} \end{cases} \tag{5.26}$$

Note that

$$\hat{u}_{jk}^\dagger = \hat{u}_{jk} \quad \hat{u}_{jk}^2 = 1 \quad \hat{u}_{jk} = -\hat{u}_{kj} \tag{5.27}$$

It can be shown easily that

$$[\hat{u}_{jk}, \hat{u}_{lm}] = 0 \quad [\widetilde{\mathcal{H}}, \hat{u}_{jk}] = 0 \quad \forall (j,k),(l,m) \tag{5.28}$$

Indeed

$$\begin{aligned}\hat{u}_{jk}\hat{u}_{lm} &= i^2 b_j^{\alpha_{jk}} b_k^{\alpha_{jk}} b_l^{\alpha_{lm}} b_m^{\alpha_{lm}} \\ &= (-1)^4 i^2 b_l^{\alpha_{lm}} b_m^{\alpha_{lm}} b_j^{\alpha_{jk}} b_k^{\alpha_{jk}} = \hat{u}_{lm}\hat{u}_{jk}\end{aligned} \tag{5.29}$$

and the commutation with $\widetilde{\mathcal{H}}$ follows directly from the commutation between these operators and the fact that there are always two $c_j$ operators in $\widetilde{\mathcal{H}}$ cancel the change in sign as

$$c_j c_k \hat{u}_{lm} = (-1)^2 \hat{u}_{lm} c_j c_k \tag{5.30}$$

Hence, the Hilbert space $\widetilde{\mathcal{L}}$ split into eigenspaces of $\hat{u}_{jk}$ index by their corresponding eigenvalues $u_{jk} = \pm 1$ — notice the removal of the hat for the eigenvalues. Therefore write

$$\widetilde{\mathcal{L}} = \bigoplus_u \widetilde{\mathcal{L}}_u \tag{5.31}$$

where the $u$ denotes the collections of all $u_{jk}$ and the sector $\widetilde{\mathcal{L}}_u$ has dimension $2^n$ now. Henceforth, the restriction of $\widetilde{\mathcal{H}}$ to $\widetilde{\mathcal{L}}_u$ is obtained by removing the hats of $\hat{u}_{jk}$. This allows to write

$$\widetilde{\mathcal{H}}_u = \frac{i}{4} \sum_{j,k} A_{jk} c_j c_k \tag{5.32}$$

which corresponds to free fermions, and then found the ground state $\left|\widetilde{\psi}_u\right\rangle$ exactly.

It is remarkable to see that

$$[\widetilde{\mathcal{H}}, D_j] = 0 \tag{5.33}$$

Thus, $D_j$ can be seen as gauge transformation of the system, since $\widetilde{\mathcal{H}}$ is invariant under $D_j$. The subspace $\widetilde{\mathcal{L}}_u$ is not gauge invariant. Indeed the gauge transformation acts as

$$u_{lm} \to D_j u_{lm} D_j^\dagger = \begin{cases} -u_{lm} & \text{if } l = j \text{ or } m = j \\ u_{lm} & \text{otherwise} \end{cases} \tag{5.34}$$

since $D_j^\dagger D_j = 1$. This is easily seen by performing the same computations as done before making use of the anticommutation relations. Then $D_j$ change the values of $u_{jk}$ on the links connecting the vertex $j$ with the three adjacent vertices $k$. Thus the state $\left|\widetilde{\psi}_u\right\rangle$ does not belong to the physical subspace. To obtain the physical ground state, symmetrize over all gauge transformations

$$|\psi_w\rangle = \prod_j \frac{1 + D_j}{2} \left|\widetilde{\psi}_u\right\rangle \in \mathcal{L} \tag{5.35}$$

where $w$ denotes the equivalence class of $u$ under the gauge transformation. To see this, $w$ is characterized by $w_p = \pm 1$ defined as, choosing a particular direction around the boundary

$$w_p = \prod_{(j,k)\in\partial p} u_{jk} \tag{5.36}$$

with $j$ in the even sublattice and $k$ the odd one. Also, $w_p$ is invariant under gauge transformation. Thus, the operators

$$\widetilde{W}_p = \prod \hat{u}_{jk} \tag{5.37}$$

commute with the gauge transformation and the Hamiltonian, and the restriction to the physical subspace coincides with the $W_p$. The variables $u_{jk}$ can be seen as a $\mathbb{Z}_2$ gauge field and $w_p$ the magnetic flux through the plaquette $p$.

## 5.3 FREE FERMIONS HAMILTONIAN

The goal is to write the Hamiltonian in a quadratic form in terms of the fermionic operators. Recall the general form (5.32)

$$\mathcal{H} = \frac{i}{4} \sum_{j,k} A_{jk} c_j c_k = c^\top A c \tag{5.38}$$

with $A$ a real antisymmetric $n \times n$ matrix, still $n = 2m$. The Hamiltonian one seeks for is

$$\mathcal{H}_{ff} = \sum_{k=1}^{m} \varepsilon_k \left( a_k^\dagger a_k - \frac{1}{2} \right) \quad \varepsilon_k \geqslant 0 \tag{5.39}$$

The ground state of such Hamiltonian is thus given by the condition $a_k |\psi\rangle = 0, \forall k$. Notice that for $A$ real antisymmetric, there exists $Q \in O(2m)$ such that

$$A = QSQ^\top \quad \text{with} \quad S = \begin{pmatrix} 0 & \varepsilon_1 & & & \\ -\varepsilon_1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & \varepsilon_m \\ & & & -\varepsilon_m & 0 \end{pmatrix} \tag{5.40}$$

and the $\{\pm\varepsilon_k\}$ are the spectrum of the Hermitian $iA$. Hence

$$c^\top A c = c^\top QSQ^\top c = b^\top S b \tag{5.41}$$

with

$$b_j = \sum_k c_k Q_{kj} \tag{5.42}$$

It can be easily shown that, again by anticommutation relations

$$\{b_i, b_j\} = 0 \quad b_j^2 = 1 \quad \forall j, k \tag{5.43}$$

Rewriting with the normal modes with a prime

$$b^\top = (b_1', b_1'', \ldots, b_m', b_m'') \tag{5.44}$$

and introducing the corresponding ladder operators

$$a_k = \frac{1}{2}(b_k' + i b_k'') \quad a_k^\dagger = \frac{1}{2}(b_k' - i b_k'') \tag{5.45}$$

satisfying the relation

$$\{a_k, b_k^\dagger\} = 1 \tag{5.46}$$

since

$$\begin{aligned} a_k a_k^\dagger + a_k^\dagger a_k &= \frac{1}{4}(2b_k'^2 + 2b_k''^2 - ib_k' b_k'' + ib_k'' b_k' + ib_k' b_k'' - ib_k'' b_k') \\ &= \frac{1}{4}(2+2) = 1 \end{aligned} \tag{5.47}$$

This finally allows to write

$$\mathcal{H} = \sum_k \varepsilon_k \left( a_k^\dagger a_k - \frac{1}{2} \right) = \frac{i}{2} \sum_k b_k' b_k'' \varepsilon_k \tag{5.48}$$

## 5.4 SPECTRUM

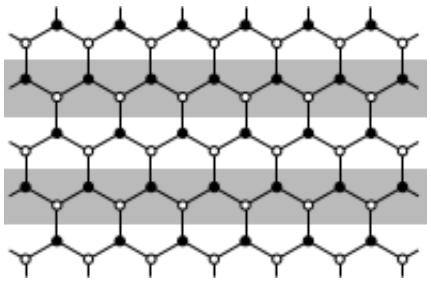

*Figure* 5.3 – Part of the lattice — shaded — considered for the action of the transformation of interest.

Take the quadratic Hamiltonian (5.25). Note that the ground state energy does not depend on the signs on the exchange constants $J_{x,y,z}$, since changing the signs can be compensated by changing the corresponding $u_{jk}$. The ground state does not even depend on the signs if $u$ is fixed. To show that, consider for instance $J_z \to -J_z$. This is equivalent to changing $u_{jk}$ for all $z$-links. But the gauge-invariant $w_p$ are constant, thus one can further apply a gauge transformation that make $u_{jk}$ back to its original value. The only effect is that $c_j \to -c_j$. The transformation acts on the shaded area on Figure 5.3. So to find the ground and excited states energy, the signs of the exchange constants do not matter.

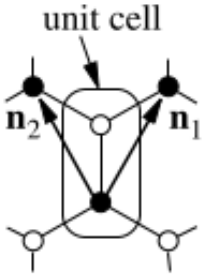


*Figure* 5.4 – Unit cell and the notation used.

A theorem by Lieb says that the energy is minimized for $w_p = 1\ \forall p$, thus choose $u_{jk} = 1$ for $j \in$ even and $k \in$ odd sublattice. This configuration has a translational symmetry and thus use Fourier transform to find the spectrum. Represent the site $j$ with $(s, \lambda)$ where $s$ refers to the unit cell and $\lambda$ to the position in the unit cell. The Hamiltonian has then the form

$$\mathcal{H} = \frac{i}{4} \sum_{s\lambda,t\mu} A_{s\lambda,t\mu} c_{s\lambda} c_{t\mu} \tag{5.49}$$

where the $A_{s\lambda,t\mu}$ dependence is on $\lambda, \mu, t - s$ by translational invariance of the $u_{jk}$. Then write

$$\widetilde{A}_{\lambda\mu}(q) = \sum_t e^{iq\cdot r_t} A_{0\lambda,t\mu} \tag{5.50}$$

and

$$a_{q,\lambda} = \frac{1}{\sqrt{2N}} \sum_s e^{-iq\cdot r_s} c_{s\lambda} \tag{5.51}$$

The Hamiltonian then becomes, by inverting the relations

$$\begin{aligned}
\mathcal{H} &= \frac{1}{2N}\frac{i}{4} \sum_{s\lambda,b\mu} \sum_{q_1} e^{-iq_1\cdot r_b} \widetilde{A}_{\lambda\mu}(q_1) \\
&\quad \cdot \sum_{q_2,q_3} e^{iq_2\cdot r_s} e^{-iq_3\cdot(r_s+r_b)} a_{q_2,\lambda} a_{q_3,\mu} \\
&= \frac{1}{2N}\frac{i}{4} \sum_{\lambda,b\mu} \sum_{q_1} e^{-iq_1\cdot r_b} \widetilde{A}_{\lambda\mu}(q_1) \sum_{q_4} e^{iq_4\cdot r_b} a_{q_4,\lambda} a_{-q_3,\mu} \\
&= \frac{i}{4} \sum_{\lambda,b\mu} \sum_q \widetilde{A}_{\lambda\mu}(q) a_{-q,\lambda} a_{q,\mu} \\
&= \frac{i}{4} \sum_{\lambda,b\mu} \sum_q \widetilde{A}_{\lambda\mu}(q) a^\dagger_{q,\lambda} a_{q,\mu}
\end{aligned} \tag{5.52}$$

The spectrum is given by the eigenvalues of $\widetilde{A}_{\lambda\mu}(q)$ which is

$$\widetilde{A}_{\lambda\mu}(q) = \begin{pmatrix} 0 & if(q) \\ -if(q) & 0 \end{pmatrix} \tag{5.53}$$

with

$$f(q) = 2(J_x e^{iq\cdot n_1} + J_y e^{iq\cdot n_2}) + J_z) \tag{5.54}$$

and $n_1, n_2$ the vectors as in Figure 5.4. Thus

$$\varepsilon(q) = \pm|f(q)| \tag{5.55}$$

Hence, either there exists a $q$ such that $f(q) = 0$, or there is a gap in the spectrum. Moreover, $f(q) = 0$ has a solution if and only if

$$\begin{cases} |J_x| \leqslant |J_y| + |J_z| \\ |J_y| \leqslant |J_x| + |J_z| \\ |J_z| \leqslant |J_x| + |J_y| \end{cases} \tag{5.56}$$

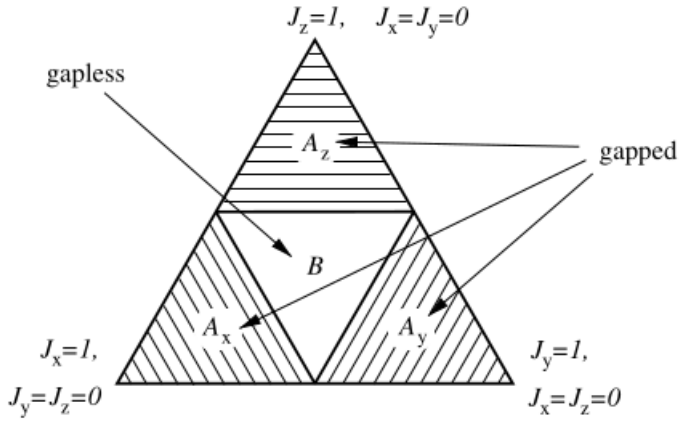


*Figure* 5.5 – Phase diagram of the model considered for the spectrum.

The region corresponding is the one that is not shaded in Figure 5.5. The 3 gapped phases are distinct but related by rotational symmetry, and there is no continuous transition between two gapped phases.

Finally, to relate to quantum spins liquids, the ground state is the superposition of many Majorana modes, thus there is a high level entanglement. Moreover,

$$\langle GS|c_j c_k|GS\rangle = \delta_{kj} - iB_{kj} \quad \text{with} \quad B = -i\,\text{sign}(iA) \tag{5.57}$$

and $A_{kj} = 0$ if $(j,k)$ is not a link, thus $B_{kj}$ too. Hence $\langle GS|c_j c_k|GS\rangle = 0$ and there is no long-range interaction, whether or not the system is gapped.

# 6 FRACTIONAL QUANTUM HALL EFFECT

## 6.1 LANDAU'S SOLUTIONS ON THE DISK AND THE CYLINDER

To begin with, just briefly recall the solutions of the Landau's problem both on the disk and the cylinder. To remind the context, one is basically just studying the movement of free $e^-$ on a plane under the action of a magnetic field. The Hamiltonian for such an $e^-$ is

$$\mathcal{H} = \frac{1}{2m}(\mathbf{p} + e\mathbf{A})^2 \tag{6.1}$$

In the Landau gauge, take the vector potential to be

$$\mathbf{A} = Bx\boldsymbol{e}_y \tag{6.2}$$

which leads to a magnetic field

$$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A} = B\boldsymbol{e}_z \tag{6.3}$$

With this gauge the Hamiltonian reads

$$\mathcal{H} = \frac{1}{2m}p_x^2 + \frac{1}{2m}(p_y + eBx)^2 \tag{6.4}$$

Hence, observe that there is an obvious translational invariance in the $y$-direction since the Hamiltonian commutes with $p_y$. Translational invariance in the $y$-direction but not in the $x$ direction means the system topologically is a cylinder. One can therefore look for energy eigenstates that are also eigenstates of $p_y$, which are of course plane waves. This means one can search for eigenstates of the following separable form

$$\psi_k(x, y) = e^{iky}\varphi_k(x) \tag{6.5}$$

Under the action of the Hamiltonian, this wavefunction becomes

$$\begin{aligned}\mathcal{H}\psi_k(x, y) &= \left[\frac{1}{2m}p_x^2 + \frac{1}{2m}(\hbar k + eBx)^2\right]\psi_k(x, y) \\ &= \mathcal{H}_k\psi_k(x, y)\end{aligned} \tag{6.6}$$

where it can be defines the following partial Hamiltonian

$$\mathcal{H}_k = \frac{p_x^2}{2m} + \frac{1}{2}m\frac{e^2B^2}{m^2}\left(x + k\frac{\hbar}{eB}\right)^2 = \frac{p_x^2}{2m} + \frac{1}{2}m\omega_C^2\left(x + kl_B^2\right)^2 \tag{6.7}$$

with $\omega_C = \frac{eB}{m}$ the cyclotron frequency and $l_B = \sqrt{\frac{\hbar}{eB}}$ the magnetic length. This is a harmonic oscillator with frequency $\omega_C$, centered at $x = -kl_B$, therefore see that the energy eigenvalues do not depend on $k$

$$E_n = \hbar\omega_C\left(n + \frac{1}{2}\right) \tag{6.8}$$

One can also consider the symmetric gauge in which the vector potential is

$$\mathbf{A} = -\frac{1}{2}\mathbf{r}\times\mathbf{B} = -\frac{By}{2}\mathbf{e}_x + \frac{Bx}{2}\mathbf{e}_y \tag{6.9}$$

Even though this choice of gauge breaks the translational symmetry in both the $x$- and the $y$-directions, one will see it does preserve rotational symmetry about the origin. The system topologically is a disk. As one will see, this also means angular momentum is a good quantum number. With an algebraic approach, one can easily prove that a basis of LLL wavefunctions are given by

$$\psi_{LLL}(z,\bar{z}) \sim \left(\frac{z}{l_B}\right)^m e^{-|z|^2/4l_B^2} \tag{6.10}$$

where $m$ is the angular momentum and $z = x - iy$. The energy, as for the Landau gauge, only depends on $n$ and not on $m$. By defining

$$\partial = \frac{1}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right) \quad \text{and} \quad \bar{\partial} = \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right) \tag{6.11}$$

one can convince oneself that the angular momentum operator is

$$L_z = i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -\hbar\left(z\partial - \bar{z}\bar{\partial}\right) \tag{6.12}$$

and then, acting on the wavefunctions yields

$$L_z\psi_{LLL}(z,\bar{z}) = -\hbar m\psi_{LLL}(z,\bar{z}) \tag{6.13}$$

So $m$ is the orbital momentum. One can derive a general expression for higher LLs which are simply quoted here

$$\psi_{nm}(z,\bar{z}) = \frac{(-1)^n}{\sqrt{2\pi}}\sqrt{\frac{n!}{2^m(m+n)!}}z^m e^{-|z|^2/4l_B^2}L_n^m\left(\frac{|z|^2}{2}\right) \tag{6.14}$$

where $L_n^m$ is the associated generalized Laguerre polynomial.

## 6.2 DEGENERACY OF FILLED LANDAU LEVELS

Each LLhas degenerate orbitals labeled by $k$ in the Landau gauge and $m$ in the symmetric gauge. This degeneracy is the same in each Landau level and depends only on the area of the sample $A$ and the magnetic field $B$. One of the advantages of the symmetric gauge is that it can provide an algebraic derivation of the degeneracies of LLs. As just seen, the wavefunctions form concentric rings around the origin. This is very different from the wavefunctions found with the Landau gauge, which were strips. The wavefunction with angular momentum $m$ is peaked on a ring of radius $R \sim \sqrt{2m}l_B$. Therefore, if one considers a disk of area $\pi R^2$, the number of states in it is roughly

$$\mathcal{N}_\phi = \frac{R^2}{2l_B^2} = \frac{A}{2\pi l_B^2} = \frac{AB}{\phi_0} = \frac{\phi}{\phi_0} \tag{6.15}$$

with

$$\phi_0 = \frac{h}{e} \simeq 4.14 \cdot 10^{-15}\ \mathrm{T/m^2} \tag{6.16}$$

the quantum of flux. For instance, consider a sample of area $A = 1\ \mathrm{cm}^2$ subjected to a magnetic field of $B = 1$ T. Then each Landau level has a total of $2.4 \cdot 10^{10}$ possible states. Therefore see that LLs are extremely degenerate.

This has an important consequence. To see this, let $\mathcal{N}_e$ be the number of $e^-$ and $\hbar\omega_I$ be the characteristic energy of the interaction. For instance, for the Coulomb interaction this energy typically is

$$\hbar\omega_I = \frac{e^2}{4\pi\varepsilon_0 l_B} \tag{6.17}$$

Without any interaction, the energy is minimized by simply filling all LLs in the ascending order. For instance, suppose one has $\mathcal{N}_e = 2\mathcal{N}_\phi$: just fill the two first LLs, *ie* 0 and 1. Now if one adds the interaction, for it to do something it has to take an $e^-$ from one of the two first LLS to the level 2, which costs either $\hbar\omega_C$ or $2\hbar\omega_C$. If $\omega_I \ll \omega_C$, this is impossible and one can just forget the interactions. Now, consider $\mathcal{N}_e = \frac{3}{2}\mathcal{N}_\phi$. The level 0 is fully filled and the level 1 is partially filled. What was just said before is still valid for the levels 0 and 2. But now the interaction can also move an $e^-$ in another state of the level 1 since it is not filled anymore. However this does not cost anything now: the interaction necessarily is the dominant term here and thus cannot be neglected anymore. Now that the interactions are no more in competition with anything else, they can give rise to interesting phases just like the FQHE's ones.

With that being said, once one has written the Hamiltonian as

$$\mathcal{H} = V = \sum A_{m_1,m_2,n_2,n_1} c^\dagger_{m_1} c^\dagger_{m_2} c_{n_2} c_{n_1} \tag{6.18}$$

one can just forget the $c^\dagger$ operators that create orbitals in the level $n = 1$. In other terms, one can project the interactions on the LLL. Basically it means that if one is studying the state $|n = 1, m_1\rangle \otimes |n = 1, m_2\rangle$, one can study the state $|n = 0, m_1\rangle \otimes |n = 0, m_2\rangle$ instead, this is just for more convenient calculations, as the wavefunctions quickly become hard to write down.

## 6.3 COULOMB INTERACTION MATRIX ELEMENTS

With all that has just been said, it is quite logical to compute the Coulomb interaction matrix elements. For convenience purposes, do this calculation on the disk and only in the LLL $n = 0$. As seen before, the wavefunctions are then

$$\psi_{0,m}(z,\bar{z}) = \frac{1}{\sqrt{2\pi 2^m m!}} z^m e^{-|z|^2/4l_B^2} \tag{6.19}$$

and the Coulomb interaction of course is

$$V(|\mathbf{r}_1 - \mathbf{r}_2|) = \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \tag{6.20}$$

In order to simplify a bit the calculations, one can take the unit of length to be the magnetic length $l_B$ and the unit of interaction energy to be $e^2/4\pi\varepsilon_0 l_B$. With this in mind, the 2-body Coulomb matrix element in the LLL is defined as

$$\begin{aligned}\langle p,q|\,V\,|m,n\rangle &= \int d^2\mathbf{r}_1\; d^2\mathbf{r}_2\; \bar{\psi}_{0,p}(\mathbf{r}_1)\bar{\psi}_{0,q}(\mathbf{r}_2)\\ &\quad\cdot\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\psi_{0,m}(\mathbf{r}_1)\psi_{0,n}(\mathbf{r}_2)\\ &= \frac{1}{\sqrt{(2\pi)^4 2^{p+q+m+n}p!q!m!n!}}\\ &\quad\cdot\int d^2z_1\; d^2z_2\;\frac{\bar{z}_1^p\bar{z}_2^q z_1^m z_2^n}{|z_1-z_2|}e^{-\frac{1}{2}(|z_1|^2+|z_2|^2)}\end{aligned} \tag{6.21}$$

where $p$, $q$, $m$ and $n$ are angular momentum quantum numbers. To compute this integral one can make the substitution which consists in transforming to the relative and center of mass coordinates

$$\begin{cases} Z &= \frac{z_1+z_2}{2}\\ z &= z_1-z_2\end{cases}\Longrightarrow\begin{cases} z_1 &= Z+\frac{z}{2}\\ z_2 &= Z-\frac{z}{2}\end{cases} \tag{6.22}$$

and similar expression for the complex conjugates. One can check the Jacobian for this substitution is unity, *ie* $d^2z_1\,d^2z_2 = d^2Z\,d^2z$. One can also easily prove

$$|z_1|^2+|z_2|^2 = z_1\bar{z}_1+z_2\bar{z_2} = 2Z\bar{Z}+\frac{1}{2}z\bar{z} = 2|Z|^2+\frac{1}{2}|z|^2 \tag{6.23}$$

allowing to make a binomial expansion

$$\begin{aligned}&\langle p,q|\,V\,|m,n\rangle\\ &= \mathcal{A}^{pq}_{mn}\int d^2Z\;d^2z\sum_{\substack{i=0,j=0\\k=0,l=0}}^{p,q,m,n}\frac{(-1)^{q+n-j-l}}{2^{p+q+m+n}}\\ &\cdot\mathcal{C}^i_p\mathcal{C}^j_q\mathcal{C}^k_m\mathcal{C}^l_n\bar{Z}^{i+j}Z^{k+l}\bar{z}^{p+q-i-j}z^{m+n-k-l}\frac{e^{-|Z|^2-\frac{1}{2}|z|^2}}{|z|}\\ &= \mathcal{A}^{pq}_{nm}\sum_{\substack{i=0,j=0\\k=0,l=0}}^{p,q,m,n}\mathcal{B}^{ijkl}_{pqmn}\int d^2Z\;d^2z\;\bar{Z}^{\mu_1}\bar{z}^{\mu_2}Z^{\mu_3}z^{\mu_4}\frac{e^{-|Z|^2-\frac{1}{2}|z|^2}}{|z|}\end{aligned} \tag{6.24}$$

So one sees that, after transforming to the center of mass and relative coordinates, typical terms in the integrand are of the form

$$\bar{Z}^{\mu_1}\bar{z}^{\mu_2}Z^{\mu_3}z^{\mu_4} \tag{6.25}$$

with $\mu_1+\mu_2 = p+q$ and $\mu_3+\mu_4 = m+n$. These integrals vanish unless $\mu_1=\mu_3$ and $\mu_2=\mu_4$ which implies $p+q=m+n$. In other terms, the Coulomb interaction conserves the total angular momentum. Explicit expressions for the precedent matrix elements can be found in the literature, one just quotes here a form particularly useful for numerical studies obtained by Tsiper:

$$\begin{aligned}\langle m+p,n|\,V\,|m,n+p\rangle &= \sqrt{\frac{(m+p)!(n+p)!}{m!n!}}\frac{\Gamma(m+n+p+\frac{3}{2})}{\pi 2^{m+n+p+2}}\\ &\quad\cdot(A^p_{mn}B^p_{nm}+B^p_{mn}A^p_{nm})\end{aligned} \tag{6.26}$$

where $A^p_{mn}$ and $B^p_{mn}$ are sums of positive terms. This means this expresses the matrix element as a sum of positive terms, which makes it numerically more stable.

## 6.4 LANDAU LEVELS QUANTIZATION ON THE SPHERE

To motivate the context, one already solved the quantization of LLs on different topologies, one will pass to the sphere for its interesting practical aspects and for the whole formalism that has been developed around it, enabling to formulate FQHE, introducing it in a sense the interactions between particles.

- No boundaries for the sphere
- Less topology degeneracy

These are the two main differences between the sphere and the other topologies — disk, cylinder, torus.

Technically, the level quantization on the sphere is represented with the behavior of charged particles on the surface of a sphere within which one assumes a punctual source of magnetic field, a monopole. Assume a radial magnetic field of strength

$$B = \frac{\hbar c s_0}{eR^2} \tag{6.27}$$

with the number of Dirac magnetic flux quanta through the sphere being

$$\frac{\Phi_{tot}}{\Phi_0} = 2s_0 \tag{6.28}$$

that must be an integer due to Dirac monopole quantization condition. The Hamiltonian is given by

$$\mathcal{H} = \frac{\boldsymbol{\Lambda}^2}{2MR^2} \tag{6.29}$$

where $\boldsymbol{\Lambda} = \mathbf{r} \times [i\nabla + e\mathbf{A}(\mathbf{r})]$ is the dynamical angular momentum. Using the definition of the vector potential and the results of spherical coordinate one gets

$$\boldsymbol{\Lambda} = -i\left(\boldsymbol{e}_\varphi \frac{\partial}{\partial\theta} - \boldsymbol{e}_\theta \frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}\right) + eR[\boldsymbol{e}_r \times \mathbf{A}(\mathbf{r})] \tag{6.30}$$

One sees that $\boldsymbol{\Lambda}$ has no radial component and is now seeking for the generator of rotations so has to look at the algebraic structure of our dynamical quantity $\boldsymbol{\Lambda}$. Get

$$[\Lambda^i, \Lambda^j] = i\varepsilon^{ijk}(\Lambda^k - s_0 e_r^k) \tag{6.31}$$

Doing the change of variable $\mathbf{L} = \boldsymbol{\Lambda} + s_0\boldsymbol{e}_r$ one gets the algebraic structure one was looking for

$$[L^i, X^j] = i\varepsilon^{ijk}X^k \tag{6.32}$$

For $\mathbf{X} = \mathbf{\Lambda}, \mathbf{L}, \boldsymbol{e}_r$. Hence it is the proper angular momentum which implies a possible quantization. Note that $\mathbf{L}$ has a radial component $L\boldsymbol{e}_r = s_0$. Taking the eigenvalue of $\mathbf{L}$ to be $s(s+1)$, thus have $s = s_0 + n$ with $n$ an integer. Finally obtain

$$\Lambda^2 = L^2 - s_0^2 \tag{6.33}$$

which gives the energy levels

$$E_n = \omega_c \left[ \left( n + \frac{1}{2} \right) + \frac{n(n+1)}{2s_0} \right] \tag{6.34}$$

The $n$ index is thus the LL.

To find the eigenstate one has to choose a gauge, the choice is made towards the latitudinal gauge

$$\mathbf{A} = -\boldsymbol{e}_\varphi \frac{s_0}{eR} \cot\theta \tag{6.35}$$

The dynamical angular momentum then becomes

$$\mathbf{\Lambda} = -i \left( \boldsymbol{e}_\varphi \frac{\partial}{\partial\theta} - \boldsymbol{e}_\theta \frac{1}{\sin\theta} \left( \frac{\partial}{\partial\varphi} - i s_0 \cos\theta \right) \right) \tag{6.36}$$

It is possible to introduce spinor coordinates for the particle position, as

$$u = \cos\frac{\theta}{2} e^{i\frac{\varphi}{2}} \quad \text{and} \quad v = \sin\frac{\theta}{2} e^{-i\frac{\varphi}{2}} \tag{6.37}$$

such that

$$\boldsymbol{e}_r = \Omega(u, v) = (u, v)\sigma \begin{pmatrix} \bar{u} \\ \bar{v} \end{pmatrix} \tag{6.38}$$

where $\sigma$ is the vector made of the three Pauli matrices. A complete orthogonal basis, spanning the LLL — $n = 0$ and $s = s_0$ — is given by

$$\Psi^s_{m,0}(u, v) = u^{s+m} v^{s-m} \tag{6.39}$$

And the following identities hold $L^z \Psi^s_{m,0} = m\Psi^s_{m,0}$ and $\mathcal{H}\Psi^s_{m,0} = \frac{1}{2}\omega_c \Psi^s_{m,0}$. One can verify this by introducing more general states with an additional quantum number $p$

$$\begin{aligned} \phi^s_{m,p}(u, v) &= \left( \cos\frac{\theta}{2} \right)^{s+m} \left( \sin\frac{\theta}{2} \right)^{s-m} e^{i(m-p)\varphi} \\ &= \begin{cases} \bar{v}^{-p} u^{s+m} v^{s-m+p} & \text{if } p < 0 \\ \bar{u}^{p} u^{s+m-p} v^{s-m} & \text{otherwise} \end{cases} \end{aligned} \tag{6.40}$$

And compute the action of $\Lambda^2$ :

$$\begin{aligned} &\Lambda^2 \phi^s_{m,p} \\ &= \left[ s - \left( \frac{s\cos\theta - m}{\sin\theta} \right)^2 + \left( \frac{s_0\cos\theta - m + p}{\sin\theta} \right)^2 \right] \phi^s_{m,p} \\ &= \left[ s + \frac{2\left(s\cos\theta - m + p\right)\left(p - n\cos\theta\right) - \left(p^2 - n^2\cos^2\theta\right)}{\sin^2\theta} \right] \phi^s_{m,p} \end{aligned} \tag{6.41}$$

Putting $p$ and $n$ to zero yields the previous results. Finally, one can see that in the LLL, the angular momentum can be written as

$$\mathbf{L} = \frac{1}{2}(u, v)\sigma \begin{pmatrix} \frac{\partial}{\partial u} \\ \frac{\partial}{\partial v} \end{pmatrix} \tag{6.42}$$

This form is actually very important for the next step, which is a generalization to higher LLs.

In his formalism Haldane restricted himself to the LLL. Now expand the results one already has. One already knows that on a plane one can describe the Hilbert space with two commuting ladder algebras $a$ and $b$. Here in the sphere topology one can by analogy present a similar formalism involving two mutually commuting SU(2) algebras. It both are angular momentum SU(2) algebras. The first one related to the cyclotron momentum $S$ — raise or lower the LL index — and the second one for the guiding center $L$ — that rotate the states while staying in the same LL. Looking at the form of $L$ and the fact that in the spinor coordinates formalism the eigenstate basis is made of power laws of $u$ and $v$, one can relate $u$, $v$, $\partial_u$ and $\partial_v$ as the Schwinger boson creation and annihilation operators. Note that since $S^2$ and $L^2$ have the same eigenvalues introducing S was not obvious even if it is mandatory to fully describe the Hilbert space and thus generalize to higher LLs. To complete the description one would also need $\bar{u}$, $\bar{v}$, $\partial_{\bar{u}}$ and $\partial_{\bar{v}}$. Using the Schwinger picture get

$$\begin{aligned} S^x + iS^y = S^+ &= u\frac{\partial}{\partial \bar{v}} - v\frac{\partial}{\partial \bar{u}} \\ S^x - iS^y = S^- &= \bar{v}\frac{\partial}{\partial u} - \bar{u}\frac{\partial}{\partial v} \\ S^z &= \frac{1}{2}\left[u\frac{\partial}{\partial u} + v\frac{\partial}{\partial v} - \bar{u}\frac{\partial}{\partial \bar{u}} - \bar{v}\frac{\partial}{\partial \bar{v}}\right] \end{aligned} \tag{6.43}$$

and the same for $L$

$$\begin{aligned} L^x + iL^y = L^+ &= u\frac{\partial}{\partial v} - \bar{v}\frac{\partial}{\partial \bar{u}} \\ L^x - iL^y = L^- &= v\frac{\partial}{\partial u} - \bar{u}\frac{\partial}{\partial \bar{v}} \\ L^z &= \frac{1}{2}\left[u\frac{\partial}{\partial u} - v\frac{\partial}{\partial v} - \bar{u}\frac{\partial}{\partial \bar{u}} + \bar{v}\frac{\partial}{\partial \bar{v}}\right] \end{aligned} \tag{6.44}$$

That can be written in the compact form

$$L = \frac{1}{2}(u, v)\sigma \begin{pmatrix} \frac{\partial}{\partial u} \\ \frac{\partial}{\partial v} \end{pmatrix} - \frac{1}{2}(\bar{u}, \bar{v})\sigma^\top \begin{pmatrix} \frac{\partial}{\partial \bar{u}} \\ \frac{\partial}{\partial \bar{v}} \end{pmatrix} \tag{6.45}$$

and

$$S = \frac{1}{2}(u, \bar{v})\sigma \begin{pmatrix} \frac{\partial}{\partial u} \\ \frac{\partial}{\partial \bar{v}} \end{pmatrix} - \frac{1}{2}(\bar{u}, v)\sigma^\top \begin{pmatrix} \frac{\partial}{\partial \bar{u}} \\ \frac{\partial}{\partial v} \end{pmatrix} \tag{6.46}$$

One gets the algebra identities

$$[S^i, S^j] = i\varepsilon^{ijk}S^k \quad [L^i, L^j] = i\varepsilon^{ijk}L^k \quad \text{and} \quad [S^i, L^j] = 0 \tag{6.47}$$

and also

$$L^2 = S^2 = s(s+1) \tag{6.48}$$

identifying

$$s = \frac{1}{2}\left[u\frac{\partial}{\partial u} + v\frac{\partial}{\partial v} + \bar{u}\frac{\partial}{\partial \bar{u}} + \bar{v}\frac{\partial}{\partial \bar{v}}\right] \tag{6.49}$$

Looking at the component of L normal to the surface of the sphere, get $\boldsymbol{e}_r L = S^z$. Hence the physical Hilbert space is limited to state that has $s_0$ as eigenvalues of $S^z$. Using $[S^+, S^-] = 2S^z$, obtain the Hamiltonian

$$\mathcal{H} = \omega_c\left(\frac{1}{2s_0}S^+S^- + \frac{1}{2}\right) \tag{6.50}$$

Thus $S^-$ and $S^+$ indeed play the role of raising and lowering operators and obtain the final result

$$\Psi^s_{m,n} = (S^-)^n \Psi^s_{m,0} \tag{6.51}$$

Now for a many-body physical system one would like to find an appropriate basis for the filling of Landau level. By some mathematical argument and the previous results one can construct it. For instance for a 2-body system, one can use the total angular momentum and the relative one as the quantum number indexing the states. Using some simple consideration on those quantum number, one can see that the projection onto the $(n+1)^{\text{th}}$ LL of any rotational invariant operator can be expanded as

$$\Pi_n V \Pi_n = \sum_l^{2s} V_l^n P_{2s-l}(L_1 + L_2) \tag{6.52}$$

where $P_j$ is the projector onto the states with total angular momentum $j(j+1)$. The coefficient $V_l^n$ are the so-called pseudopotentials. One can use that to express the effect of an interaction potential such as a Coulomb one which gives as pseudopotential coefficients in the LLL

$$V_l^0 = \frac{\binom{2l}{l}\binom{8s+2-2l}{4s+1-l}}{\binom{4s+2}{2s+1}} \tag{6.53}$$

## 6.5 INTRODUCTION OF PSEUDOPOTENTIALS

Start with a general interaction Hamiltonian in the LLL for the many-body system

$$\mathcal{H} = \sum_{\substack{m_1+m_2 \\ =m_3+m_4}} A^{m_3,m_4}_{m_1,m_2} \langle m_3, m_4|V|m_1, m_2\rangle \, c^\dagger_{m_3} c^\dagger_{m_4} c_{m_1} c_{m_2} \tag{6.54}$$

and focus on the 2-body matrix element in the basis $|M, m\rangle$, with $M$ the total angular momentum and $m$ the relative angular momentum. One can relate

$$|m_1, m_2\rangle = \sum_{M,m} N^{M,m}_{m_1,m_2} |M, m\rangle \tag{6.55}$$

with in terms of the Clebsch-Gordan coefficients. Now seeking for a central potential $V(\mathbf{r})$, it must be diagonal in the basis $|M, m\rangle$ since it must conserve the $M$ and $m$. Also, it should depend only on $m$. Then

$$\langle M', m'|V(\mathbf{r})|M, m\rangle = \delta_{M'M}\delta_{m'm}\,\langle m|V(\mathbf{r})|m\rangle \tag{6.56}$$

which allows to write the interaction

$$\mathcal{H} = \sum_{M,m} V_m\,|M, m\rangle\langle M, m| \tag{6.57}$$

with the Haldane's pseudopotentials

$$V_m = \langle m|V(\mathbf{r})|m\rangle \tag{6.58}$$

## 6.6 EXACT GROUND STATE

Here the aim is to find a potential that emerges from simple considerations, which turns out to give the Laughlin states as being the daughter states of the interaction and from which can be written any other central potential. First take a 2D central potential, and write its Fourier transform

$$\begin{aligned} V(\mathbf{k}) &= \int d^2r\; V(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}} \\ &= \int_0^\infty dr\; rV(r)\int_0^{2\pi} d\vartheta\; e^{ikr\cos\vartheta} \\ &= 2\pi\int_0^\infty dr\; rV(r)J_0(kr) \end{aligned} \tag{6.59}$$

where the Bessel functions of the first kind have been introduced. Recalling their expression

$$J_n(x) = \sum_{p=0}^{\infty} \frac{(-1)^p x^{2p+n}}{2^{2p+n}p!\Gamma(p+n+1)} \tag{6.60}$$

and not focusing on the multiplying factors, one can expand

$$V(\mathbf{k}) = \sum_{p=0}^{\infty} B_p(-k^2)^p \tag{6.61}$$

Remembering the identification $\nabla^2 \leftrightarrow -k^2$ since

$$\widehat{\nabla^2\delta}(\mathbf{r}) = \int d^2k\;(-k^2)e^{i\mathbf{k}\cdot\mathbf{r}} \tag{6.62}$$

the potential recover its real-space-form as

$$V(\mathbf{r}) = \sum_{p=0}^{\infty} A_p\nabla^{2p}\delta(\mathbf{r}) \tag{6.63}$$

Now it is possible to relate any other central potential to the one in (6.63) by finding the $A_p$. First write the pseudopotentials in the Fourier space

$$V_m = \int \frac{d^2k}{(2\pi)^2}\; V(\mathbf{k})\,\langle m|e^{i\mathbf{k}\cdot\mathbf{r}}|m\rangle \tag{6.64}$$

Perform the transformation

$$\mathbf{k}\cdot\mathbf{r} = \frac{\bar{k}z + k\bar{z}}{2} = \frac{\bar{k}(a + b^\dagger) + k(a^\dagger + b)}{\sqrt{2}} \tag{6.65}$$

and neglect the $a, a^\dagger$ since they do not contribute in the LLL, to give

$$\begin{aligned}
\langle m|e^{-i\mathbf{k}\cdot\mathbf{r}}|m\rangle &= \langle m|e^{i\frac{\bar{k}b^\dagger + kb}{\sqrt{2}}}|m\rangle \\
&= e^{-\frac{k\bar{k}}{2}}\langle m|e^{i\frac{\bar{k}b^\dagger}{\sqrt{2}}}e^{i\frac{kb}{\sqrt{2}}}|m\rangle \\
&= e^{-\frac{k^2}{2}}\sum_{j=0}^{\infty}\frac{1}{(j!)^2}\langle m|\left(i\frac{\bar{k}b^\dagger}{\sqrt{2}}\right)^j\left(i\frac{kb}{\sqrt{2}}\right)^j|m\rangle \\
&= e^{-\frac{k^2}{2}}\sum_{j=0}^{m}\frac{(-k^2)^j}{2^j j!}\frac{m!}{j!(m-j)!} \\
&= e^{-\frac{k^2}{2}}L_m\left(\frac{k^2}{2}\right)
\end{aligned} \tag{6.66}$$

having used the relation for $j \leqslant m$

$$b^j|m\rangle = \sqrt{\frac{m!}{(m-j)!}}|m-j\rangle \tag{6.67}$$

and introduced the Laguerre polynomials in the closed form

$$L_m(x) = \sum_{j=0}^{m}\binom{m}{j}\frac{(-1)^j x^j}{j!} \tag{6.68}$$

From this one can expand again

$$V(\mathbf{r}) = \sum_{j=0}^{\infty} V_j L_j(-\nabla^2)\delta(\mathbf{r}) \tag{6.69}$$

and thus possible to relate to the (6.63) as

$$A_p = \sum_{j=p}^{\infty}\binom{j}{j-p}\frac{V_j}{p!} \tag{6.70}$$

Why are these $\nabla^{2p}\delta(\mathbf{r})$ potentials interesting ? They are the most simple non-trivial potentials for fermions, taking $p$ odd. They appear to be almost local but mostly short-range. To observe how these two-points potentials act on Laughlin states, take their form in the disk geometry

$$\psi_{M,m} = \langle\mathbf{r}|M,m\rangle \sim (z_1+z_2)^M(z_1-z_2)^m e^{-\frac{|z_1|^2+|z_2|^2}{4}} \tag{6.71}$$

having set $l_B = 1$. Perform the change of variables

$$Z = \frac{z_1+z_2}{2} \quad \text{and} \quad z = z_1 - z_2 \tag{6.72}$$

and take into account the normalization, get

$$\psi_{M,m} = \frac{Z^M}{\sqrt{\pi M!}}\frac{z^m}{\sqrt{2\pi 2^{2m+1}m!}}e^{-\frac{|z|^2}{8}-\frac{|Z|^2}{2}} \tag{6.73}$$

Consider only the dependence on $m$ in the state and the interaction (6.63) with $p = 1$. Then

$$\begin{aligned} V_m &= \langle m|\nabla^2\delta^{(2)}(\mathbf{r})|m\rangle \\ &= \int dz d\bar{z}\ \nabla^2\delta^{(2)}(\mathbf{r})|\psi_m|^2 \\ &\overset{\text{IBP}}{=} \int dz d\bar{z}\ \delta(z)\delta(\bar{z})\nabla^2|\psi_m|^2 \end{aligned} \tag{6.74}$$

First notice that the boundary terms have been neglected, since the dependence on a Gaussian. Then

$$\nabla^2 = \partial_x^2 + \partial_y^2 = (\partial_x + i\partial_y)(\partial_x - i\partial_y) = \partial_z\partial_{\bar{z}} \tag{6.75}$$

which allows to compute

$$\begin{aligned} \nabla^2|\psi_m|^2 &\sim \partial_z(z^m\bar{z}^{m-1} + z^{m+1}\bar{z}^m)e^{-z\bar{z}} \\ &\sim (z^{m-1}\bar{z}^{m-1} + z^m\bar{z}^m + z^{m+1}\bar{z}^{m+1})e^{-z\bar{z}} \end{aligned} \tag{6.76}$$

and plugin it into the integral, the term $V_m$ vanishes unless $m = 1$, since any dependence in $z$ or $\bar{z}$ gives $0$ due to the Dirac $\delta$. This forces the conclusion that the Laughlin-$\frac{1}{3}$ state is the most compact ground state of the interaction, which is then the parent Hamiltonian of this system of interacting fermions. The most compact since any multiplication by a non-constant symmetric polynomial in $z, \bar{z}$ makes the radius $R \sim \sqrt{2m}$ increase and the $m = 0$ no longer used. Hence pursuing the derivation

$$\nabla^{2p}|\psi_m|^2 \sim \sum_{j=-p}^{p} c_j z^{m-j}\bar{z}^{m-j}e^{-z\bar{z}} \tag{6.77}$$

and the states with $m > p$ will have no contribution. Avoiding the singularities, take the only vanishing term is $m = p$. That confirms the focus on the $p$ odd terms.

There is also a connection to make with these matrix elements in the higher LLs. Indeed,
electron interacting with a $V(\mathbf{r})$ in higher LLs is equivalent to take a effective potential $V_{\text{eff}}(\mathbf{r})$ the LLL

$$\langle n, m_1'; n, m_2'|V(\mathbf{r})|n, m_1; n, m_2\rangle = \langle m_1', m_2'|V_{\text{eff}}(\mathbf{r})|m_1, m_2\rangle \tag{6.78}$$

with, derived in the same way as in (6.66),

$$V_{\text{eff}}(\mathbf{k}) = L_n^2\left(\frac{k^2}{2}\right)V(\mathbf{k}) \tag{6.79}$$

# Part II

# NUMERICAL

# 7 EXACT DIAGONALIZATION

## 7.1 GENERALITIES

Exact diagonalization of the Hamiltonian enables to reach the complete knowledge of a quantum spin system. In general, every finite system can be diagonalized numerically, but limited to small system because computationally inefficient since the size of the basis increases exponentially in the system size. To reach the thermodynamic limit, one needs to seek for block-diagonalization first, as shown on Figure 7.1. The symmetries are of great interest, and one shall not use group theory to reduce the Hamiltonian but rather introduce a more practical approach.

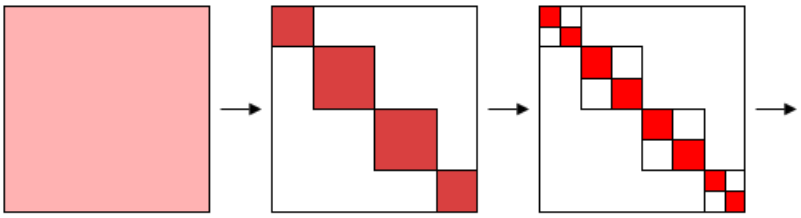

*Figure* 7.1 – Schematic picture of the block-diadonalization process, reducing their size after applying a symmetry of the Hamiltonian.

For the rest of the discussion, one takes the $S = 1/2$ antiferromagnetic Heisenberg Hamiltonian

$$\begin{aligned}\mathcal{H} &= J \sum_{i=0}^{N-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} \\ &= J \sum_{i=0}^{N-1} S_i^z S_{i+1}^z + \frac{J}{2} \sum_{i=0}^{N-1} [S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+]\end{aligned} \tag{7.1}$$

with periodic boundary conditions $\mathbf{S}_N = S_0$. Also, work with the states $\left|S_0^z, \ldots, S_{N-1}^z\right\rangle$.

Now discuss the symmetries.

## 7.2 TRANSLATION

Define the translation operator as

$$T \left|S_0^z, \ldots, S_{N-1}^z\right\rangle = \left|S_{N-1}^z, S_0^Z, \ldots, S_{N-2}^z\right\rangle \tag{7.2}$$

which corresponds tot decreasing the spin index by one at each site. It is important to note that the Hamiltonian (7.1) is invariant under the action of T, that is

$$[\mathcal{H}, T] = 0 \tag{7.3}$$

Therefore, one can construct the momentum states $|a(k)\rangle$ as

$$T|a(k)\rangle = e^{ik}|a(k)\rangle \tag{7.4}$$

with the momentum allowed being

$$k = \frac{2\pi}{N}m \quad \text{with} \quad m = -N/2+1,\dots,N/2 \tag{7.5}$$

since $T^N = \mathbb{1}$ and lattice constant equal to 1. Then, it is possible to introduce a reference state $|a\rangle$, which is a single state in the $z$-component basis, giving

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}}\sum_{r=0}^{N-1} e^{-ikr}T^r|a\rangle \tag{7.6}$$

To find a complete set of normalizable orthogonal states, start by seeing that

$$\langle a(k)|b(k)\rangle = 0 \iff T^r|a\rangle \neq |b\rangle \ \ \forall r \tag{7.7}$$

Hence, only one of the states in the set of translated states $T^r|a\rangle$ can be chosen as a representative.

If all $T^r|a\rangle$ are distinct, then $N = N_a$. But if the periodicity is less than $N$, it can be chosen as the smallest $R_a$ such that

$$T^{R_a}|a\rangle = |a\rangle \quad \text{with} \quad R_a \in \{1,\dots,N\} \tag{7.8}$$

To correctly relate the normalization factor to $R_a$ instead of restricting the summation up to $r = R_a$, take the sum of the phases

$$\begin{aligned} F(k,R_a) &= \sum_{n=0}^{N/R_a-1} e^{-iknR_a} \\ &= \begin{cases} N/R_a & \text{if } kR_a \equiv 0 \mod 2\pi \\ 0 & \text{otherwise} \end{cases} \end{aligned} \tag{7.9}$$

Thus

$$N_a = R_a|F(k,R_a)|^2 \tag{7.10}$$

This means that $F(k,R_a) = 0$ is not allowed, and hence for a given $|a\rangle$, $k = \frac{2\pi}{R_a}m$ with $m = 0,\dots,R_a-1$ and

$$N_a = \frac{N^2}{R_a} \tag{7.11}$$

Now construct the Hamiltonian matrix in the momentum basis. To simplify, define

$$\mathcal{H} = J\sum_{j=0}^{N}\mathcal{H}_j \tag{7.12}$$

with

$$\mathcal{H}_0 = \sum_{i=0}^{N-1} S_i^z S_{i+1}^z \quad \text{and} \quad \mathcal{H}_j = \frac{1}{2}[S_j^+S_{j+1}^- + S_j^-S_{j+1}^+] \tag{7.13}$$

and set $J = 1$. Then, according to (7.3), write

$$\begin{aligned}\mathcal{H}\,|a(k)\rangle &= \frac{1}{\sqrt{N_a}}\sum_{r=0}^{N-1} e^{-ikr}T^r\mathcal{H}\,|a\rangle \\ &= \frac{1}{\sqrt{N_a}}\sum_{j=0}^{N}\sum_{r=0}^{N-1} e^{-ikr}T^r\mathcal{H}_j\,|a\rangle\end{aligned} \tag{7.14}$$

This allows to write

$$\begin{aligned}\mathcal{H}_j\,|a\rangle &= h_j(a)\,\left|b'_j\right\rangle \\ &= h_j(a)T^{-l_j}\,\left|b'_j\right\rangle \quad \text{with} \quad l_j = 0,\ldots,N-1\end{aligned} \tag{7.15}$$

giving finally

$$\begin{aligned}\mathcal{H}\,|a(k)\rangle &= \sum_{j=0}^{N}\frac{h_j(a)}{\sqrt{N_a}}\sum_{r=0}^{N-1} e^{-ikr}T^{r-l_j}\,\left|b_j\right\rangle \\ &= \sum_{j=0}^{N} h_j(a)e^{-ikl_j}\sqrt{\frac{N_{b_j}}{N_a}}\,\left|b_j(k)\right\rangle\end{aligned} \tag{7.16}$$

Therefore, the matrix elements are

$$\left\langle b_j(k)\middle|\mathcal{H}_j\middle|a(k)\right\rangle = h_j(a)e^{-ikl_j}\sqrt{\frac{N_{b_j}}{N_a}} \tag{7.17}$$

Overall, trading $h_j(a)$ by the values of the diagonal and off-diagonal elements, get

$$\begin{aligned}\langle a(k)|\mathcal{H}_0|a(k)\rangle &= \sum_{j=1}^{N} S_j^z S_j^z \\ \text{and} \quad \left\langle b_j(k)\middle|\mathcal{H}_{j>0}\middle|a(k)\right\rangle &= \frac{e^{-ikl_j}}{2}\sqrt{\frac{R_a}{R_{b_j}}}\end{aligned} \tag{7.18}$$

## 7.3 INVERSION

Define the magnetization in the direction of the quantization axis $z$ as

$$m_z = \sum_{j=0}^{N-1} S_j^z \tag{7.19}$$

For the case $m_z = 0$ for $N$ even, one can block-diadonalize using a discrete subspace of all the possible spin-rotations, the spin inversion symmetry that is the invariance with respect to flipping all the spins. It is defined as

$$Z\left|S_0^z,\ldots,S_{N-1}^z\right\rangle = \left|-S_0^Z,\ldots,-S_{N-1}^z\right\rangle \tag{7.20}$$

For this operator, one has $Z^2 = \mathbb{1}$. It is thus possible to block-diadonalize the Hamiltonian in the $m_z = 0$ sector. Denote by$z = \pm 1$ the eigenvalues of $Z$. Since

$$[Z, T] = 0 \tag{7.21}$$

one can further reduce the size of the blocks by writing first

$$|a(k,z)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r [1 + zZ] |a\rangle \tag{7.22}$$

with the normalization constant

$$N_a = \frac{2N^2}{R_a} \begin{cases} 1 & T^m Z |a\rangle \neq |a\rangle \ \ \forall m \\ 1 + z\cos km & T^m Z |a\rangle = |a\rangle \end{cases} \tag{7.23}$$

The Hamiltonian then acts as

$$\mathcal{H}_j |a\rangle = h_j(a) Z^{g_j} T^{-l_j} \left|b_j\right\rangle \quad \text{with} \quad g_j = 0, 1 \tag{7.24}$$

giving the matrix elements

$$\left\langle b_j(k,z)\right|\mathcal{H}_j\left|a(k,z)\right\rangle = h_j(a) z^{g_j} e^{-ikl_j} \sqrt{\frac{N_{b_j}}{N_a}} \tag{7.25}$$

valid $\forall k$

## 7.4 PARITY

The Hamiltonian also commutes with the parity operator

$$P \left|S_0^z, \ldots, S_{N-1}^z\right\rangle = \left|S_{N-1}^Z, \ldots, -S_1^z, S_0^z\right\rangle \tag{7.26}$$

with $P^2 = \mathbb{1}$ and thus the eigenvalues $p = \pm 1$. But

$$[P, T] \neq 0 \tag{7.27}$$

in general, but they commute for $k = 0, \pi$. To show that, write

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r [1 + pP] |a\rangle \tag{7.28}$$

Since $PT = T^{-1}P$, one has

$$\begin{aligned} P |a(k,p)\rangle &= \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^{-}r [1 + P] |a\rangle \\ &= p \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{ikr} T^r [1 + pP] |a\rangle \end{aligned} \tag{7.29}$$

which is (7.28) for $k = 0, \pi$ and in this cases the block-diadonalization can be made using the both parity and translational invariance.

But one is interesting in block-diadonalization for the general case. Hence, it is possible to mix momentum states with $\pm k$ and thereby consider the semi-momentum states

$$|a^\sigma(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} C_k^\sigma(r) T^r |a\rangle \tag{7.30}$$

where $\sigma$ stands for the spin $\sigma = \pm 1$ and

$$C_k^\sigma(r) = \begin{cases} \cos kr & \sigma = +1 \\ \sin kr & \sigma = -1 \end{cases} \tag{7.31}$$

Consider only half of the first Brillouin zone $0 \leqslant k \leqslant \pi$. With some workaround not interesting here for the normalization and orthogonality, one can find

$$|a^\sigma(k,p)\rangle = \frac{1}{\sqrt{N_a^\sigma}} \sum_{r=0}^{N-1} C_k^\sigma(r)[1 + pP]T^r |a\rangle \tag{7.32}$$

and pursue the computation to fanilly find the matrix elements for the semi-momentum states.

## 7.5 THE LANCZOS METHOD

Performing complete diagonalization becomes rapidly time consuming. It is therefore sometimes useful to restrict to only find the ground state and possibly some excited states. The Lanczos algorithm is a Krylov-space technique that allows this.

The Krylov space is a subspace of the full Hilbert space such that the low-lying excited states are well approximated within it. Consider a random state $|\psi\rangle$ and $M$ the dimension of the full Hilbert space. Then express it as a linear combination of the eigenstates $|\psi_n\rangle$ of the Hamiltonian

$$\begin{aligned} \mathcal{H}^\Lambda |\psi\rangle &= \sum_{n=0}^{M-1} c_n E_n^\Lambda |\psi_n\rangle \\ &= c_{max} E_{max}^\Lambda \left[ |\psi_{max}\rangle + \sum_{n \neq n_{max}} \frac{c_n}{c_{max}} \left( \frac{E_n}{E_{max}} \right)^2 |\psi_n\rangle \right] \end{aligned} \tag{7.33}$$

For a large $\Lambda$, the state with eigenvalue $|E_{max}|$ will dominate the sum provided $c_{max} \neq 0$ obviously. Hence, acting with the Hamiltonian many times will project out the eigenvector with the largest-magnitude eigenvalue. To reach the ground state $|\psi_0\rangle$, one must apply $(-c)^\Lambda$ instead, with $c$ ensuring that $|E_0 - c| > |E_{M-1} - c|$, typically $c = E_{max}$. In what follows, assume such constant is already absorbed in the Hamiltonian if needed.

A more efficient way to obtain the ground state for $\Lambda \to \infty$ is to consider the whole subspace spanned by the set of $\mathcal{H}^m |\psi\rangle$ with $m = 0, \ldots, \Lambda$. This composes the Krylov space. The Lanczos method consists in constructing an orthogonal basis using linear combination of the states in the Krylov space such that the Hamiltonian is tridiagonal in it. This procedure is like the Gram-Schmidt orthonormalization. Start with a random state normalized $|\phi_0\rangle$. Then

$$|\phi_1\rangle = \frac{1}{\sqrt{N_1}} \underbrace{[\mathcal{H}|\phi_0\rangle - a_0 |\phi_0\rangle]}_{|\gamma_1\rangle} \tag{7.34}$$

so that $\langle\phi_0|\phi_1\rangle = 0$ and $\langle\phi_0|\mathcal{H}|\phi_0\rangle = a_0$, which gives $N_1 = \langle\gamma_1|\gamma_1\rangle$. Repeat the procedure to have in general

$$|\phi_{m+1}\rangle = \frac{1}{\sqrt{N_{m+1}}} \underbrace{[\mathcal{H}\,|\phi_m\rangle - a_m\,|\phi_m\rangle - \sqrt{N_m}\,|\phi_{m-1}\rangle]}_{|\gamma_{m+1}\rangle} \tag{7.35}$$

with

$$a_m = \langle\phi_m|\mathcal{H}|\phi_m\rangle \quad \text{and} \quad N_m = \langle\gamma_m|\gamma_m\rangle \tag{7.36}$$

requiring it to be orthogonal to all the previous states. Indeed

$$\begin{aligned}
\langle\phi_{m+1}|\phi_{m-k}\rangle &= \frac{1}{\sqrt{N_{m+1}}}\,\langle\phi_m|\mathcal{H}|\phi_{m-k}\rangle \\
&= \frac{1}{\sqrt{N_{m+1}}}[\sqrt{N_{m-k+1}}\,\langle\phi_m|\phi_{m-k+1}\rangle \\
&+ a_{m-k}\,\langle\phi_m|\phi_{m-k}\rangle \\
&+ \sqrt{N_{m-k}}\,\langle\phi_m|\phi_{m-k-1}\rangle] \\
&= 0
\end{aligned} \tag{7.37}$$

supposing all the previously generated states are orthogonal to each other. Therefore

$$\mathcal{H}\,|\phi_m\rangle = \sqrt{N_{m+1}}\,|\phi_{m+1}\rangle + a_m\,|\phi_m\rangle + \sqrt{N_m}\,|\phi_{m-1}\rangle \tag{7.38}$$

or writing in tridiagonal form, with $b_m = \sqrt{N_{m+1}}$

$$\mathcal{H} \doteq \begin{pmatrix} a_0 & b_0 & & \\ b_0 & a_1 & b_1 & \\ & b_1 & a_2 & \ddots \\ & & \ddots & \ddots \end{pmatrix} \tag{7.39}$$

# 8 MONTE CARLO

## 8.1 MONTE CARLO INTEGRATION

Classical integration methods can be given by the Riemann sum, or better by the trapezoidal formula or the Simpson rule. For d-dimensional of N-body simulations, the convergence is slow, even slower for higher d. This implies finding a better method for carrying integrations. The Monte Carlo provides this.

In general, consider a quantity $f$ distributed with a Gaussian with mean value $\langle f \rangle$ and variance $\sigma^2$. Then, an unbiased estimator for $\langle f \rangle$ is

$$\bar{f} = \frac{1}{N} \sum_{i=1}^{N} f_i \tag{8.1}$$

and the error of this estimator is

$$\Delta = \frac{\sigma}{\sqrt{N}} \tag{8.2}$$

To compute this, use the unbiased estimator the variance and thus the standard error of averages from uncorrelated estimates is

$$\Delta = \sqrt{\frac{\left\langle \overline{f^2} - \bar{f}^2 \right\rangle}{N-1}} \tag{8.3}$$

Often, the function integrated is peaked around a small region of the phase space and has a large variance, hence a large error, and a lot a time is wasted to compute the integral is the regions where $f$ does not lie. Hence, instead of picking $x_i$ randomly uniformly, choose them according to a probability distribution $p(x)$. This is called this importance sampling.

The integral can be taken approximately as

$$\langle f \rangle = \frac{1}{\Omega} \int dx\, f(x) \overset{\text{estimator}}{=} \frac{1}{N} \sum_{i=1}^{N} f(x_i) \tag{8.4}$$

but this method is not ideal. Hence, via importance sampling, write

$$\langle f \rangle = \frac{1}{\Omega} \int dx\, \frac{f(x)}{p(x)} p(x) \overset{\text{estimator}}{=} \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{p(x_i)} \tag{8.5}$$

taking $p$ similar to $f$, which leads to the ratio $\frac{f}{p}$ being almost constant so that the its variance and hence its error being small.

## 8.2 METROPOLIS–HASTINGS ALGORITHM

Before introducing the Metropolis-Hastings algorithm, first present the Markov chain. A Markov chain is a Markov process that allows to create a $p$-distributed configurations from scratch. The chain is constructed as

$$x_0 \to x_1 \to x_2 \to \cdots \to x_n \to x_{n+1} \to \cdots \tag{8.6}$$

staying in 1D for simplicity. It must have the property that

$$\mathcal{P}(x_{n+1} = j | x_n = i_n, \ldots, x_0 = i_0) = \mathcal{P}(x_{n+1} = j | x_n = i_n) \tag{8.7}$$

meaning that the information from the previous steps is not relevant for the next step; this is memoryless. Define the transition probability as

$$w_{ij} = \mathcal{P}(x_1 = j | x_0 = i) \tag{8.8}$$

and the chain is said to be homogeneous if

$$\mathcal{P}(x_{n+1} = j | x_n = i) = \mathcal{P}(x_n = j | x_{n-1} = i) \tag{8.9}$$

which is the one one will consider from now on. The transition matrix of the chain is given by $W = (w_{ij})$. The goal here is to find the distribution $p$, to which the Markov chain must converge. Hence, the Markov chain Monte Carlo method aims at generating randomly $N$ states $(x_1, \ldots, x_N)$ according to the distribution $p$, creating $x_{n+1}$ only from $x_n$, thus creating the transition matrix $W$ so that for any distribution $\mu$

$$W^k \mu \xrightarrow{k \to \infty} p \tag{8.10}$$

thus, so that $\mu$ converges towards the distribution $p$ one wants to sample.

The Metropolis-Hastings algorithm ensures that the Markov chain converges towards $p$. It requires some properties. These are, noting the notation $W_{xy} = W(x|y)$

**NORMALIZATION** $\sum_y W(x|y) = 1$

**ERGODICITY** $\forall x, y,\ \exists n \mid W^n(x|y) \neq 0$

**DETAILED BALANCE** $p(x)W(y|x) = p(y)W(x|y)$

The ergodicity condition means that it is possible to reach any configuration $x$ from any other $y$ in a finite number of Markov steps. The algorithm is done by splitting $W$ into two factors. When moving from $x$ to $y$, first select $y$ with probability $g(y|x) \neq 0$ and accept or reject the candidate with acceptance probability $A(y|x)$ as

$$W(y|x) = \begin{cases} g(y|x)A(y|x) & y \neq x \\ 1 - \sum_{x' \neq x} W(x'|x) & y = x \end{cases} \tag{8.11}$$

The detailed balance condition then becomes

$$\frac{A(y|x)}{A(x|y)} = \frac{p(y)}{p(x)} \frac{g(x|y)}{g(y|x)} \tag{8.12}$$

so that $A$ has to be chosen as

$$A(y|x) = \begin{cases} F\left(\frac{p(y)}{p(x)}\frac{g(x|y)}{g(y|x)}\right) & \text{if } g(y|x) \neq 0 \\ 0 & \text{otherwise} \end{cases} \tag{8.13}$$

with $F : ]0, \infty] \to ]0, 1]$ satisfying

$$F(k) = kF\left(\frac{1}{k}\right) \tag{8.14}$$

and thus here one can choose $F(k) = \min(1, k)$. The algorithm is therefore as follows

- generate the initial state $x_0$
- at step $n$, generate $y_{n+1}$ with the law $g(y_{n+1}|x_n)$
- select a number $a \in [0, 1]$ with uniform probability
- if $a < A(y_{n+1}|x_n)$ accept the candidate $x_{n+1} = y_{n+1}$, else reject it $x_{n+1} = x_n$

As an example of relevant Metropolis-Hastings algorithms for spin lattices, consider the single-spin-flip algorithm. It enables to study thermodynamics of spin systems at equilibrium. Hence, sample the states with Boltzmann distribution

$$p(x) = \frac{1}{Z}e^{-\beta E(x)} \tag{8.15}$$

on an Ising model of $N$ spins. Then, the selection is taken as

$$g(y|x) = \begin{cases} \frac{1}{N} & \text{if } x \text{ and } y \text{ differ by a single spin flip} \\ 0 & \text{otherwise} \end{cases} \tag{8.16}$$

and the acceptance

$$A(y|x) = \min\left(1, \frac{p(y)}{p(x)}\right) = \min\left(1, e^{-\beta[E(y)-E(x)]}\right) \tag{8.17}$$

## 8.3 AUTOCORRELATIONS

As saw in the beginning, the error is easily computed when the observations are uncorrelated. But for Monte Carlo process, one needs to take into account the correlations between configurations. Denote by $f(t)$ the measurement of $f$ at the $t$-th Monte Carlo step. Taking $N \to \infty$, the error becomes

$$\begin{aligned} \Delta^2 &= \frac{\left\langle \overline{f^2} - \overline{f}^2 \right\rangle}{N-1} + \frac{2}{N^2}\sum_{t=1}^{N}\sum_{\delta t=1}^{N-t} \langle f(t)f(t+\delta)\rangle - \langle f\rangle^2 \\ &= \frac{\left\langle \overline{f^2} - \overline{f}^2 \right\rangle}{N-1}[1 + 2\tau_f] \end{aligned} \tag{8.18}$$

assuming that

$$\langle f(t)f(t+\delta t)\rangle - \langle f\rangle^2 \propto e^{-\frac{\delta t}{\tau_f}} \tag{8.19}$$

with the autocorrelation time

$$\tau_f = \frac{\sum_{\delta t=1}^{\infty} \langle f(t)f(t+\delta)\rangle - \langle f\rangle^2}{\langle f^2\rangle - \langle f\rangle^2} \tag{8.20}$$

To find a more reliable way to estimate the autocorrelation time, use the binning analysis. Starting for the original measurements $f_i^{(0)}$, $i = 1,\ldots,N$ iteratively create binned series by averaging over consecutive entries

$$f_i^{(l)} = \frac{1}{2}\left[f_{2i-1}^{(l-1)} + f_{2i}^{(l-1)}\right] \quad \text{with} \quad i = 1,\ldots,N_l \tag{8.21}$$

with $N_l = 2^{-l}N$. Basically, the bin averages $f_i^{(l)}$ are less correlated than the original values, keeping the mean value intact. The errors now become

$$\Delta^{(l)} = \sqrt{\frac{\left\langle \overline{f^{(l)\,2}} - \overline{f^{(l)}}^2 \right\rangle}{N_l - 1}} \tag{8.22}$$

and increases as a function of the bin size $2^l$. For $2^l \gg \tau_f$recover the correct error estimate

$$\Delta = \lim_{l\to\infty} \Delta^{(l)} \tag{8.23}$$

The autocorrelation time is found, if convergence, as

$$\tau_f = \lim_{l\to\infty} \frac{1}{2}\left[\left(\frac{\Delta^{(l)}}{\Delta^{(0)}}\right)^2 - 1\right] \tag{8.24}$$

But if no convergence is obtained, $\tau_f$ is much longer and must run longer simulation to find reliable error estimates.

For functions of measurements like

$$\langle U\rangle = \frac{\langle A\rangle}{\langle B\rangle} \tag{8.25}$$

it becomes difficult to perform binning analysis because of error propagation and cross-correlations. Therefore, us Jackknife analysis instead. Again split the measurements into $M$ bins of size $\frac{N}{M} \gg \tau$. Now, instead of evaluating $U$ in each of the bins obtaining the error estimate out of the variance of these estimates, which is not good since too small number of measurements lie in each bin, use the following. Work with $M+1$ evaluations of $U$, $U_0$ being the estimate using all bins and $U_i$, $i = 1,\ldots,M$ when all bins except the $i$-th are used. Then a larger data set is used. Hence the resulting estimation for $U$ is

$$\langle U\rangle = U_0 - (M-1)(\overline{U} - U_0) \quad \text{with} \quad \overline{U} = \frac{1}{M}\sum_{i=1}^{M} U_i \tag{8.26}$$

with error

$$\begin{aligned}\Delta &= \sqrt{\frac{M-1}{M}\sum_{i=1}^{M} u_i^2 - \overline{u}^2} \\ &= \sqrt{(M-1)\left(\overline{u^2} - \overline{u}^2\right)}\end{aligned} \tag{8.27}$$

Finally, one can talk about equilibration, or thermalization. The Markov chain converges only asymptotically. Hence, Monte Carlo measurements should be started only after a large number of steps which mist be much larger than the thermalization time

$$\tau_f^{(th)} = \frac{\sum_{\delta t=1}^{\infty} \langle f(0) f(\delta t)\rangle - \langle f\rangle^2}{\langle f(0)\rangle \langle f(\delta t)\rangle - \langle f\rangle^2} \tag{8.28}$$

It can be shown that the thermalization time is the maximum of all autocorrelation times. In practice, thermalize at least 10 times $\tau_f^{(th)}$ before starting measurements.

# 9 STOCHASTIC SERIES EXPANSION

## 9.1 PATH INTEGRAL

The path integral offers a way to deal with the Boltzmann operator $e^{-\beta\mathcal{H}}$ and especially its trace. This is useful when exact diagonalization becomes hard to be done.

Start with writing

$$Z = \operatorname{tr} e^{-\beta\mathcal{H}} = \operatorname{tr} \prod_{l=1}^{L} e^{-\Delta_\tau \mathcal{H}} \tag{9.1}$$

with $\Delta_\tau = \frac{\beta}{L}$. A complete basis can be inserted between each branch, since the trace can be expressed as a sum of diagonal elements in any basis

$$\begin{aligned} Z &= \sum_{\alpha_0} \cdots \sum_{\alpha_{L-1}} \langle \alpha_0 | e^{-\Delta_\tau \mathcal{H}} | \alpha_{L-1} \rangle \cdots \langle \alpha_1 | e^{-\Delta_\tau \mathcal{H}} | \alpha_0 \rangle \\ &= \sum_{\{\alpha\})} W(\{\alpha\})) \end{aligned} \tag{9.2}$$

The argument in the exponential can be viewed as the Schrödinger time evolution operator $e^{-it\mathcal{H}}$ with the identification $\hbar = 1$ and the imaginary time $t = -i\Delta_\tau$. The $W(\{\alpha\})$ are the weights of a world line configuration $\{\alpha\})$.

## 9.2 SERIES EXPANSION REPRESENTATION

Before the path integral was introduced in this subject, the series expansion of the operator was predominant. Then a more general method, the stochastic series expansion, revived it to compute traces exactly by also sampling them. Construct a configuration space for MC sampling by Taylor expanding the operator

$$e^{-\beta\mathcal{H}} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \mathcal{H}^n \tag{9.3}$$

Introducing a complete basis

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_n} \langle \alpha_0 | \mathcal{H} | \alpha_{n-1} \rangle \cdots \langle \alpha_1 | \mathcal{H} | \alpha_0 \rangle \tag{9.4}$$

Taking a boson system with only the kinetic energy, the Hamiltonian is

$$\mathcal{H} = -\sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) \tag{9.5}$$

and in this case, all the matrix element are the same so that

$$W(\{\alpha\}_n) = \frac{\beta^n}{n!} \tag{9.6}$$

Also, the weights are positive definite, for bosons systems and quantum spins without frustration in the off-diagonal terms. Follow under this assumption.

The energy is expressed as

$$\begin{aligned} E &= -\frac{\partial \ln Z}{\partial \beta} = \langle \mathcal{H} \rangle = \frac{1}{Z} \operatorname{tr} \mathcal{H} e^{-\beta \mathcal{H}} \\ &= \frac{1}{Z} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_{n+1}} \langle \alpha_0 | \mathcal{H} | \alpha_n \rangle \cdots \langle \alpha_1 | \mathcal{H} | \alpha_0 \rangle \\ &= -\frac{1}{Z} \sum_{n=1}^{\infty} \frac{(-\beta)^n}{n!} \frac{n}{\beta} \sum_{\{\alpha\}_n} \langle \alpha_0 | \mathcal{H} | \alpha_n \rangle \cdots \langle \alpha_1 | \mathcal{H} | \alpha_0 \rangle \\ &= -\frac{1}{Z} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \frac{n}{\beta} \sum_{\{\alpha\}_n} \langle \alpha_0 | \mathcal{H} | \alpha_n \rangle \cdots \langle \alpha_1 | \mathcal{H} | \alpha_0 \rangle \end{aligned} \tag{9.7}$$

and (9.4) and (9.7) match considering $\frac{n}{\beta}$ as the energy estimator. Thus

$$E = -\frac{\langle n \rangle}{\beta} \tag{9.8}$$

If the Hamiltonian is written as

$$\mathcal{H} = -\sum_i \mathcal{H}_i \tag{9.9}$$

then there is an expression for the expectation value of an individual $\mathcal{H}_i$ which is the average number of times it appears in the expansion of the partition function

$$\langle \mathcal{H}_i \rangle = \frac{\langle n_i \rangle}{\beta} \tag{9.10}$$

Actually, one can take $n = \infty$ in the expression for the energy. But one can truncate it at $n_{max} \propto N\beta$ in practice. Take for instance the specific heat

$$C = \frac{\partial E}{\partial \beta} = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle \tag{9.11}$$

When $T \to 0$, $C \to 0$ and then $\langle n^2 \rangle - \langle n \rangle^2 \sim \langle n \rangle$. Hence, the variance of the distribution of $n$ goes like $\langle n \rangle$ and therefore the distribution vanishes exponentially beyond some $n_{max}$.

## 9.3 SSE FOR THE $S = \frac{1}{2}$ HEISENBERG MODEL

Consider the Heisenberg Hamiltonian as a sum of bond operators

$$\mathcal{H}_b = J_b \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)} \tag{9.12}$$

with the lattice encoded as a list of sites $[i(b), j(b)]$ connected by the bond $b = 1, \ldots, N_b$. A positive definite SSE can be constructed for any bipartite lattice, for $i(b)$ in sublattice A and $j(b)$ in B. Take $J_b = J > 0$.

One can further divide the Heisenberg interaction into its diagonal and off-diagonal parts in the $z$-component of the spin. Thus define bond operators

$$\begin{aligned} \mathcal{H}_{1,b} &= \frac{1}{4} - S^z_{i(b)} S^z_{j(b)} \\ \mathcal{H}_{2,b} &= \frac{1}{2}[S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}] \end{aligned} \tag{9.13}$$

which implies the Hamiltonian

$$\mathcal{H} = \frac{JN_b}{4} - J \sum_{b=1}^{N_b} [\mathcal{H}_{1,b} - \mathcal{H}_{2,b}] \tag{9.14}$$

The starting point of the SSE algorithm for this Hamiltonian is to write the partition function as

$$Z = \sum_{\alpha} \sum_{n=0}^{\infty} (-1)^{n_2} \frac{\beta^n}{n!} \sum_{S_n} \langle \alpha | \prod_{p=0}^{n-1} \mathcal{H}_{a(p),b(p)} | \alpha \rangle \tag{9.15}$$

with $\beta = \frac{J}{T}$ having absorbed the coupling, $S_n$ the product of the bond operators

$$S_n = [a(0), b(0)], [a(1), b(1)], \ldots, [a(n-1), b(n-1)] \tag{9.16}$$

and $n_2$ is the number of off-diagonal operators. The action on the state

$$|\alpha\rangle = \left| S^z_1, \ldots, S^Z_N \right\rangle \tag{9.17}$$

by the string of operators, one gets a succession, propagated states

$$|\alpha(n)\rangle \propto \prod_{p=0}^{n-1} \mathcal{H}_{a(p),b(p)} |\alpha\rangle \tag{9.18}$$

It is useful to observe that

$$\begin{aligned} \mathcal{H}_{1,b} \left| \uparrow_{i(b)} \uparrow_{j(b)} \right\rangle &= 0 \qquad \mathcal{H}_{1,b} \left| \downarrow_{i(b)} \downarrow_{j(b)} \right\rangle = 0 \\ \mathcal{H}_{2,b} \left| \uparrow_{i(b)} \uparrow_{j(b)} \right\rangle &= 0 \qquad \mathcal{H}_{2,b} \left| \downarrow_{i(b)} \downarrow_{j(b)} \right\rangle = 0 \end{aligned} \tag{9.19}$$

and then the configurations $(\alpha, S_n)$ contributing to $Z$ must involve antiparallel spins, since

$$\begin{aligned} \left\langle \uparrow_{i(b)} \downarrow_{j(b)} \middle| \mathcal{H}_{1,b} \middle| \uparrow_{i(b)} \downarrow_{j(b)} \right\rangle &= \frac{1}{2} \quad \left\langle \downarrow_{i(b)} \uparrow_{j(b)} \middle| \mathcal{H}_{1,b} \middle| \uparrow_{i(b)} \downarrow_{j(b)} \right\rangle = \frac{1}{2} \\ \left\langle \uparrow_{i(b)} \downarrow_{j(b)} \middle| \mathcal{H}_{2,b} \middle| \uparrow_{i(b)} \downarrow_{j(b)} \right\rangle &= \frac{1}{2} \quad \left\langle \uparrow_{i(b)} \downarrow_{j(b)} \middle| \mathcal{H}_{2,b} \middle| \downarrow_{i(b)} \uparrow_{j(b)} \right\rangle = \frac{1}{2} \end{aligned} \tag{9.20}$$

The propagation has to satisfy the periodicity condition

$$|\alpha(n)\rangle = |\alpha(0)\rangle = |\alpha\rangle \tag{9.21}$$

for the partition function to be non-zero.

It is practically useful to introduce a cut-off L, which should not cause any error. Define the unity operator as $\mathcal{H}_{0,0} = \mathbb{1}$ and including $[a(p), b(p)] = [0, 0]$ in the list, the partition function reads

$$Z = \sum_{\alpha} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L-n)!}{L!} \langle \alpha | \prod_{p=0}^{L-1} \mathcal{H}_{a(p),b(p)} | \alpha \rangle \tag{9.22}$$

with $n$ the number of non-unity elements in the string in the fixed-length $S_L$. This formulation is useful since it fixes the number of operators to $n < L$ large enough, putting the remaining $L - n$ to unity, instead of changing the number $n$ of useful ones always. This explains the introduction of the $\binom{L}{n}$ since the unity operators can be put anywhere in the string. The weights become

$$W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!} \tag{9.23}$$

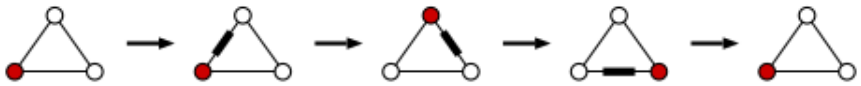

*Figure* 9.1 – Example of three off-diagonal operations bringing all spins back to their original states, each operator associated to a negative sign.

where the factor $\frac{1}{2}$ comes from all the non-zero amplitude and where $(-1)^{n_2}$ has been removed since they are taken to be always positive for a bipartite lattice. This is called the sign problem, which is not really a problem. Indeed, always an even number $n_2$ is required to satisfy the time periodicity condition (9.21). However, for frustrated systems such as the ones forming loops with an odd number of sites as in Figure 9.1, the overall sign will be negative.

## 9.4 MC SAMPLING

During the Monte Carlo sampling one will need to access operators and some properties of the propagated states also in non-sequential order—given an operator and the spins it acts on, one will need to to know which operators act on those spins next. It would be prohibitively time consuming to propagate a single state back and forth to extract this information, and also it would not be practical to store all the propagated states. Therefore use also another kind of data structure, in which the connectivity of the operators is explicit and represented as a network in a compact way. This linked vertex structure is illustrated in Figure 9.2. For the Heisenberg Hamiltonian considered, the vertices allowed are in Figure 9.3. The goal here is to MC sample the partition function.

The diagonal updates are the updates of single diagonal operators that can be carried out sequentially at locations $p = 0, \ldots, L-1$ in $S_L$. There is not constraint in the update $[1, b]_p \to [0, 0]_p$ corresponding to the removal of

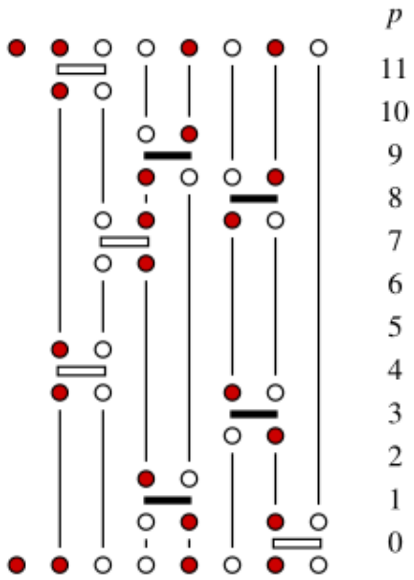


*Figure* 9.2 – Linked vertex storage configuration.

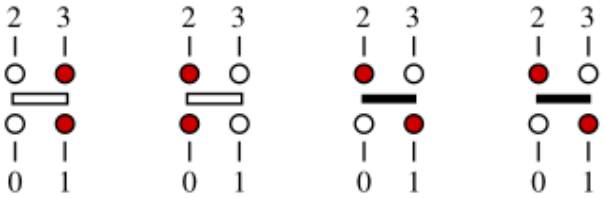


*Figure* 9.3 – Allowed vertices for the Heisenberg model considered.

a diagonal operator. The insertion of a diagonal operator $[0,0]_p \to [1,b]_p$ is nonetheless constrained by the fact the the spins on bond $b$ must be antiparallel in the propagated state $|\alpha(p)\rangle$. The transition probabilities come from the expression for the weights. But one need to be careful that the selection probabilities depend on the choice of update. Writing

$$P(A \to B) = P_{\text{select}}(B) P_{\text{accept}}(A \to B) \tag{9.24}$$

with the selections

$$\begin{aligned} [1,b]_p \to [0,0]_p &\implies P_{\text{select}}([1,b]_p \to [0,0]_p) = 1 \\ [0,0]_p \to [1,b]_p &\implies P_{\text{select}}([0,0]_p \to [1,b]_p) = \frac{1}{N_b} \end{aligned} \tag{9.25}$$

since the diagonal operators can be put on the bond $b$ among all $N_b$ possible whereas there only one way to update to unity. Therefore

$$\begin{aligned} P_{\text{accept}}([1,b]_p \to [0,0]_p) &= \min\left[\frac{W(\alpha, S_L, n-1)}{W(\alpha, S_L, n)} \frac{1}{N_b}, 1\right] \\ &= \min\left[\frac{2(L-n+1)}{\beta N_b}, 1\right] \\ P_{\text{accept}}([0,0]_p \to [1,b]_p) &= \min\left[\frac{W(\alpha, S_L, n+1)}{W(\alpha, S_L, n)} N_b, 1\right] \\ &= \min\left[\frac{\beta N_b}{2(L-n)}, 1\right] \end{aligned} \tag{9.26}$$

where $n$ is the number of operators before the update. This satisfies the detailed balance condition, which can be checked quite easily.

The off-diagonal updates have to involve at least two operators. In fact, involve an even number of them by periodicity conditions. For the Heisenberg model considered, use the loop updates that correspond to constructing a loop of generators connected by the links. For instance, an operator-loop is shown on Figure 9.4. The goal is to flip the loop, that is flipping the spins along the loop as well as operators themselves. A loop cannot cross an operator since parallel spins acted upon by an operator are prohibited. To explore all phase space — ergodicity — one cannot just put and off-diagonal operator, then take the spins in a found loop and flip them with operators.

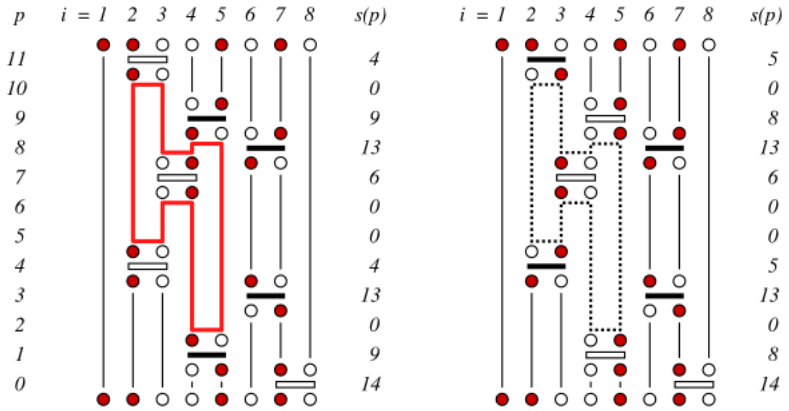


*Figure* 9.4 – SSE configuration with one loop shown before (left) and after (right) the operation of flipping spins and operators has been performed.

A MC step is then defined as

- Start with a randomly initialized spin state and initialize $S_L$ so that its elements are $[0, 0]$ for all.
- By sequentially going through all elements of $S_L$, insert and remove diagonal operators according to the acceptance probabilities.
- After a full sequence of diagonal updates, construct and flip/accept a loop with a certain probability — $\frac{1}{2}$ in the case of the Heisenberg model considered.

## 9.5 OBSERVABLES

In general, the thermal expectation value is

$$\langle O \rangle = \frac{1}{Z} \operatorname{tr} O e^{-\beta \mathcal{H}} \tag{9.27}$$

and since the trace is cyclic, one can put the $O$ anywhere. For $O$ diagonal $O\,|\alpha(p)\rangle = O_p\,|\alpha(p)\rangle$, the estimator of $O$ can be taken as

$$\langle \bar{O} \rangle = \frac{1}{L} \sum_{p=0}^{L-1} O_p \tag{9.28}$$

In practice, one can take the partial summation over every $N^{th}$ time slice for instance since states separated by a small number of slices are not very different in contrast to states separated by a large number of them.

Finally, the energy is such that

$$E = -\frac{\langle n \rangle}{\beta} \tag{9.29}$$

and thus the more the non-trivial — non-identity — operators, the smaller the energy.

# 10 TENSOR NETWORKS

## 10.1 INTRODUCTION

Tensor Network methods provide flexible ways to study quantum systems. They manage to become necessary despite the wide variety of numerical studies of strongly correlated systems. Indeed, they are not limited by the size of the systems, provide a good way to deal with entanglement and offer diagram visualization of quantum states. Moreover, it has been shown that geometry and curvature can emerge form the entanglement representation.

Luckily enough, not all quantum states in the Hilbert space of a many-body system are equal. Some are more relevant than others. To be specific, many important Hamiltonians in Nature are such that the interactions between the different particles tend to be local *eg* nearest or next-to-nearest neighbors. And locality of interactions turns out to have important consequences. In particular, one can prove that low-energy eigenstates of gapped Hamiltonians with local interactions obey the so-called area-law for the entanglement entropy. This means that the entanglement entropy of a region of space tends to scale, for large enough regions, as the size of the boundary of the region and not as the volume. And this is a very remarkable property, because a quantum state picked at random from a many-body Hilbert space will most likely have a entanglement entropy between subregions that will scale like the volume, and not like the area. In other words, low-energy states of realistic Hamiltonians are not just any state in the Hilbert space: they are heavily constrained by locality so that they must obey the entanglement area-law. By turning around the above consideration, one finds a dramatic consequence. It means that not any quantum state in the Hilbert space can be a low-energy state of a gapped, local Hamiltonian. Only those states satisfying the area-law are valid candidates. Yet, the manifold containing these states is just a tiny, exponentially small, corner of the gigantic Hilbert space. This corner is, therefore, the corner of relevant states. And if one aims to study states within this corner, then one better finds a tool to target it directly instead of messing around with the full Hilbert space. Here is where the good news come. It is the family of TN states the one that targets this most relevant corner of states. Moreover, recall that Renormalization Group methods for many-body systems aim to, precisely, identify and keep track of the relevant degrees of freedom to describe a system. Thus, it looks just natural to devise RG methods that deal with this relevant corner of quantum states, and are therefore based on TN states.

## 10.2 REPRESENTATION OF TN

For a d-dimensional, an index contraction is the sum over all possible values of repeated indices of set of tensors, as for instance

$$E_{\alpha\beta\gamma\delta} = \sum_{\mu,\nu,\rho,\sigma,\tau=1}^{d} A_{\mu\nu\rho\delta} B_{\nu\alpha\tau} C_{\rho\sigma\tau\beta} D_{\sigma\gamma\mu} \tag{10.1}$$

and open indices are those that are not contracted. A TN is a set of tensors that have their, but not necessarily all, indices contracted. For instance, (10.1) describes a TN, which has 4 open indices and thus results in a rank-4 tensor.

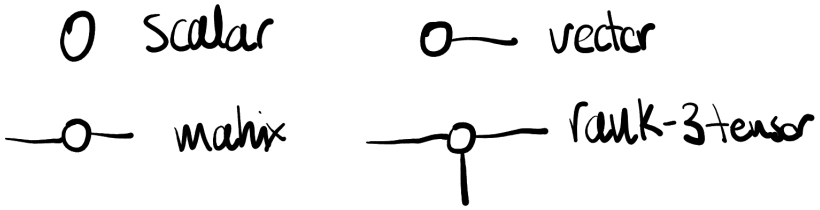


*Figure* 10.1 – Diagram representation of tensors. The tensors are the shapes and their indices are the lines emerging from.

Introduce a diagrammatic way to visual them, as in Figure 10.1. A TN thus consists in interconnected such shapes. The lines between two different tensors corresponds to contracted indices, and those which do not connect two tensors are open indices. For instance, the trace of a product of 6 matrices in represented in Figure 10.2

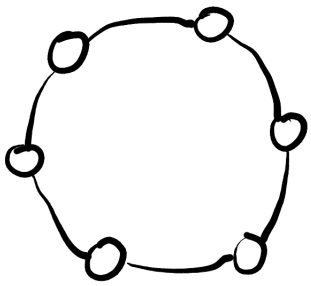

*Figure* 10.2 – Example of a trace of a product of 6 matrices.

## 10.3 MATRIX PRODUCT STATES

For the Heisenberg antiferromagnet for example, the Hilbert space grows like $2^L$ with L the number of sites. The ground state is hidden in a sea of non-relevant states for the problem. It lies in the corner of the Hilbert space one has already made allusion to, and can be found using methods that shall be presented later on. This corner can be represented by a matrix product state.

First recall the singular value decomposition. In the compact form, a $n \times m$ matrix $M$ can be decomposed as

$$M = USV^\dagger \tag{10.2}$$

with $U$ having orthonormal columns, $V^\dagger$ orthonormal rows and $S$ diagonal containing the singular values of $M$ order in descending way. The further goal is to approximate $M$ of rank $r$ — that is the number of non-zero singular values — by $M'$ of rank $r' < r$ by keeping only the largest singular values of $M$.

With sites $i = 1, \ldots, L$, write local $d$-dimensional states as $\{\sigma_i\}$. Take for now $d = 1$, and write the most general pure state

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c_{\sigma_1,\ldots,\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle \tag{10.3}$$

The goal is to find a notation that that enhances the locality of the states while preserving the non-locality of the state due to its quantum nature. Use SVD. One way of doing this is by left-canonical matrix product state. Reshape the states with $d^L$ components to one with $d \times d^{L-1}$, with coefficients

$$\Psi_{\sigma_1,(\sigma_2,\ldots,\sigma_L)} = c_{\sigma_1,\ldots,\sigma_L} \tag{10.4}$$

Perform a SVD on $\Psi$

$$\begin{aligned} c_{\sigma_1,\ldots,\sigma_L} &= \Psi_{\sigma_1,(\sigma_2,\ldots,\sigma_L)} \\ &= \sum_{a_1=1}^{r_1} U_{\sigma_1,a_1} S_{a_1,a_1} (V^\dagger)_{a_1,(\sigma_2,\ldots,\sigma_L)} \\ &= \sum_{a_1=1}^{r_1} U_{\sigma_1,a_1} c_{a_1\sigma_2,\ldots,\sigma_L} \end{aligned} \tag{10.5}$$

where $r_1 \leqslant d$. Decompose $U$ in $d$ row vectors $A^{\sigma_1}$ as $A^{\sigma_1}_{a_1} = U_{\sigma_1,a_1}$. Reshape again $c_{a_1\sigma_2,\ldots,\sigma_L}$ into a $r_1 d \times d^{L-2}$ matrix $\Psi_{(a_1\sigma_2),(\sigma_3,\ldots,\sigma_L)}$ to get

$$c_{\sigma_1,\ldots,\sigma_L} = \sum_{a_1=1}^{r_1} A^{\sigma_1}_{a_1} \Psi_{(a_1\sigma_2),(\sigma_3,\ldots,\sigma_L)} \tag{10.6}$$

Continue this procedure as

$$\begin{aligned} c_{\sigma_1,\ldots,\sigma_L} &= \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} A^{\sigma_1}_{a_1} U_{(a_1\sigma_2),a_2} S_{a_2,a_2} (V^\dagger)_{a_2,(\sigma_3,\ldots,\sigma_L)} \\ &= \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \Psi_{(a_2\sigma_3),(\sigma_4,\ldots,\sigma_L)} \end{aligned} \tag{10.7}$$

with $A^{\sigma_2}_{a_1,a_2} = U_{(a_1\sigma_2),a_2}$ and $A^{\sigma_2}$ a $r_1 \times r_2$ matrix. Also, $\Psi_{(a_2\sigma_3),(\sigma_4,\ldots,\sigma_L)}$ a $r_2 d \times d^{L-3}$ matrix, with $r_2 \leqslant r_1 d$. Continue to have

$$\begin{aligned} c_{\sigma_1,\ldots,\sigma_L} &= \sum_{a_1,\ldots,a_{L-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} A^{\sigma_L}_{a_{L-1}} \\ &= A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_{L-1}} A^{\sigma_L} \end{aligned} \tag{10.8}$$

Finally giving

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle \tag{10.9}$$

However, considering L even for simplicity, the maximum dimension of the $A$ matrices is $d^{L/2-1} \times d^{L/2}$ which makes the computation untenable.

## 10.4 AKLT AS A MPS

Recall the parent Hamiltonian of the model as in Figure 10.3

$$\mathcal{H} = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}[\mathbf{S}_i \cdot \mathbf{S}_{i+1}]^2 \tag{10.10}$$

Taking $S = 1$ symmetrized states at the sites as pairs of spins-$\frac{1}{2}$ and singlet linking them, one has for the $S = 1$ states

$$\begin{aligned} |+\rangle &= |\uparrow\uparrow\rangle \\ |-\rangle &= |\downarrow\downarrow\rangle \\ |0\rangle &= \frac{1}{2}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle] \end{aligned} \tag{10.11}$$

and for the valence bond singlets $\frac{1}{2}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]$. In the language of 2L spin-$\frac{1}{2}$ states, a state is

$$|\psi\rangle = \sum_{a,b} c_{a,b} |a, b\rangle \tag{10.12}$$

Moreover, a state on site $i$ is

$$|\Sigma^i\rangle = \sum_{b_i, a_{i+1}} \Sigma_{ba} |b_i\rangle |a_{i+1}\rangle \tag{10.13}$$

and introducing the matrix $\Sigma$ as

$$\Sigma = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \tag{10.14}$$

Hence, write the state with singlets on all bonds

$$|\psi_\Sigma\rangle = \sum_{a,b} \Sigma_{b_1 a_2} \Sigma_{b_2 a_3} \cdots \Sigma_{b_L a_1} |a, b\rangle \tag{10.15}$$

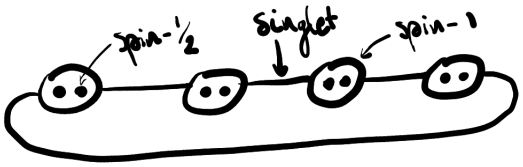


*Figure* 10.3 – Example of AKLT model for $S = 1$ states with periodic BCs.

All is written is the spin-$\frac{1}{2}$ language, thus map $|a_i\rangle |b_i\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}^{\otimes 2}$ to the physical spin-1 states $|\sigma_i\rangle \in \{|+\rangle, |0\rangle, |-\rangle\}$. Thus to represent (10.11), introduce matrices

$$\begin{aligned} M^+ &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ M^0 &= \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \\ M^- &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \tag{10.16}$$

Then, one finds

$$|\sigma\rangle = \sum_{a,b} M^{\sigma}_{ab} |a, b\rangle \tag{10.17}$$

Therefore, one has the mapping

$$\begin{aligned} |\psi_\Sigma\rangle &\to \sum_{\mathbf{a},\mathbf{b},\boldsymbol{\sigma}} M^{\sigma_1}_{a_1 b_1} \cdots M^{\sigma_L}_{a_L b_L} |\boldsymbol{\sigma}\rangle \langle \boldsymbol{\sigma}|\mathbf{a}, \mathbf{b}\rangle \\ &= \sum_{\mathbf{a},\mathbf{b},\boldsymbol{\sigma}} M^{\sigma_1}_{a_1 b_1} \Sigma_{b_1 a_2} \cdots M^{\sigma_L}_{a_L b_L} \Sigma_{b_L a_1} |\boldsymbol{\sigma}\rangle \\ &= \sum_{\boldsymbol{\sigma}} \mathrm{tr}[M^{\sigma_1} \Sigma M^{\sigma_2} \Sigma \cdots M^{\sigma_L} \Sigma] |\boldsymbol{\sigma}\rangle \\ &= |\psi\rangle \end{aligned} \tag{10.18}$$

Simply by further denoting $\widetilde{A}^\sigma = M^\sigma \Sigma$ with

$$\begin{aligned} \widetilde{A}^+ &= \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix} \\ \widetilde{A}^0 &= \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \\ \widetilde{A}^- &= \begin{pmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \end{aligned} \tag{10.19}$$

giving

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{tr}\left[\widetilde{A}^{\sigma_1} \cdots \widetilde{A}^{\sigma_L}\right] |\boldsymbol{\sigma}\rangle \tag{10.20}$$

which is not normalized. Thus left-normalize the $\widetilde{A}^\sigma$. Since

$$\sum_\sigma \widetilde{A}^{\sigma\dagger} \widetilde{A}^\sigma = \frac{3}{4} \mathbb{1} \tag{10.21}$$

Hence rescale to obtain $A^\sigma$ matrices as

$$\begin{aligned} A^+ &= \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{pmatrix} \\ A^0 &= \begin{pmatrix} -\frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{pmatrix} \\ A^- &= \begin{pmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0 \end{pmatrix} \end{aligned} \tag{10.22}$$

This allows finally to compute

$$\begin{aligned}
\langle\psi|\psi\rangle &= \sum_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} \operatorname{tr}\left[A^{\sigma_1'}\cdots A^{\sigma_L'}\right]^\dagger \operatorname{tr}[A^{\sigma_1}\cdots A^{\sigma_L}]\left\langle\boldsymbol{\sigma}'|\boldsymbol{\sigma}\right\rangle \\
&\overset{[1]}{=} \sum_{\boldsymbol{\sigma}} \operatorname{tr}[A^{\sigma_1}\cdots A^{\sigma_L}]^* \operatorname{tr}[A^{\sigma_1}\cdots A^{\sigma_L}] \\
&\overset{[2]}{=} \sum_{\boldsymbol{\sigma}} \operatorname{tr}\left[A^{\sigma_1^*}\cdots A^{\sigma_L^*}\right] \operatorname{tr}[A^{\sigma_1}\cdots A^{\sigma_L}] \\
&\overset{[3]}{=} \sum_{\boldsymbol{\sigma}} \operatorname{tr}\left[(A^{\sigma_1^*}\cdots A^{\sigma_L^*})\otimes(A^{\sigma_1}\cdots A^{\sigma_L})\right] \\
&\overset{[4]}{=} \operatorname{tr}\left[\left(\sum_{\sigma_1} A^{\sigma_1^*}\otimes A^{\sigma_1}\right)\cdots\left(\sum_{\sigma_1} A^{\sigma_L^*}\otimes A^{\sigma_L}\right)\right] \\
&= \operatorname{tr} E^L \\
&= 1+3\left(-\frac{1}{3}\right)^L \xrightarrow{L\to\infty} 1
\end{aligned} \tag{10.23}$$

where

$$E = \sum_{\sigma} A^{\sigma^*}\otimes A^{\sigma} = \begin{pmatrix} \frac{1}{3} & 0 & 0 & \frac{2}{3} \\ 0 & -\frac{1}{3} & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & 0 \\ \frac{2}{3} & 0 & 0 & \frac{1}{3} \end{pmatrix} \tag{10.24}$$

that has eigenvalues $1, -\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}$. The relations used are the following

[1] $\rightarrow$ $\operatorname{tr} A^\dagger = \operatorname{tr} A$

[2] $\rightarrow$ $\operatorname{tr}(A)^* = \operatorname{tr} A^*$

[3] $\rightarrow$ $\operatorname{tr} A\otimes B = \operatorname{tr} A \operatorname{tr} B$

[4] $\rightarrow$ $(AB)\otimes(CD) = (A\otimes C)(B\otimes D)$

Hence, it has been possible to express the AKLT model as a $d = 2$ matrix product state.

## 10.5 ENTANGLEMENT ENTROPY

Here, one derives the Schmidt decomposition of a general quantum state. First, a pure state is written

$$|\psi\rangle = \sum_{ij} \Psi_{ij} |i\rangle_A |j\rangle_B \tag{10.25}$$

on $\mathcal{H}_A\otimes\mathcal{H}_B$, with basis $\dim\{|i\rangle_A\} = N_A$ and $\dim\{|j\rangle_B\} = N_B$, which has density operator $\hat{\rho} = |\psi\rangle\langle\psi|$. The reduced density operators are thus the partial traces

$$\hat{\rho}_A = \operatorname{tr}_B |\psi\rangle\langle\psi| \quad \text{and} \quad \hat{\rho}_B = \operatorname{tr}_A |\psi\rangle\langle\psi| \tag{10.26}$$

Perform SVD on matrix $\Psi$, then

$$\begin{aligned}|\psi\rangle &= \sum_{ij} \sum_{a=0}^{\min(N_1,N_B)} U_{ia} S_{aa} V^*_{ja} |i\rangle_A |j\rangle_B \\ &= \sum_{a=0}^{\min(N_1,N_B)} \left(\sum_i U_{ia} |i\rangle_A\right) s_a \left(\sum_j V^*_{ja} |j\rangle_B\right) \\ &= \sum_{a=0}^{\min(N_1,N_B)} s_a |a\rangle_A |a\rangle_B\end{aligned} \tag{10.27}$$

Truncate to the $r \leqslant \min(N_1, N_B)$ largest singular values to get

$$|\psi\rangle = \sum_{a=1}^{r} s_a |a\rangle_A |a\rangle_B \tag{10.28}$$

and this is the Schmidt decomposition. For $r > 1$ the system is entangled. The reduced density operators then read

$$\hat{\rho}_A = \sum_{a=1}^{r} s_a^2 |a_A\rangle\langle a_A| \quad \text{and} \quad \hat{\rho}_B = \sum_{a=1}^{r} s_a^2 |a_B\rangle\langle a_B| \tag{10.29}$$

The eigenvalues being $s_a^2$ and the eigenvectors left- and right-singular vectors, allow to write the von Neumann entropy of entanglement defined as $S(\rho) = -\operatorname{tr} \rho \ln \rho$, as

$$S_A(|\psi\rangle) = -\operatorname{tr} \hat{\rho}_A \ln \hat{\rho}_A = -\sum_{a=1}^{r} s_a^2 \ln s_a^2 \tag{10.30}$$

and note that $S_B(|\psi\rangle) = S_A(|\psi\rangle)$.

## 10.6 CORRELATION LENGTH FOR AKLT

To calculate observables, one defines the operators that act as

$$\hat{O}^{[l]} = \sum_{\sigma_l, \sigma'_l} O^{\sigma_l, \sigma'_l} |\sigma_l\rangle\langle\sigma'_l| \tag{10.31}$$

The goal her is to calculate the correlations on a translationally invariant state with left-normalized site-independent A matrices and thus E matrices=. Then

$$\begin{aligned}&\langle\psi|\hat{O}^{[i]}\hat{O}^{[j]}|\psi\rangle \\ &= \operatorname{tr}\left[E^{[1]} \cdots E^{[i-1]} E_O^{[i]} E^{[i+1]} \cdots E^{[j-1]} E_O^{[j]} E^{[j+1]} \cdots E^{[L]}\right] \\ &= \operatorname{tr}\left[E_O^{[i]} E^{j-i-1} E_O^{[j]} E^{L-j+i-1}\right] \\ &= \sum_{k,l} \langle l|E_O^{[i]}|k\rangle \lambda_k^{j-i-1} \langle k|E_O^{[j]}|l\rangle \lambda_l^{L-j+i-1} \\ &\xrightarrow{L\to\infty} \sum_k \langle 1|E_O^{[i]}|k\rangle \lambda_k^{j-i-1} \langle k|E_O^{[j]}|1\rangle\end{aligned} \tag{10.32}$$

with $E_O$ having the interposed operator $\hat{O}$ and since $\lambda_1 = 1$ and $|\lambda_k| < 1\ \forall k > 1$. Hence, if $\langle 1|E_O^{[i]}|1\rangle$ are finite, the correlations can be long-ranged, else they are a superposition of exponentials with decay length $\xi_k = -\frac{1}{\ln \lambda_k}$, thus

$$\frac{\langle\psi|\hat{O}^{[i]}\hat{O}^{[j]}|\psi\rangle}{\langle\psi|\psi\rangle} = c_1 + \sum_{k=2}^{D^2} c_k e^{\frac{r}{\xi_k}} \tag{10.33}$$

with $r = |j - i - 1|$ and $c_k = \langle 1|E_O^{[i]}|k\rangle\ \langle k|E_O^{[j]}|1\rangle$. For AKLT and $i < j$,

$$\left\langle S_i^z S_j^z \right\rangle = \frac{12}{9}(-1)^{j-i} e^{-(j-i)\ln 3} \tag{10.34}$$

hence $\xi = \frac{1}{\ln 3}$.

## 10.7 BRING A MPS TO CANONICAL FORM

Start with a general MPS without normalization

$$\begin{aligned}
|\psi\rangle &= \sum_{\sigma_1,\ldots,\sigma_L} M^{\sigma_1} M^{\sigma_2} \cdots M^{\sigma_{L-1}} M^{\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle \\
&= \sum_{\boldsymbol{\sigma}} \sum_{a_1,\ldots,a_{L-1}} M^{\sigma_1}_{1,a_1} M^{\sigma_2}_{a_1,a_2} \cdots M^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} M^{\sigma_L}_{a_{L-1},1} |\boldsymbol{\sigma}\rangle \\
&= \sum_{\boldsymbol{\sigma}} \sum_{a_1,\ldots,a_{L-1}} M_{(\sigma_1,1),a_1} M^{\sigma_2}_{a_1,a_2} \cdots M^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} M^{\sigma_L}_{a_{L-1},1} |\boldsymbol{\sigma}\rangle \\
&\overset{\text{SVD}}{=} \sum_{\boldsymbol{\sigma}} \sum_{a_1,\ldots,a_{L-1}} \sum_{s_1} A_{(\sigma_1,1),s_1} S_{s_1,s_1} V^\dagger_{s_1,a_1} M^{\sigma_2}_{a_1,a_2} \cdots |\boldsymbol{\sigma}\rangle \\
&= \sum_{\boldsymbol{\sigma}} \sum_{a_2,\ldots,a_{L-1}} \sum_{s_1} A^{\sigma_1}_{1,s_1} \underbrace{\left[\sum_{a_1} S_{s_1,s_1} V^\dagger_{s_1,a_1} M^{\sigma_2}_{a_1,a_2}\right]}_{\widetilde{M}^{\sigma_2}_{s_1,a_2}} M^{\sigma_3}_{a_2,a_3} \cdots |\boldsymbol{\sigma}\rangle
\end{aligned} \tag{10.35}$$

and $A^\dagger A = \mathbb{1}$ due to SVD is left-normalization. Iterate the procedure to get MPS with $\widetilde{M}$s. To do so, reshape $\widetilde{M}^{\sigma_2}_{s_1,a_2}$ to $\widetilde{M}^{(\sigma_2,s_1),a_2}$, do SVD to get $A_{(\sigma_2,s_1),a_2}$ which is reshape to a left-normalized $A^{\sigma_2}_{s_1,s_2}$. Multiply the two right matrices of this SVD with the left $M$ matrix to repeat the process. In the end, has left-normalized $A^{\sigma_i}_{s_{i-1},s_i}$ on all site except the last one having a remaining scalar $S_{1,1}V^\dagger_{1,1}$ which corresponds to the norm of $|\psi\rangle$.

## 10.8 MATRIX PRODUCT OPERATOR

An operator $\hat{O} : H \to H$ with $\{|A_i\rangle\}$ an orthonormal basis of $H$ can be written as

$$\begin{aligned}
\hat{O} &= \sum_i |A_i\rangle\langle A_i|\, \hat{O} \sum_j |A_j\rangle\langle A_j| \\
&= \sum_{ij} O_{ij} |A_i\rangle\langle A_j|
\end{aligned} \tag{10.36}$$

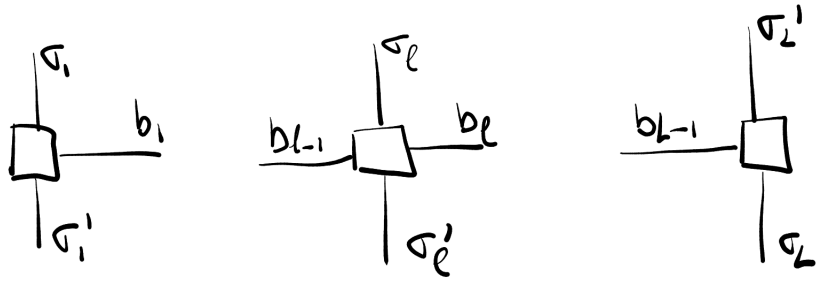


*Figure* 10.4 – Elements of a matrix product operator with physical indices pointing up and down.

and writing $H = \otimes_{i=1}^{L} H_s$ one gets

$$\hat{O} = \sum_{\sigma,\sigma'} O_{(\sigma_1,\ldots,\sigma_L),(\sigma'_1,\ldots,\sigma'_L)} \left|\sigma_1,\ldots,\sigma_L\right\rangle\!\left\langle\sigma'_1,\ldots,\sigma'_L\right| \tag{10.37}$$

the general form of an operator in tensorial state. Reshaping

$$O_{(\sigma_1,\ldots,\sigma_L),(\sigma'_1,\ldots,\sigma'_L)} = c_{(\sigma_1,\sigma'_1),\ldots,(\sigma_L,\sigma'_L)} \tag{10.38}$$

enables to decompose in canonical form as for the MPS to get a MPO

$$\hat{O} = \sum_{\sigma,\sigma'} W^{\sigma_1,\sigma'_1} \cdots W^{\sigma_L,\sigma'_L} \left|\sigma\right\rangle\!\left\langle\sigma'\right| \tag{10.39}$$

Now, instead of having one physical state, there are two, shown on Figure 10.4, and thus the MPO looks as in Figure 10.5.

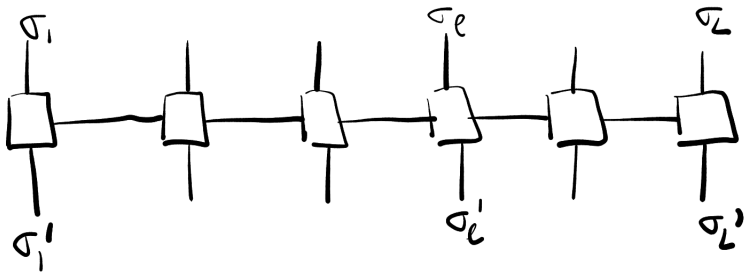


*Figure* 10.5 – A MPO acting on a chain, ready to be applied to a MPS.

Now apply the MPO to a MPS

$$\begin{aligned}
\hat{O}\left|\psi\right\rangle &= \sum_{\sigma,\sigma'} W^{\sigma_1,\sigma'_1} \cdots W^{\sigma_L,\sigma'_L} \left|\sigma\right\rangle \left\langle\sigma'\right|\left.\psi\right\rangle \\
&= \sum_{\sigma,\sigma'} W^{\sigma_1,\sigma'_1} \cdots W^{\sigma_L,\sigma'_L} M^{\sigma'_1} \cdots M^{\sigma'_L} \left|\sigma\right\rangle \\
&= \sum_{\sigma,\sigma'} \sum_{a,b} \left(W^{\sigma_1,\sigma'_1}_{1,b_1} W^{\sigma_2,\sigma'_2}_{b_1,b_2} \cdots\right) \left(M^{\sigma'_1}_{1,a_1} M^{\sigma'_2}_{a_1,a_2} \cdots\right) \left|\sigma\right\rangle \\
&= \sum_{\sigma,\sigma'} \sum_{a,b} \left(W^{\sigma_1,\sigma'_1}_{1,b_1} M^{\sigma'_1}_{1,a_1}\right) \left(W^{\sigma_2,\sigma'_2}_{b_1,b_2} M^{\sigma'_1}_{1,a_1}\right) \cdots \left|\sigma\right\rangle \\
&= \sum_{\sigma} \sum_{a,b} N^{\sigma_1}_{(1,1),(b_1,a_1)} N^{\sigma_2}_{(b_1,a_1),(b_2,a_2)} \cdots \left|\sigma\right\rangle \\
&= \sum_{\sigma} N^{\sigma_1} N^{\sigma_2} \cdots \left|\sigma\right\rangle
\end{aligned} \tag{10.40}$$

which is still a MPS !

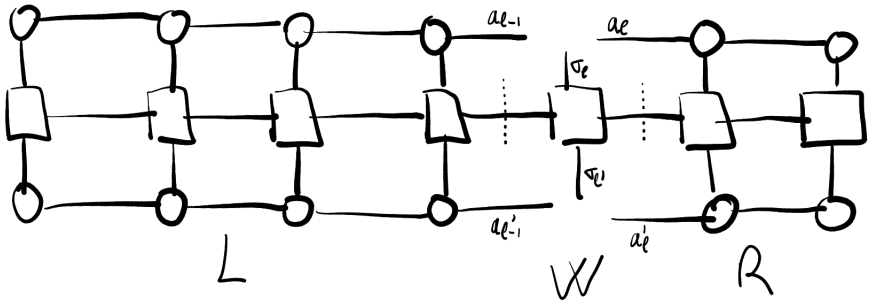


*Figure* 10.6 – Representation of the DRMG Hamiltonian matrix element in MPS/MPO language.

To apply a Hamiltonian MPO on a mixed canonical state, consider the MPS

$$\begin{aligned} |\psi\rangle &= \sum_{\boldsymbol{\sigma}} A^{\sigma_1} \dots A^{\sigma_{\ell-1}} \Psi^{\sigma_\ell} B^{\sigma_{\ell+1}} \dots B^{\sigma_L} |\boldsymbol{\sigma}\rangle \\ &= \sum_{a_{\ell-1}, a_\ell} |a_{\ell-1}\rangle_A \, \Psi^{\sigma_\ell}_{a_{\ell-1}, a_\ell} \, |a_\ell\rangle_B \end{aligned} \tag{10.41}$$

Then apply the Hamiltonian

$$\begin{aligned} \mathcal{H}|\psi\rangle &= \sum_{a_{\ell-1}, a_\ell} \Psi^{\sigma_\ell}_{a_{\ell-1}, a_\ell} \mathcal{H} |a_{\ell-1}, \sigma_\ell, a_\ell\rangle \\ &= \sum_{a_{\ell-1}, a_\ell} \sum_{a'_{\ell-1}, \sigma'_\ell, a'_\ell} \Psi^{\sigma_\ell}_{a_{\ell-1}, a_\ell} \left\langle a'_{\ell-1}, \sigma'_\ell, a'_\ell \middle| \mathcal{H} \middle| a_{\ell-1}, \sigma_\ell, a_\ell \right\rangle \left| a'_{\ell-1}, \sigma'_\ell, a'_\ell \right\rangle \end{aligned} \tag{10.42}$$

where one writes, as in Figure 10.6,

$$\left\langle a'_{\ell-1}, \sigma'_\ell, a'_\ell \middle| \mathcal{H} \middle| a_{\ell-1}, \sigma_\ell, a_\ell \right\rangle = \sum_{b_{\ell-1}, b_\ell} L^{a'_{\ell-1}, a_{\ell-1}}_{b_{\ell-1}} W^{\sigma'_\ell, \sigma_\ell}_{b_{\ell-1}, b_\ell} R^{a'_\ell, a_\ell}_{b_\ell} \tag{10.43}$$

## 10.9 DMRG

Consider spin-$\frac{1}{2}$ nearest-neighbors Heisenberg antiferromagnetic chain of length $L$ with open BCs. DMRG prefers open BCs, and is for $L$ finite. iDMRG is for $L \to \infty$. The goal is to find the ground state energy of a Hamiltonian $\mathcal{H}$. It is adequate to run a two steps algorithm that starts with iDMRG to go to DMRG. Note that here the dimension of the Hilbert space is $d^L$, with $d = 2$.

The iDMRG is proceeded as follows. The assumption is that there exists a reduced state that can describe the relevant physics and there exists a procedure to find it. Basically, consider a chain of increasing length an discard number of states to keep the algorithm efficient with manageable Hilbert space size. This is the decimation procedure. The iDMRG is sum up in Figure 10.7. Introduce left and right blocks $A$ and $B$, which in a first step may

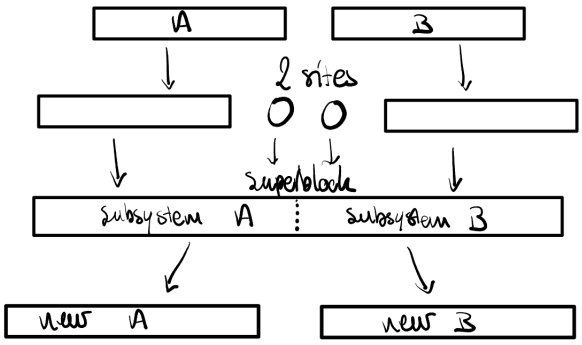


*Figure* 10.7 – iDMRG algorithm represented.

consist of one spin each, such that total chain length is 2. Longer chains are now built iteratively from the left and right end, by inserting pairs of spins between the blocks, such that the chain grows to length 4, 6, and so on. At each step, previous spins are absorbed into the left and right blocks, such that block sizes grow as 1, 2, 3, and so on, leading to exponential growth of the dimension of the full block state space as $2^\ell$, where $\ell$ is the current block size. The chains then always have a block-site-site-block structure, $A \bullet\bullet B$. To find the ground state, say that any state in the superblock is

$$\begin{aligned} |\psi\rangle &= \sum_{a_A=1}^{D} \sum_{\sigma_A=1}^{d} \sum_{\sigma_B=1}^{d} \sum_{a_B=1}^{D} \Psi_{a_A,\sigma_A,\sigma_B,a_B} |a\rangle_A |\sigma\rangle_A |\sigma\rangle_B |a\rangle_B \\ &= \sum_{i_A j_B} \Psi_{i_A,j_B} |i\rangle_A |j\rangle_B \end{aligned} \tag{10.44}$$

where D is chosen to be the dimension of the reduced Hilbert space of each block, and $\{|a\rangle_A\}$ forming a D-dimensional basis of the block A for instance. Then minimize the energy

$$E = \frac{\langle\psi|\mathcal{H}_{A\bullet\bullet B}|\psi\rangle}{\langle\psi|\psi\rangle} \tag{10.45}$$

with respect to the Hamiltonian of the superblock, to find the coefficients $\psi_{a_A,\sigma_A,\sigma_B,a_B}$ to have a good approximation of the ground state energy. If now the states $\{|i\rangle_A\}$ as the basis of the blocks $A\bullet$, the dimension of this basis is then $Dd$. To avoid exponential growth, truncate the basis back to D. To motivate, one wants to find the state $|\tilde{\psi}\rangle$ such that $\langle\psi|\tilde{\psi}\rangle$ is minimized.

The finite-size DMRG is shown on Figure 10.8. It continues the growth process of *eg* block B following the same prescription as before. But it does so at the expense of block A, which shrinks *ie* old shorter blocks A are reused. This is continued until A is so small as to have a complete Hilbert space. Then the growth direction is reversed. A grows at the expense of B, including new ground state determinations and basis choices for A, until B is small enough to have a complete Hilbert space, which leads to yet another reversal of growth direction. This sweeping through the system is continued until energy converges. The intuitive motivation for this procedure is that after each sweep, blocks A or B are determined in the presence of an ever improved embedding.

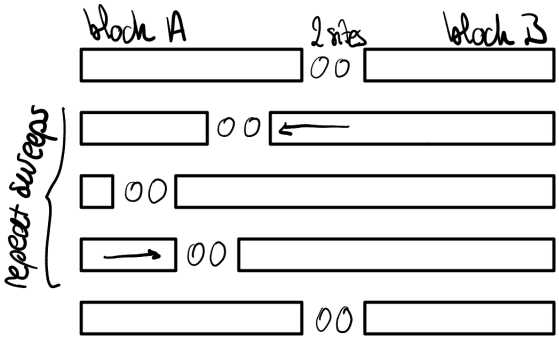


*Figure* 10.8 – DMRG algorithm summed up.

The ground state can be found using an iterative method by minimizing the energy $E = \frac{\langle\psi|\mathcal{H}|\psi\rangle}{\langle\psi|\psi\rangle}$ thus finding

$$\min_{|\psi\rangle,\lambda} \langle\psi|\mathcal{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle \tag{10.46}$$

The problem is that if one considers all the matrices M, the problem is highly non-linear. But one can proceed by keeping all the matrices on the sites except the one considered fixed. Of course, this is computationally worth — quadratic form — but not optimal. To calculate the terms of the minimization, note that it can be recast into a generalized eigenvalue problem

$$\hat{\mathcal{H}}v - \lambda\hat{\mathcal{N}}v = 0 \tag{10.47}$$

with $v_{\sigma_\ell,a_{\ell-1},a_\ell} = M^{\sigma_\ell}_{a_{\ell-1},a_\ell}$, which is represented in Figure 10.9. If $|\psi\rangle$ is mixed canonical, thus left-normalized at the left of the site $\ell$ and right-normalized on the right, then $\mathcal{N} = \mathbb{1}$, so that the problem reduces to Figure 10.10.

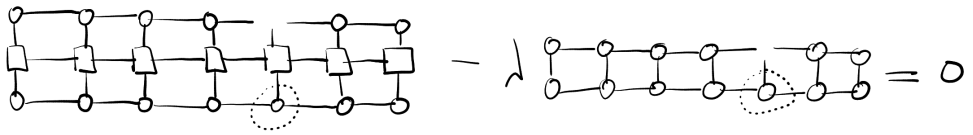

*Figure* 10.9 – Generalized eigenvalue problem for the optimization of $v$.

The algorithm is as follows

- start for a random $|\psi\rangle$
- right-normalize it
- run the optimization from $\ell = 1$ to $L-1$, that is, solve the eigenvalue problem for $M^{\sigma_\ell}$, then left-normalize it to $A^{\sigma_\ell}$ by SVD, absorb the $SV^\dagger$ into the $M^{\sigma_{\ell+1}}$, then move to the $\ell+1$ site and repeat until $L-1$
- start from $\ell = L$ to 2, and do the same but right-normalizing
- repeat the sweeps until convergence, but can fall in local minimum thus seek for the null error on the energy

$$
\begin{aligned}
& M_0 B_0 B_0 B_0 \cdots B_0 \\
\xrightarrow{\text{optimize}} & M_1 B_0 B_0 B_0 \cdots B_0 \xrightarrow{\text{SVD}} A_1 M_0 B_0 B_0 \cdots B_0 \\
\xrightarrow{\text{optimize}} & A_1 M_1 B_0 B_0 \cdots B_0 \xrightarrow{\text{SVD}} A_1 A_1 M_0 B_0 \cdots B_0 \\
\xrightarrow{\text{optimize}} & A_1 A_1 M_1 B_0 \cdots B_0 \xrightarrow{\text{SVD}} A_1 A_1 A_1 M_0 \cdots B_0 \\
\xrightarrow{\cdots} & A_1 A_1 A_1 A_1 \cdots M_0 \\
\xrightarrow{\text{optimize}} & A_1 A_1 A_1 A_1 \cdots M_1 \xrightarrow{\text{SVD}} A_1 A_1 A_1 A_1 \cdots B_1 \\
\xrightarrow{\cdots} & A_1 A_1 A_1 M_1 \cdots B_1 \\
\xrightarrow{\text{optimize}} & A_1 A_1 A_1 M_2 \cdots B_1 \xrightarrow{\text{SVD}} A_1 A_1 M_1 B_2 \cdots B_1 \\
\xrightarrow{\text{optimize}} & A_1 A_1 M_2 B_2 \cdots B_1 \xrightarrow{\text{SVD}} A_1 M_1 B_2 B_2 \cdots B_1 \\
\xrightarrow{\text{optimize}} & A_1 M_2 B_2 B_2 \cdots B_1 \xrightarrow{\text{SVD}} M_1 B_2 B_2 B_2 \cdots B_1 \\
\xrightarrow{\cdots} &
\end{aligned}
\tag{10.48}
$$

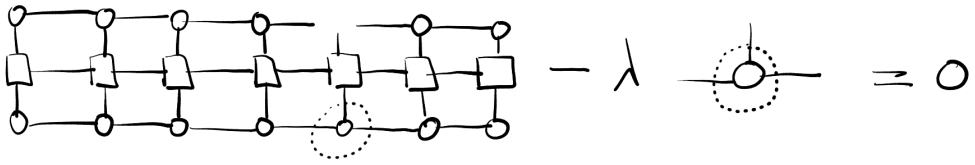

*Figure* 10.10 – Standard eigenvalue problem for the optimization of $v$.

## 10.10 CONTRACTIONS OF PEPS

Projected entangled pair states have an number of properties. They are translationally invariant, dense in the Hilbert space and increasing D the bond dimension makes the corner increase in size, satisfy the area law of entanglement entropy. But they can have infinite correlation length, thus have no canonical form, and computing expectation values on them is exponentially costly. Hence, the order of contractions matters.

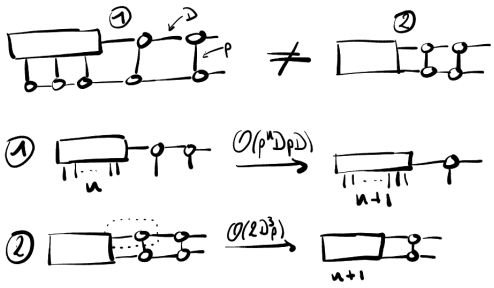

*Figure* 10.11 – Oder of contractions matters for the PEPS.

To see the difference in the order of contractions, look at Figure 10.11. This is based on the property of contractions cost that is shown in Figure 10.12.

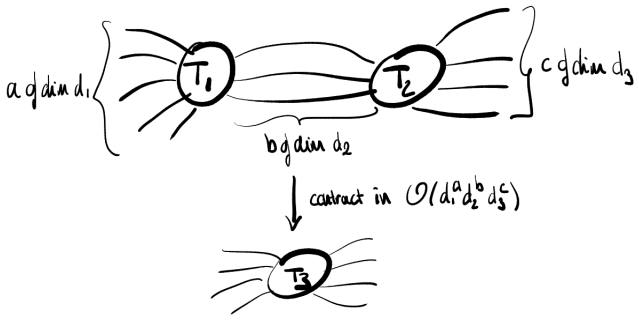


*Figure* 10.12 – Property of the contractions cost for tensor networks.

For a PEPS with bond dimension D, the contraction shown on Figure 10.13 is increasing exponentially in the linear number of sites, and this is anyway unavoidable.

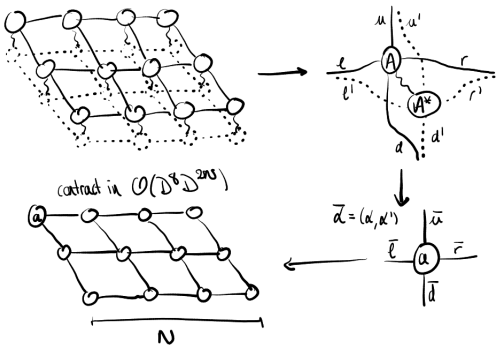


*Figure* 10.13 – Exponential cost of the PEPS contraction.

## 10.11 CTMRG

There are basically two methods to find the ground state of a Hamiltonian, via imaginary time evolution of using a variational approach. In either case, the computations must be approximated, and this is where the corner transfer matrix renormalization group comes. This involves the computation of the environment of the system considered, and it becomes mandatory in the case of the infinite PEPS.

For a square lattice as used before, the environment is presented on Figure 10.14. Then, the goal is to compute an effective environment since the exact computation is to costly. The algorithm is therefore on Figure 10.15. Only one step is shown, 3 others must be performed on each side — or $\bar{\alpha}$ bond — to complete one iteration.

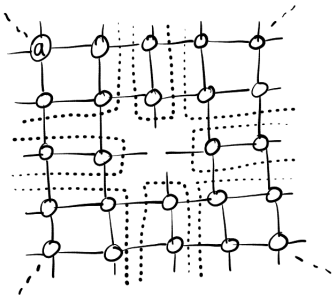

*Figure* 10.14 – Environment of a tensor in the context of CTMRG.

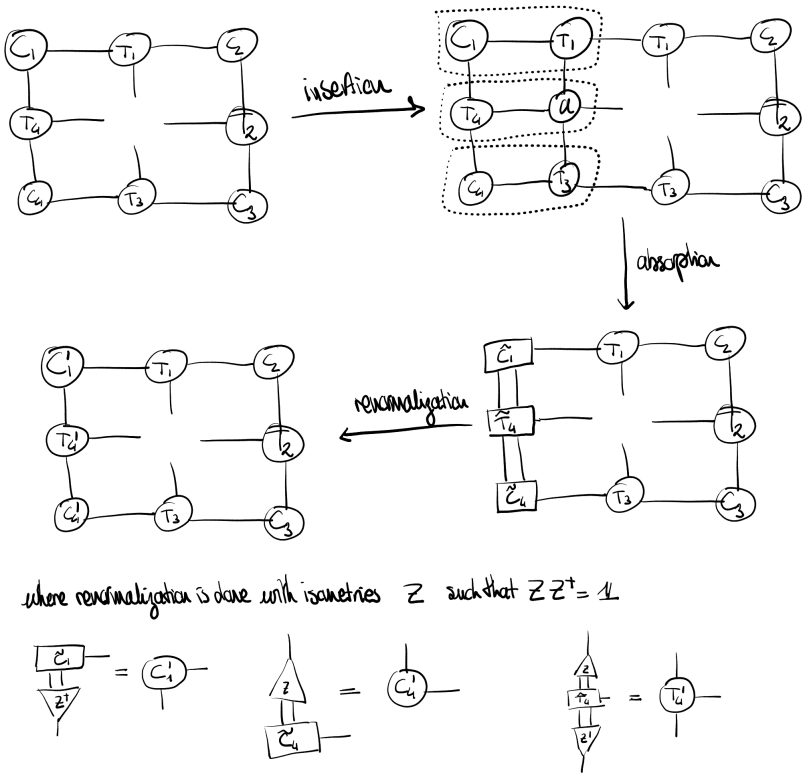


*Figure* 10.15 – CTMRG algorithm.

## 10.12 GROUND STATE RESEARCH

Now that the structural ansatz of TN were established and that one knows how to approximate many-body state of a physical system. One is interested in finding the ground state of such systems. So will present two methods and we will focus on the second one which is widely used in a lot of fields in physics.

First, the variational approach, that is based on the fact that the energy associated to the ground state is the lowest so that

$$E_0 < \frac{\langle\Psi|\, H \,|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{10.49}$$

Thus minimizing the RHS of this inequality will give approximation of the ground state. In a TN formalism one could choose a family of state $\mathcal{F}$ — MPS, PEPS... — and minimize with respect to it. Only have one constraint

which is the norm of the state to equal one. Thus introduce one Lagrange multiplier $\lambda$

$$\min_{|\Psi\rangle \in \mathcal{F}} (\langle\Psi| \mathcal{H} |\Psi\rangle - \lambda \langle\Psi|\Psi\rangle) \tag{10.50}$$

If the state are defined as MPS state for example one should take every parameters of every tensor of the network as the variational parameters. Instead, fix every tensor but one and minimize with respect to it then move to another one and so on. In practice, perform that several times before reaching an acceptable approxiamtion of the ground state. So now fixing all the tensors but one gives

$$\min_{|\Psi\rangle \in \mathbb{F}} (\langle\Psi| H |\Psi\rangle - \lambda \langle\Psi|\Psi\rangle) = \min_{A} (\vec{A}^{\dagger} H_{eff} \vec{A} - \lambda \vec{A}^{\dagger} N \vec{A}) \tag{10.51}$$

where $\vec{A}$ is the vectorly ordered tensor A, $\mathcal{H}_{\text{eff}}$ is an effective Hamiltonian and $\mathcal{N}$ a normalisation matrix. Usually $\mathcal{H}_{\text{eff}}$ and N are respectively the TNs approximation of $\langle\Psi| \mathcal{H} |\Psi\rangle$ and $\langle\Psi|\Psi\rangle$. Finally minimizing leads to the generalized eigenvalue problem

$$\mathcal{H}_{\text{eff}} \vec{A} = \lambda \mathcal{N} \vec{A} \tag{10.52}$$

Note that for MPS with open boundary conditions, one just recovers the DMRG algorithm.

A second method is the imaginary time evolution. The idea is taking a random state with non-zero overlap with the ground state and let it evolve with respect to an imaginary time such that

$$|GS\rangle = \lim_{\tau \to \infty} \frac{e^{-\tau \mathcal{H}} |\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}} \tag{10.53}$$

In order to prove this, take the Schrödinger equation

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \mathcal{H}\psi(x,t) \tag{10.54}$$

The global solution is given by

$$\psi(x,t) = \sum_n c_n(0) e^{-iE_n t/\hbar} \psi_n \tag{10.55}$$

where $\psi_n$ are the eigenstates of the Hamiltonian, found by solving the eigenvalue problem. The time dependence is such that the eigenstates are oscillating in the representation of the evolving state one is considering. Now make the change of coordinate $t \to it = \tau$. The Schrödinger equation becomes

$$-\hbar \frac{\partial \psi(x,\tau)}{\partial \tau} = \mathcal{H}\psi(x,\tau) \tag{10.56}$$

So that the general solution recasts as

$$\psi(x,t) = \sum_n c_n(0) e^{-E_n \tau/\hbar} \psi_n \tag{10.57}$$

The interesting thing with that transformation is that one no longer has a superposition of oscillating eigenstate but an exponentially decaying superposition of those. So finally, if the random state chosen has a non-zero overlapping with the ground state, it belongs to the superposition and for a long imaginary time the dominating term would be $e^{-E_0\tau/\hbar}$. Hence end up with

$$\psi(x,\tau \gg 1) \simeq c_0(0)e^{E_0\tau/\hbar}|\psi_0\rangle \tag{10.58}$$

Re-normalising this state gives an approximation of the ground state.

## 10.13 TROTTER–SUSUKI DECOMPOSITION

Having the Imaginary time evolution method, one would like to apply the evolution operator on a MPS state one can take the case of a 1D chain and consider only first neighbours interaction as

$$\hat{\mathcal{H}} = \sum_n \hat{h}_{n,n+1} \tag{10.59}$$

One can perform a subdivision on the imaginary time $\tau$ so that the evolution factor becomes

$$e^{-\tau\mathcal{H}} = \left(e^{-\delta\tau\mathcal{H}}\right)^m \tag{10.60}$$

Now in order to expand this exponentiation of operator, need the Trotter formula

$$e^{A+B} = \lim_{n\to\infty}\left(e^{\frac{A}{n}\frac{B}{n}}\right)^n \tag{10.61}$$

One will need a generalisation of this expression since there are more than two non-commuting operators in the exponential. This generalisation has been proposed by Suzuki. First propose a systematic approximate for the exponential function based on its two equivalent formulations.

$$e^x = \lim_{n\to\infty}\left(1+\frac{x}{n}\right)^n \tag{10.62}$$

and

$$e^x = \lim_{m\to\infty}\sum_k^m \frac{x^k}{k!} \tag{10.63}$$

Thus define the double index sequence

$$e_{n,m}(x) = \left(\sum_k^m \frac{\left(\frac{x}{n}\right)^k}{k!}\right)^n \tag{10.64}$$

This sequence converges for both $n$ and $m$ to the exponential of $x$ as one can find the relation

$$|e^x - e_{n,m}(x)| \leqslant \frac{|x|^{m+1}}{n^m(m+1)!}e^{|x|} \tag{10.65}$$

For any operator in a Banach algebra this identity holds. Now for a collection of operator $A_j$ in a Banach algebra, get the following inequality which is the main result of Suzuki that is interesting here

$$\left\| \exp\left\{ \sum_j^p A_j \right\} - f_n(A_j) \right\| \leqslant \frac{2}{n} \left( \sum_j^p \|A_j\| \right)^2 \exp\left\{ \frac{n+2}{n} \sum_j^p \|A_j\| \right\} \quad (10.66)$$

where $p$ is an integer and $f_n(A_j) = [e^{A_1/n} e^{A_2/n} e^{A_3/n} ... e^{A_p/n}]^n$. Thus one sees that for $p = 2$ one retrieves the Trotter formula and now a well-defined generalisation of this result that can applies of the factor $e^{-\tau H}$. Finally the first order Trotter-Suzuki decomposition reads

$$e^{-\delta\tau\mathcal{H}} = \prod_n e^{-\delta\tau h_{n,n+1}} + O(\delta\tau^2) \quad (10.67)$$

There are several ways to apply that imaginary time evolution on an MPS state and thanks to the Trotter-Suzuki decomposition it takes a quite straightforward from as is Figure 10.16.

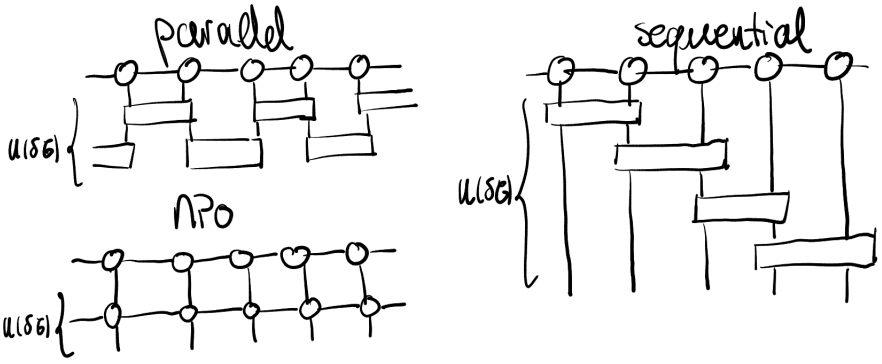


*Figure* 10.16 – Application of the imaginary time evolution operator on an MPS state/

## 10.14 ITEBD IN 1D

So far, we have only used MPS notation based on one set of matrices — the A-matrices — per site, but there also exists other useful notations, such as the one introduced by Vidal which takes the form

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} \Gamma^{\sigma_1} \lambda^{[1]} \Gamma^{\sigma_2} \lambda^{[2]} \ldots \Gamma^{\sigma_{L-1}} \lambda^{[L-1]} \Gamma^{\sigma_L} |\vec{\sigma}\rangle \quad (10.68)$$

where was introduced on each site $\ell$ a set of $d$ matrices $\Gamma^{\sigma_\ell}$ and on each bond $\ell$ one diagonal matrix $\lambda^{[\ell]}$. This is just another way of reshaping the wavefunction coefficients. These matrices are specified by the demand that for arbitrary $\ell$ ($1 \leqslant \ell < L$) one can read off the Schmidt decomposition

$$|\psi\rangle = \sum_{a_\ell}^{r} s_{a_\ell} |a_\ell\rangle_A |a_\ell\rangle_B \quad (10.69)$$

with r the Schmidt rank and where the Schmidt coefficients are the diagonal elements of $\lambda^{[\ell]}$, namely $s_{a_\ell} = \lambda^{[\ell]}_{a_\ell a_\ell}$ and the states on A and B are given as

$$|a_\ell\rangle_A = \sum_{\sigma_1,\ldots,\sigma_\ell} \left(\Gamma^{\sigma_1}\lambda^{[1]}\Gamma^{\sigma_2}\ldots\lambda^{[\ell-1]}\Gamma^{\sigma_\ell}\right)_{a_\ell} |\sigma_1,\ldots,\sigma_\ell\rangle \,,$$
$$|a_\ell\rangle_B = \sum_{\sigma_{\ell+1},\ldots,\sigma_L} \left(\Gamma^{\sigma_{\ell+1}}\lambda^{[\ell+1]}\Gamma^{\sigma_{\ell+2}}\ldots\lambda^{[L-1]}\Gamma^{\sigma_L}\right)_{a_\ell} |\sigma_{\ell+1},\ldots,\sigma_L\rangle \,,$$

where the states on A and B are orthonormal respectively, similarly to the constructions of A and B matrices. Graphically, the new notation can be represented as in Figure 10.17.

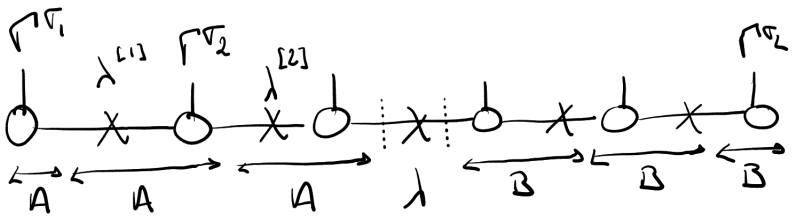


*Figure* 10.17 – Pictural representation of the $\Gamma - \lambda$ notation.

The crucial difference to the decomposition into A-matrices is that each A is decomposed, using the knowledge of $\lambda^{[\ell-1]}$ obtained in the previous step, into

$$A^{\sigma_\ell}_{a_{\ell-1},a_\ell} = \lambda^{[\ell-1]}_{a_{\ell-1},a_{\ell-1}}\Gamma^{\sigma_\ell}_{a_{\ell-1},a_\ell} \tag{10.70}$$

Similarly, decompose from the right using the right-normalization of B-matrices, the same state is obtained with a grouping

$$B^{\sigma_\ell}_{a_{\ell-1},a_\ell} = \Gamma^{\sigma_\ell}_{a_{\ell-1},a_\ell}\lambda^{[\ell]}_{a_\ell,a_\ell} \tag{10.71}$$

The TEBD algorithm, which stands for Time-Evolving Block Decimation, is a numerical scheme to simulate the evolution of a 1D finite lattice. But bulk properties of matter are best studied in an infinite system, where they are not contaminated by finite-size corrections or boundary effects. However, for most algorithms the cost of a simulation grows with the system size, and the thermodynamic limit can only be reached by extrapolating results for increasingly large systems. Present here the infinite TEBD, conveniently abridged iTEBD, a noticeably simple and fast algorithm to simulate infinite systems directly, without even resorting to extrapolations.

As presented before, the Trotter-Suzuki decomposition allows to expand the evolution operator as a sequence of small two-site gates

$$\mathcal{U}_{\ell,\ell+1} \equiv \exp\{-ih_{\ell,\ell+1}\delta t\}, \quad \delta t \ll 1 \tag{10.72}$$

In the TEBD algorithm, arrange the evolution operator into two gates $\mathcal{U}^{AB}$ and $\mathcal{U}^{BA}$

$$\mathcal{U}^{AB} \equiv \bigotimes_{\ell\in\mathbb{Z}} \mathcal{U}_{2\ell,2\ell+1} \,, \quad \mathcal{U}^{BA} \equiv \bigotimes_{\ell\in\mathbb{Z}} \mathcal{U}_{2\ell-1,2\ell} \,. \tag{10.73}$$

The wavefunction $|\psi\rangle$ is shift invariant, therefore it can be represented with an MPS where $\Gamma^{\sigma_\ell}$ and $\lambda^{[\ell]}$ are actually independent of $\ell$. However, one will partially break this translational symmetry in order to simulate the action of the two previous gates on $|\psi\rangle$. To this end, choose an MPS of the form

$$\Gamma^{\sigma_{2\ell}} = \Gamma^A, \quad \lambda^{[2\ell]} = \lambda^A \tag{10.74}$$

$$\Gamma^{\sigma_{2\ell+1}} = \Gamma^B, \quad \lambda^{[2\ell+1]} = \lambda^B, \quad \ell \in \mathbb{Z} \tag{10.75}$$

The TEBD considers a finite L sites case, where the simulation of the time evolution is achieved by updating the MPS with repeated applications of gates $\mathcal{U}^{AB}$ and $\mathcal{U}^{BA}$ on $|\psi\rangle$. For the infinite TEBD, that is for $L = \infty$, the action of the gates preserves the invariance of the evolved state under shifts of two sites, as shown in Figure 10.18. In the first part, one has drawn a tensor network representation containing both an MPS for $|\psi\rangle$ and two-site gates $\mathcal{U}$ acting on each pair of sites $\{2\ell, 2\ell+1\}$. On the second part, drawn the new MPS obtained, which is $\mathcal{U}^{AB}|\psi\rangle$. Notice that both structures are invariant under shifts by two lattice sites and are completely specified by a handful of tensors, despite the fact that they represent a state of an infinite 1D lattice.

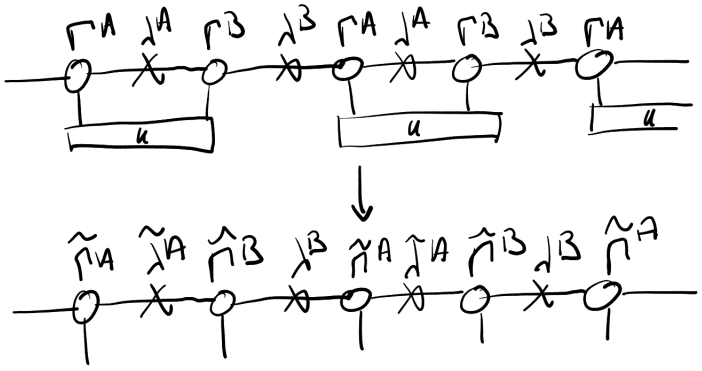


*Figure* 10.18 – Shift-invariance of the structure.

Therefore only tensors $\Gamma^A$, $\Gamma^B$, $\lambda^A$, and $\lambda^B$ need to be updated, which can be achieved through simple matrix manipulations shown in Figure 10.19. In order to update the MPS after gate $\mathcal{U}$ has been applied, first contract the tensor network into a single tensor $\Theta_{\alpha i j \gamma}$. Then perform an SVD of $\Theta$ according to the index bipartition $(\alpha i) : (j\gamma)$, namely

$$\Theta = \sum_\beta X_{(\alpha i),\beta} \tilde{\lambda}^A_\beta Y_{\beta (j\gamma)} \,. \tag{10.76}$$

We can introduce $\lambda^B$ back into the network using the inverse matrix $(\lambda^B)^{-1}$ and we can form tensors $\tilde{\Gamma}^A$ and $\tilde{\Gamma}^B$ by attaching X and Y to it.

For L sites, the TEBD algorithm requires $\mathcal{O}(Ldr^2)$ space to store an MPS and $\mathcal{O}(Ld^3r^3)$ time to simulate a small evolution $\exp\{-iH\delta t\}$. For L sites, the iTEBD requires computational space and time that scale just as $\mathcal{O}(d^2r^2)$ and $\mathcal{O}(d^3r^3)$. The key to such a drastic cost reduction by a factor L is that, in contrast to other approaches, here use an MPS based on the Schmidt decomposition, allowing for a parallelized and local update of tensors $\Gamma$ and $\lambda$.

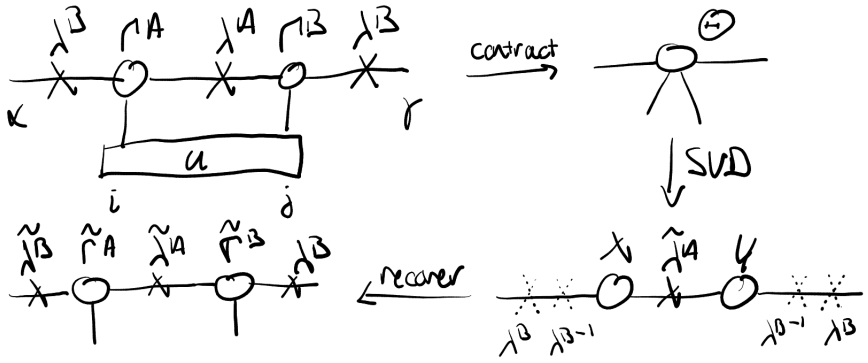


*Figure* 10.19 – MPS update in iTEBD.

Finally, evolution in imaginary time can also be simulated with iTEBD by simply replacing the two-site unitary gates $\exp\{-ih\delta t\}$ with non-unitary gates $\exp\{-h\delta\tau\}$, $\delta\tau \ll 1$.
Note that nonunitary gates destroy the Schmidt decomposition. A parallelized and local update of tensors should no longer be possible. For small $\delta\tau$, however, gate $\exp\{-h\delta\tau\}$ is close to the identity, and proceeding with a local update introduces only small errors that vanish as $\delta\tau \longrightarrow 0$. An accurate MPS for the ground state $|GS\rangle$ is then achieved by simulating imaginary time evolution with decreasingly small values of $\delta\tau$.//

There are simple extensions of the algorithm, which include, only to name a few

- Interactions $h$ with longer range. Here only considered next-nearest neighbor interactions.
- Interactions involving more than just two sites *eg* $h_{\ell,\ell+1,\ell+2}$.
- Time-dependent hamiltonians.
- Systems invariant under shifts by $m$ sites, with $m > 1$, *ie*. a larger unit cell.

## 10.15 EVOLUTION OF IPEPS

The goal is to find the ground state of an Hamiltonian with only the nearest-neighbor interactions in a 2D lattice. To do so, use iPEPS to find an approximation. The procedure consists in projecting-out the ground state via the imaginary time evolution as

$$|\psi_0\rangle = \lim_{\tau\to\infty} \frac{e^{-\tau\mathcal{H}}|\psi\rangle}{\|e^{-\tau\mathcal{H}}|\psi\rangle\|} \tag{10.77}$$

The goal is to apply the gate successively, exactly as for MPS in the iTEBD. But for MPS the truncation can be done in an optimal way casting them in canonical form and doing SVD. For iPEPS, no canonical form exist. It can be viewed by the iPEPS having loops in general, then the environment is not separable. Hence, use approximation in the truncation via simple or full update.

## 10.16 SIMPLE UPDATE

Consider as an example that will guide the description of the procedure, the spin-$\frac{1}{2}$ Heisenberg model on the honeycomb lattice. The Hamiltonian can be written

$$\begin{aligned}\mathcal{H} &= \sum_{\langle ij\rangle} \mathcal{H}_{ij} \\ &= \sum_{\langle ij\rangle} J\mathbf{S}_i \cdot \mathbf{S}_j - \frac{h}{2}\left[(-1)^i S_i^z + (-1)^j S_j^z\right]\end{aligned} \tag{10.78}$$

Schematically, the TN state is as in Figure 10.20, having attached diagonal matrices $\lambda_\alpha$, $\alpha = x, y, z$ to the bonds, that will be used to take into account an effective environment through them.

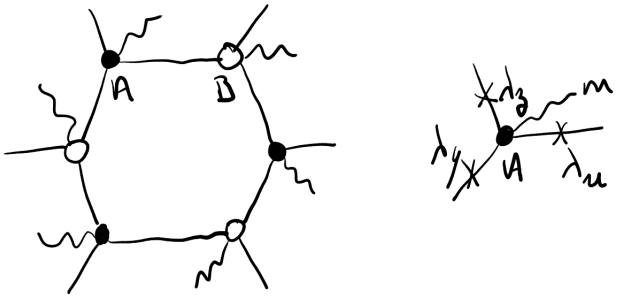


*Figure* 10.20 – Spin-$\frac{1}{2}$ Heisenberg model on the honeycomb lattice as a tensor network.

The system considered for the update is of the form given in Figure 10.21. It is important to note that the bond indices $\alpha_i$ can take D values.

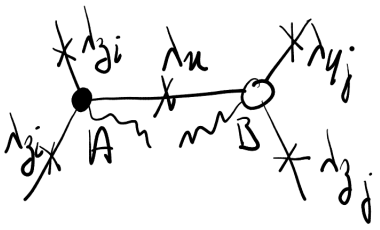


*Figure* 10.21 – System considered for the simple update.

Now, assume the state

$$|\psi\rangle = \mathrm{tr} \prod_{i\in b, j\in w} \lambda_{x_i}\lambda_{y_i}\lambda_{z_i} A^{m_i}_{x_i y_i z_i} B^{m_j}_{x_j y_j z_j} \left|m_i, m_j\right\rangle \tag{10.79}$$

with the trace the sum over all spin configurations and all bonds indices. Divide the Hamiltonian

$$\mathcal{H} = \sum_{\alpha=x,y,z} \mathcal{H}_\alpha \quad \text{with} \quad \mathcal{H}_\alpha = \sum_{i\in b} \mathcal{H}_{i,i+\alpha} \tag{10.80}$$

Apply the Trotter-Susuki formula to split the evolution operator as

$$e^{-\tau\mathcal{H}} = e^{-\tau\mathcal{H}_x} e^{-\tau\mathcal{H}_y} e^{-\tau\mathcal{H}_z} + \mathcal{O}(\tau^2) \tag{10.81}$$

and noticing by commutation

$$e^{-\tau\mathcal{H}_\alpha} = \prod_{i\in b} \underbrace{e^{-\tau\mathcal{H}_{i,i+\alpha}}}_{\text{gate}} \tag{10.82}$$

To represent the simple update with diagrams, follow Figure 10.22, where only the bond $x$ has been considered.

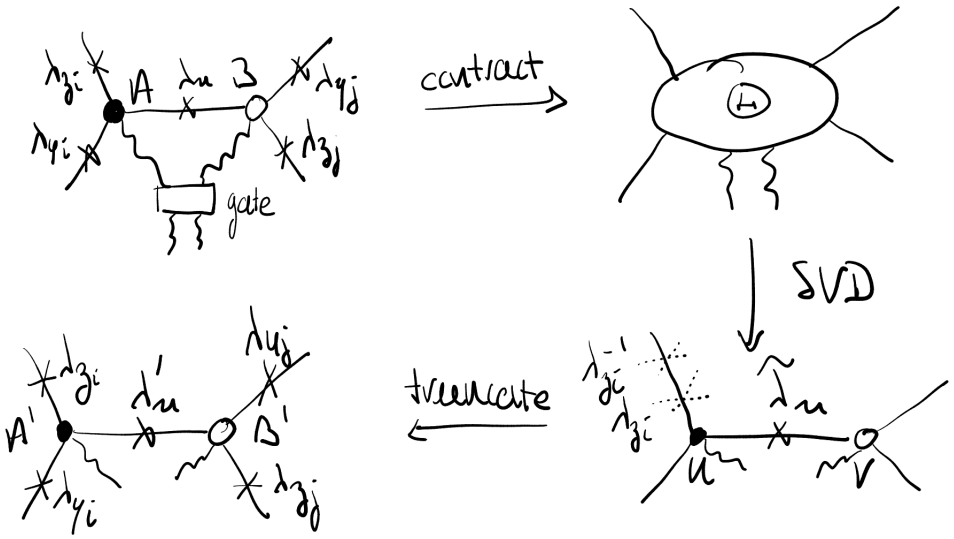


*Figure* 10.22 – Procedure of the simple update on the honeycomb lattice, only for the bond $x$ for simplicity.

Then, apply the same procedure for on the $y$- and $z$-bonds, being careful to the fact that the $\lambda$ matrices are only changed on the bond considered, keeping all the others unchanged, as mean-field.

With equations, one reads

$$\begin{aligned} e^{-\tau\mathcal{H}_x}|\psi\rangle = \mathrm{tr} \prod_{i\in b, j=i+x} \sum_{m_i', m_j'} \langle m_i', m_j' | \overbrace{e^{-\tau\mathcal{H}_{ij}}}^{\text{gate}} | m_i, m_j \rangle \\ \cdot \lambda_{x_i}\lambda_{y_i}\lambda_{z_i} A^{m_i}_{x_i y_i z_i} B^{m_j}_{x_j y_j z_j} | m_i', m_j' \rangle \end{aligned} \tag{10.83}$$

The contraction gives a $D^2 d \times D^2 d$ matrix, with $d = 2$ here as the dimension of the basis of a single-state Hilbert space,

$$\begin{aligned} \Theta_{y_i z_i m_i', y_j z_j m_j'} &= \sum_{m_i, m_j} \sum_x \langle m_i', m_j' | e^{-\tau\mathcal{H}_{ij}} | m_i, m_j \rangle \\ &\quad \cdot \lambda_{y_i}\lambda_{z_i} A^{m_i}_{x y_i z_i} \lambda_x B^{m_j}_{x y_j z_j} \lambda_{y_j}\lambda_{z_j} \\ &\overset{\text{SVD}}{=} \sum_x U_{y_i z_i m_i, x} \tilde{\lambda}_x V^\dagger x, y_j z_j m_j \end{aligned} \tag{10.84}$$

Then truncate the bond $\tilde{\lambda}_x$ of dimension $D^2 d$ back to $\lambda_x'$ of dimension $D$ and update

$$\begin{aligned} A'^{m_i}_{x y_i z_i} &= \lambda_{y_i}^{-1}\lambda_{z_i}^{-1} U_{y_i z_i m_i, x} \\ B'^{m_j}_{x y_j z_j} &= \lambda_{y_j}^{-1}\lambda_{y_j}^{-1} V_{y_j z_j m_j, x} \end{aligned} \tag{10.85}$$

## 10.17 FULL UPDATE

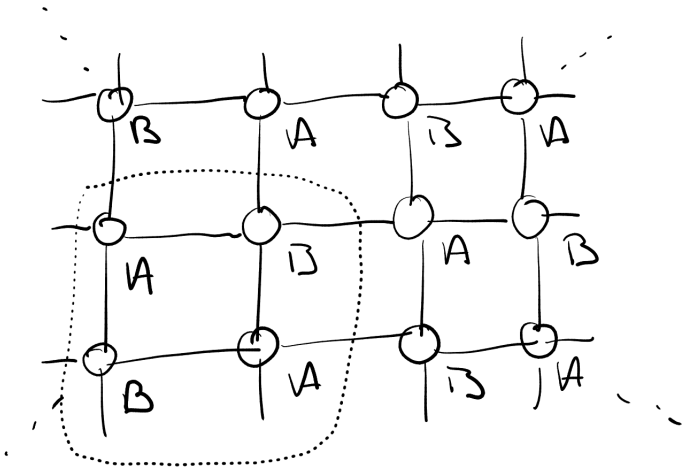


*Figure* 10.23 – Lattice considered for the full update procedure here.

To consider the full update, focus on one link with tensors $A$ and $B$ on Figure 10.23. The iPEPS and its evolution is as

$$|\psi_{AB}\rangle \xrightarrow{\text{apply gate}} |\psi_{A'B'}\rangle \xrightarrow{\text{truncate to } D} |\psi_{\tilde{A}\tilde{B}}\rangle \tag{10.86}$$

where only $A, B$ are changed, all the rest is fixed. The truncation is necessary to avoid the exponential increase of the bond dimension. A good way to perform this approximation is to find $\tilde{A}, \tilde{B}$ such that

$$d(\tilde{A}, \tilde{B}) = \| |\psi_{A'B'}\rangle - |\psi_{\tilde{A}\tilde{B}}\rangle \|^2 \tag{10.87}$$

is minimized. To solve this problem, one needs to

[1] calculate the effective environment

[2] update the system

For [1], there are various approaches but focus on CTM methods.
For [2], the process is as follows

- fix $\tilde{B}$ to rewrite

$$d(\tilde{A}, \tilde{A}^\dagger) = \tilde{A}^\dagger R \tilde{A} - \tilde{A}^\dagger S - S^\dagger \tilde{A} + T \tag{10.88}$$

  with $\tilde{A}$ having bond dimension $D$. The tensors $R$, $S$ and $T$ are given in Figure 10.24.

- find $\min_{\tilde{A}^\dagger} d(\tilde{A}, \tilde{A}^\dagger)$ thus

$$\frac{\partial d(\tilde{A}, \tilde{A}^\dagger)}{\partial \tilde{A}^\dagger} = 0 \implies \tilde{A} = R^{-1} S \tag{10.89}$$

- fix $\tilde{A}$ and do the same for $\tilde{B}$

- replace $\tilde{A}, \tilde{B}$ over the entire lattice to represent the effect of all the corresponding gates

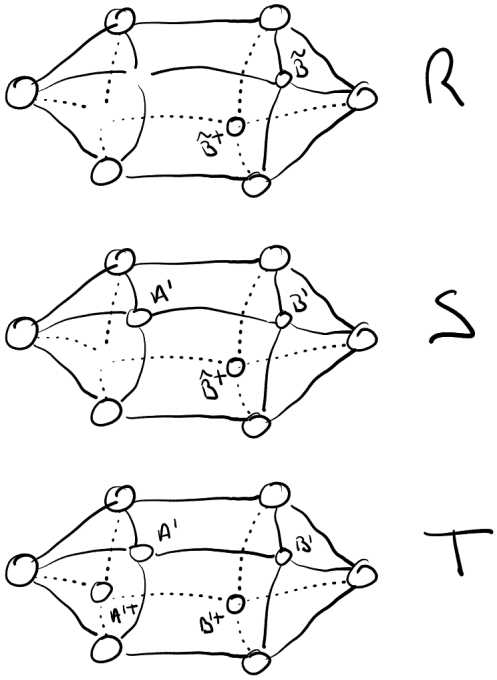


*Figure* 10.24 – Tensors involved in the computation of the effective environment in the full update.

- repeat for the other 3 bonds

There are number of ways to make it faster

- optimize the computation of $R^{-1}$
- (applicable to simple update) do QR/LQ or SVD on A and B and apply the gate on those that have less components
- fast full update, where the effective environment and the tensors are updated simultaneously
- gauge fixing, which improves stability too
- ...

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