Numerical analysis of superconducting phases in the extended Hubbard model with non-local pairing

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Abstract

[To be continued...]

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Appendix A

Mean-Field Theory in Hubbard lattices

In this Appendix the Mean-Field solutions to the Hubbard hamiltonian,

$$\hat{H} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \qquad t, U > 0$$

are described. The discussion is limited to the two-dimensional square lattice. The two-dimensional square lattice extension of the two-sites model can be studied by the means of Mean Field Theory. We have:

$$\begin{aligned} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} &= \left(\langle \hat{n}_{i\uparrow} \rangle + \delta\hat{n}_{i\uparrow}\right)\left(\langle \hat{n}_{i\downarrow} \rangle + \delta\hat{n}_{i\downarrow}\right) \\ &\simeq \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle + \delta\hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle + \langle \hat{n}_{i\uparrow} \rangle \delta\hat{n}_{i\downarrow} + \mathcal{O}\left(\delta n^2\right) \\ &= -\langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle + \hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle + \langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + \mathcal{O}\left(\delta n^2\right) \end{aligned}$$

where $\delta\hat{n}_{i\sigma} \equiv \hat{n}_{i\sigma} - \langle \hat{n}_{i\sigma} \rangle$ and orders higher than first have been ignored, assuming negligible fluctuations around the equilibrium single-site population. The first term of the above three can be neglected at fixed particles number, being a pure energy shift.

A.1 Ferromagnetic solution

The Mean-Field Theory ferromagnetic solution prescribes an uniformly magnetized lattice,

$$\langle \hat{n}_{i\uparrow} \rangle = n + m \qquad \langle \hat{n}_{i\downarrow} \rangle = n - m$$

where n is the site electron density and m is the density unbalance, leading to a magnetization per site $2m$. The mean-field hamiltonian with these substitutions becomes:

$$\begin{aligned} \hat{H} &\simeq -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \left[\hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle + \langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow}\right] \\ &= -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + nU \sum_{i} \left[\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}\right] + mU \sum_{i} \left[\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}\right] \end{aligned}$$

Fourier transforming,

$$\begin{aligned} -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} &= -2t \sum_{\mathbf{k}\sigma} \left[\cos(k_x) + \cos(k_y)\right] \hat{n}_{\mathbf{k}\sigma} \\ nU \sum_{i} \left[\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}\right] &= nU \sum_{\mathbf{k}\sigma} \hat{n}_{\mathbf{k}\sigma} \\ mU \sum_{i} \left[\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}\right] &= mU \sum_{\mathbf{k}\sigma} \left[\hat{n}_{\mathbf{k}\uparrow} - \hat{n}_{\mathbf{k}\downarrow}\right] \end{aligned}$$

having used adimensional lattice momenta. For a square lattice, the Brillouin Zone is delimited by

$$\mathbf{k} \in [-\pi, \pi] \times [-\pi, \pi]$$

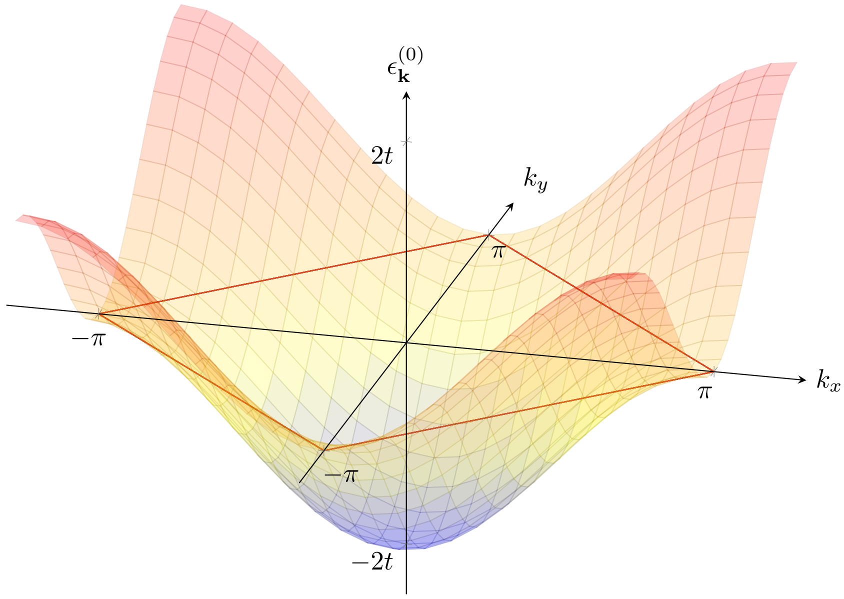

Figure A.1 | Depiction of the Hubbard square lattice hopping band $\epsilon_{\mathbf{k}}^{(0)} = -2t[\cos(k_x) + \cos(k_y)]$. The red lines mark the zero-energy intersection.

The hopping single-state energy is given by

$$\epsilon_{\mathbf{k}}^{(0)} = -2t\left[\cos(k_x) + \cos(k_y)\right]$$

represented as a band in Fig. A.1. At $U = 0$, the mean-field ferromagnetic state fills the band bottom-up. The single-state energy becomes:

$$\begin{aligned}\epsilon_{\mathbf{k}\uparrow} &= U\,(n+m) - 2t\left[\cos(k_x) + \cos(k_y)\right]\\ \epsilon_{\mathbf{k}\downarrow} &= U\,(n-m) - 2t\left[\cos(k_x) + \cos(k_y)\right]\end{aligned}$$

Now it is a matter of finding the optimal value for m, minimizing the total energy at fixed filling $\rho = 2n$. Notice that said minimization is performed parametrically varying the magnetization m, inside the ferromagnetic-polarized space. As it turns out, for strong local repulsion $U/t \gg 1$, antiferromagnetic ordering is preferred. Comparison is needed in order to assess which magnetic ordering is preferred.

Consider the half-filling situation. An unpolarized system will have $n = 1/4$, $m = 0$: this implies $\langle \hat{n}_{i\uparrow}\rangle = \langle \hat{n}_{i\downarrow}\rangle = 1/4$. A perfectly up-ferromagnetic system, $n = 1/4$, $m = 1/4$: then $\langle \hat{n}_{i\uparrow}\rangle = 1/2$ and $\langle \hat{n}_{i\downarrow}\rangle = 0$. [To be continued...]

Unclear: numerically, it turns out the paramagnetic phase ($m = 0$) is preferred. Let $\Delta \equiv Um$ and ignore the constant contribution to energies Un: graphically, the $\uparrow$ band is shifted by Δ, the $\downarrow$ band by $-\Delta$. At half-filling the Fermi energy remains fixed. For each quadrant (top view of the bands), the DoS is inversion-symmetric with respect to the anti-diagonal (red lines in Fig. A.1), thus filling the bands bottom-up while performing the shifts should leave the total energy unchanged. Why is $m = 0$ preferred?

A.2 Antiferromagnetic solution

Consider now an AF mean-field solution. Let me change notation for a brief moment, indicating each site as

$$i \to \mathbf{r} = (x, y) \qquad x, y \in \mathbb{N}$$

The mean-field AF solution at half-filling is the uniform-modulated magnetization

$$m_{\mathbf{r}} = (-1)^{x+y} m \qquad m \in [-1, 1]$$

and a mean-field Ansatz

$$\langle \hat{n}_{\mathbf{r}\uparrow} \rangle = n + m_{\mathbf{r}} \qquad \langle \hat{n}_{\mathbf{r}\downarrow} \rangle = n - m_{\mathbf{r}}$$

With respect to the solution presented above, the only detail changing is the last term,

$$\hat{H} = -t \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{\mathbf{r}\sigma} \hat{c}_{\mathbf{r}'\sigma} + nU \sum_{\mathbf{r}} \left[\hat{n}_{\mathbf{r}\uparrow} + \hat{n}_{\mathbf{r}\downarrow} \right] + mU \sum_{\mathbf{r}} (-1)^{x+y} \left[\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow} \right]$$

Fourier-transforming, the phase factor can be absorbed in the destruction operator inside of $\hat{n}_{\mathbf{r}\sigma}$:

$$\begin{aligned}
\sum_{\mathbf{r}} (-1)^{x+y} \hat{n}_{\mathbf{r}\sigma} &= \sum_{\mathbf{r}} (-1)^{x+y} \hat{c}^{\dagger}_{\mathbf{r}\sigma} \hat{c}_{\mathbf{r}\sigma} \\
&= \sum_{\mathbf{r}} e^{i\boldsymbol{\pi}\cdot\mathbf{r}} \frac{1}{N} \sum_{\mathbf{k}\in\mathrm{BZ}} e^{i\mathbf{k}\cdot\mathbf{r}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \frac{1}{N} \sum_{\mathbf{k}'\in\mathrm{BZ}} e^{-i\mathbf{k}'\cdot\mathbf{r}} \hat{c}_{\mathbf{k}'\sigma} \\
&= \sum_{\mathbf{k}\in\mathrm{BZ}} \sum_{\mathbf{k}'\in\mathrm{BZ}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}'\sigma} \frac{1}{N^2} \sum_{\mathbf{r}} e^{-i[\mathbf{k}'-(\mathbf{k}+\boldsymbol{\pi})]\cdot\mathbf{r}} \\
&= \sum_{\mathbf{k}\in\mathrm{BZ}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\sigma}
\end{aligned}$$

where $\boldsymbol{\pi} = (\pi, \pi)$. It follows:

$$mU \sum_{\mathbf{r}} (-1)^{x+y} \left[\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow} \right] = \Delta \sum_{\mathbf{k}} \left[\hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} - \hat{c}^{\dagger}_{\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\downarrow} \right]$$

Here $\Delta \equiv mU$. [To be continued...]

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