Solutions for Assignment 2

3. Weak coupling: spin density wave

(a)The substitution is easy. Since

$$n_{\mathbf{r}\uparrow} = O_{\mathbf{r}\uparrow} + \delta O_{\mathbf{r}\uparrow}, \quad n_{\mathbf{r}\downarrow} = O_{\mathbf{r}\downarrow} + \delta O_{\mathbf{r}\downarrow} \tag{1}$$

the interaction term in the Hamiltonian reads

$$\begin{aligned}
U\sum_{\mathbf{r}} n_{\mathbf{r}\uparrow}n_{\mathbf{r}\downarrow} &= U\sum_{\mathbf{r}} O_{\mathbf{r}\uparrow}O_{\mathbf{r}\downarrow} + O_{\mathbf{r}\uparrow}\delta O_{\mathbf{r}\downarrow} + \delta O_{\mathbf{r}\uparrow}O_{\mathbf{r}\downarrow} + \delta O_{\mathbf{r}\uparrow}\delta O_{\mathbf{r}\downarrow} \\
&= U\sum_{\mathbf{r}} O_{\mathbf{r}\uparrow}O_{\mathbf{r}\downarrow} + O_{\mathbf{r}\uparrow}(n_{\mathbf{r}\downarrow} - O_{\mathbf{r}\downarrow}) + (n_{\mathbf{r}\uparrow} - O_{\mathbf{r}\uparrow})O_{\mathbf{r}\downarrow} + \text{higher order in fluctuation} \\
&\approx U\sum_{\mathbf{r}} O_{\mathbf{r}\uparrow}n_{\mathbf{r}\downarrow} + O_{\mathbf{r}\downarrow}n_{\mathbf{r}\uparrow} - O_{\mathbf{r}\uparrow}O_{\mathbf{r}\downarrow} \ , \qquad (2)
\end{aligned}$$

because operators of up and down spin commute.

(b)Using the transformation given in the exercise, we have

$$O_{\mathbf{r}\uparrow} = \bar{n}_{\mathbf{r}} + \Omega^z_{\mathbf{r}}, \quad O_{\mathbf{r}\downarrow} = \bar{n}_{\mathbf{r}} - \Omega^z_{\mathbf{r}} \tag{3}$$

and the substitution into Eq.(2) dictates, for the interaction part of the Hamiltonian

$$U\sum_{\mathbf{r}} \left[\bar{n}_{\mathbf{r}}(n_{\mathbf{r}\uparrow} + n_{\mathbf{r}\downarrow}) - \Omega^z_{\mathbf{r}}(n_{\mathbf{r}\uparrow} - n_{\mathbf{r}\downarrow}) - (\bar{n}_{\mathbf{r}})^2 + (\Omega^z_{\mathbf{r}})^2\right] \ , \tag{4}$$

where we used $[\bar{n}_{\mathbf{r}}, \Omega^z_{\mathbf{r}}] = 0$.

(c) In terms of the A and B sublattices, the Hamiltonian can be rewritten

$$\begin{aligned}
\hat{\mathcal{H}}^{\mathrm{HF}}_{\mathrm{Neel}} &= t\sum_{\mathbf{r}\boldsymbol{\delta}\sigma} c^\dagger_{\mathbf{r}\sigma}c_{\mathbf{r}+\boldsymbol{\delta},\sigma} + U\sum_{\mathbf{r}\in A}[(\bar{n}-\Omega)n_{\mathbf{r}\uparrow} + (\bar{n}+\Omega)n_{\mathbf{r}\downarrow} - (\bar{n}-\Omega)(\bar{n}+\Omega)] \\
&\qquad + U\sum_{\mathbf{r}\in B}[(\bar{n}+\Omega)n_{\mathbf{r}\uparrow} + (\bar{n}-\Omega)n_{\mathbf{r}\downarrow} - (\bar{n}+\Omega)(\bar{n}-\Omega)] \\
&= t\sum_{\mathbf{r}\boldsymbol{\delta}\sigma} c^\dagger_{\mathbf{r}\sigma}c_{\mathbf{r}+\boldsymbol{\delta},\sigma} + \sum_{\mathbf{r}\in A}\left[\epsilon_{A\uparrow}n_{\mathbf{r}\uparrow} + \epsilon_{A\downarrow}n_{\mathbf{r}\downarrow} - \frac{1}{U}\epsilon_{A\uparrow}\epsilon_{A\downarrow}\right] + \sum_{\mathbf{r}\in B}\left[\epsilon_{B\uparrow}n_{\mathbf{r}\uparrow} + \epsilon_{B\downarrow}n_{\mathbf{r}\downarrow} - \frac{1}{U}\epsilon_{B\uparrow}\epsilon_{B\downarrow}\right]
\end{aligned} \tag{5}$$

where we have introduced $\epsilon_{A\uparrow} = U(\bar{n}-\Omega)$, $\epsilon_{A\downarrow} = U(\bar{n}+\Omega)$, $\epsilon_{B\uparrow} = U(\bar{n}+\Omega)$ and $\epsilon_{B\downarrow} = U(\bar{n}-\Omega)$. We notice that this is just a Hamiltonian for electrons on sublattices A and B with spin-dependent on-site energies $\epsilon_{A,B\sigma}$, just like a tight-binding model; the on-site repulsion which will be disregarded.

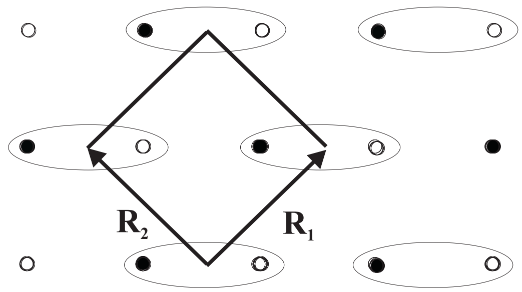

FIG. 1: Checkboard lattice. Atom A and atom B are represented by filled and empty dots.

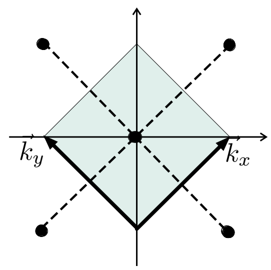

FIG. 2: The Brillouin Zone(filled square) of the checkboard lattice.

In the case of half-filling, the condition $n_{\mathbf{r}\sigma} + n_{\mathbf{r}\bar{\sigma}} = 1$ is fulfilled, then the above Hamiltonian describes the situation of one orbital per site. The unit cell contains one A atom and one B atom. As depicted in Fig. 1, the Bravais lattice can be built up by two vectors $\mathbf{R}_1 = (1, 1)$ and $\mathbf{R}_2 = (-1, 1)$. The reciprocal lattice $(\mathbf{Q}_i)$is defined as $\mathbf{Q}_i \cdot \mathbf{R}_j = 2\pi\delta_{ij}$, which gives

$$\mathbf{Q}_1 = 2\pi \left(\frac{1}{2}, \frac{1}{2}\right), \quad \mathbf{Q}_2 = 2\pi \left(-\frac{1}{2}, \frac{1}{2}\right) \quad . \tag{6}$$

The Brillouin Zone is depicted in Fig.2, which is the same shape as the Bravais lattice in the real space. Considering the hopping between the nearest neighbors, as in Fig.3 then the Hamiltonian

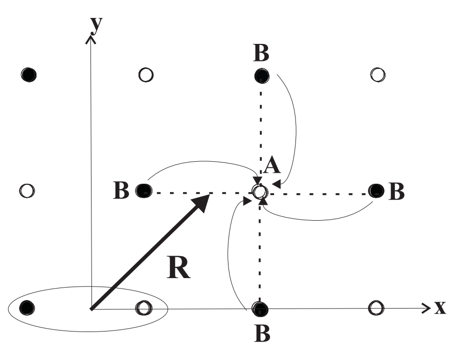

FIG. 3: Nearest neighbor jumping from the surrounding B sites to A site.

in the real space reads,

$$\hat{\mathcal{H}} = t\sum_{\mathbf{r}\in A\boldsymbol{\delta}\sigma} c^\dagger_{A\mathbf{r}\sigma}c_{B\mathbf{r}+\boldsymbol{\delta}\sigma} + \sum_{\mathbf{r}}(\sum_{\sigma}\epsilon_{A\sigma}n_{\mathbf{r}\sigma} - \frac{1}{U}\epsilon_{A\uparrow}\epsilon_{A\downarrow})$$
$$+t\sum_{\mathbf{r}\in B\boldsymbol{\delta}\sigma} c^\dagger_{B\mathbf{r}\sigma}c_{A\mathbf{r}+\boldsymbol{\delta}\sigma} + \sum_{\mathbf{r}}(\sum_{\sigma}\epsilon_{B\sigma}n_{\mathbf{r}\sigma} - \frac{1}{U}\epsilon_{B\uparrow}\epsilon_{B\downarrow})\ . \tag{7}$$

where we have dropped some constant terms like $\epsilon_{A(B),\sigma}\epsilon_{A(B),\bar{\sigma}}/U$ and the lattice constant is taken as $a = 1$. Now the Fourier transformations to transfer the operators from the real space into k-space(within the first Brillouin zone), i.e.,

$$c^\dagger_{A(B),\mathbf{r},\sigma} = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} c^\dagger_{A(B),\mathbf{k},\sigma}, \quad c_{A(B),\mathbf{r},\sigma} = \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} c_{A(B),\mathbf{k},\sigma}\ , \tag{8}$$

gives for the hopping term $\sum c^\dagger_{A\mathbf{r}\sigma}c_{B\mathbf{r}+\boldsymbol{\delta}\sigma}$

$$\sum_{\mathbf{r}\boldsymbol{\delta}\sigma} c^\dagger_{A\mathbf{r}\sigma}c_{B\mathbf{r}+\boldsymbol{\delta}\sigma} = \sum_{\mathbf{r}\mathbf{k}\mathbf{k}'\boldsymbol{\delta}\sigma} c^\dagger_{A\mathbf{k}\sigma}c_{B\mathbf{k}+\boldsymbol{\delta}\sigma} e^{i\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')} e^{i\boldsymbol{\delta}\cdot\mathbf{k}'} \tag{9}$$
$$= \sum_{\mathbf{k}\boldsymbol{\delta}\sigma} c^\dagger_{A\mathbf{k}\sigma}c_{B\mathbf{k}+\boldsymbol{\delta}\sigma} e^{i\boldsymbol{\delta}\cdot\mathbf{k}}, \tag{10}$$

and similar for the other one, where we used $\sum_{\mathbf{r}} e^{i\mathbf{r}\cdot\mathbf{k}} = \delta(\mathbf{k})$. Now we define a function $\gamma(\mathbf{k})$ as

$$\gamma(\mathbf{k}) \equiv \frac{1}{z}\sum_{\boldsymbol{\delta}} e^{i\boldsymbol{\delta}\cdot\mathbf{k}}\ . \tag{11}$$

Here z is the coordination number, number of nearest neighbours, which is equal to 4 in our case. For two dimensions, $\boldsymbol{\delta}$ takes the values $\{(1,0);(0,1);(-1,0);(0,-1)\}$ and we find

$$4\gamma(\mathbf{k}) = (e^{ik_x} + e^{-ik_x}) + (e^{ik_y} + e^{-ik_y}) = 2\cos k_x + 2\cos k_y\ . \tag{12}$$

The Fourier transformations of the potential terms just turn $\mathbf{r}$'s into $\mathbf{k}$'s. Substitution of the above into the Hamiltonian gives

$$\hat{\mathcal{H}} = \sum_{\mathbf{k}\sigma}\left[2t(\cos k_x + \cos k_y)\left(c^\dagger_{A\mathbf{k},\sigma}c_{B\mathbf{k},\sigma} + c^\dagger_{B\mathbf{k},\sigma}c_{A\mathbf{k},\sigma}\right) + \epsilon_{A\sigma}c^\dagger_{A\mathbf{k},\sigma}c_{A\mathbf{k},\sigma} + \epsilon_{B\sigma}c^\dagger_{B\mathbf{k},\sigma}c_{B\mathbf{k},\sigma}\right]$$
$$= \sum_{\mathbf{k}\sigma}(c^\dagger_{A\mathbf{k}\uparrow}, c^\dagger_{B\mathbf{k}\uparrow}, c^\dagger_{A\mathbf{k}\downarrow}, c^\dagger_{B\mathbf{k}\downarrow})\begin{pmatrix} \epsilon_{A\uparrow} & 4t\gamma(\mathbf{k}) & 0 & 0 \\ 4t\gamma(\mathbf{k}) & \epsilon_{B\uparrow} & 0 & 0 \\ 0 & 0 & \epsilon_{A\downarrow} & 4t\gamma(\mathbf{k}) \\ 0 & 0 & 4t\gamma(\mathbf{k}) & \epsilon_{B\downarrow} \end{pmatrix}\begin{pmatrix} c_{A\mathbf{k}\uparrow} \\ c_{B\mathbf{k}\uparrow} \\ c_{A\mathbf{k}\downarrow} \\ c_{B\mathbf{k}\downarrow} \end{pmatrix}\ . \tag{13}$$

Noticing that these two blocks have identical eigenvalues, we can calculate from the characteristic polynomial

$$(\epsilon_{A\uparrow} - \omega)(\epsilon_{B\uparrow} - \omega) - 16t^2\gamma(\mathbf{k})^2 = 0 \tag{14}$$

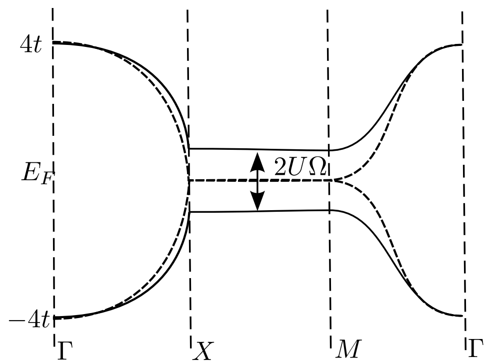

FIG. 4: Band structure for $\Omega = 0$ and $U\Omega$ small. In the latter case a gap opens up, with the Fermi surface exactly in the middle.

to derive two dispersion relations (using $\epsilon_{A\uparrow} + \epsilon_{B\uparrow} = 2U\bar{n}$ and $\epsilon_{A\uparrow}\epsilon_{B\uparrow} = U^2\bar{n}^2 - U^2\Omega^2$)

$$\begin{aligned} \omega_{\mathbf{k}}^{\pm} &= \frac{\epsilon_{A\uparrow} + \epsilon_{B\uparrow}}{2} \pm \sqrt{\frac{(\epsilon_{A\uparrow} + \epsilon_{B\uparrow})^2}{4} - \epsilon_{A\uparrow}\epsilon_{B\uparrow} + 16t^2\gamma(\mathbf{k})^2} \\ &= U\bar{n} \pm \sqrt{U^2\Omega^2 + 4t^2(\cos k_x + \cos k_y)^2} \ . \end{aligned} \tag{15}$$

For $\Omega = 0$,

$$\omega_{\mathbf{k}}^{\pm} = U\bar{n} \pm 2t|\cos k_x + \cos k_y|^2 \ . \tag{16}$$

For half-filling, the Fermi surface lies half-way the extrema, and is nested (see Fig. 4), i.e. it coincides with the boundary of the Brillouin Zone everywhere. For Ω small but finite, a gap opens everywhere. The lower band is completely filled, while the upper band is totally empty (at least at $T = 0$).

When $\Omega = 0$, the distinction between the A- and B-lattices (and corresponding Hamiltonian terms) vanishes. We might as well just consider the lattice as one, leaving a tight-binding model with square-lattice potential. In this case, the cells of the Bravais lattice become twice as small, each containing just one lattice site, so that the area of the Brillouin Zone ($\sim \frac{2\pi}{a}$) is doubled. To compare the two approaches, the first Brillouin Zone of the single-band model corresponds to the first and second Brillouin Zones of the staggered model.

To obtain the band structure of the staggered model from that of the single-band model, one 'folds' the band at the zone boudaries (of the staggerd model) inward. This happens automatically in the repeated zone scheme.

(d)At half-filling, the low-lying energy band should be filled up while the other is empty, then the classical energy is

$$E(\bar{n},\Omega) = \frac{1}{N}\sum_{\mathbf{k}\in BZ}\omega_{\mathbf{k}}^{-}(\bar{n},\Omega) + U(\Omega^2-\bar{n}^2) \tag{17}$$

where the last term can be regarded as potential energy, which was dropped in obtaining the Hamiltonian (3.8). To minimize the classical energy, we have the saddle-point equations

$$\begin{aligned}\frac{\partial E(\bar{n},\Omega)}{\partial\bar{n}} &= -2\bar{n}U + \frac{1}{N}\sum_{\mathbf{k}\in BZ}\frac{\partial}{\partial\bar{n}}\omega_{\mathbf{k}}^{-}(\bar{n},\Omega)\\ \frac{\partial E(\bar{n},\Omega)}{\partial\Omega} &= 2U\Omega + \frac{1}{N}\sum_{\mathbf{k}\in BZ}\frac{\partial}{\partial\Omega}\omega_{\mathbf{k}}^{-}(\bar{n},\Omega)\ .\end{aligned} \tag{18}$$

According to the dispersion relation and $\partial E/\partial\bar{n} = 0$, we immediately obtain $(1-2\bar{n})U = 0$ and since U finite, $2\bar{n} = 1$. Because we have already assumed that the charge density is uniform, which means on every site the charge density is the same, i.e., $2\bar{n}$. At half-filling, we should certainly expect $2\bar{n} = 1$ without doing any calculations. As to the equation concerning Ω, the derivative is

$$\frac{\partial}{\partial\Omega}\omega_{\mathbf{k}}^{-} = -\frac{U^2\Omega}{\sqrt{U^2\Omega^2+4t^2(\cos k_x+\cos k_y)^2}}\ . \tag{19}$$

Making use of the identity $\cos k_x + \cos k_y = 2\cos(\frac{k_x+k_y}{2})\cos(\frac{k_x-k_y}{2})$ and taking into account the Jacobian for transforming integration variables from $\mathbf{k}$ to $h_{x(y)}$, which is $|\partial k_i/\partial h_j| = 2$, we shall have

$$\Omega = \frac{2}{\pi^2}\int_0^{\pi/2}dh_x\int_0^{\pi/2}dh_y\frac{1}{\sqrt{1+\left(\frac{4t}{U\Omega}\cos h_x\cos h_y\right)^2}}\ . \tag{20}$$

The transformation of the sum to the integral over $\mathbf{h}$ goes like

$$\begin{aligned}\frac{1}{N}\sum_{\mathbf{k}\in\mathrm{BZ}} &\mapsto \frac{1}{V_{\mathrm{BZ}}}\int_{k\in V_{\mathrm{BZ}}}\mathrm{d}^2k \mapsto \frac{2}{V_{\mathrm{BZ}}}\int_{h\in V'_{\mathrm{BZ}}}\mathrm{d}^2h = \frac{2}{V_{\mathrm{BZ}}}\int_{-\pi/2}^{\pi/2}\mathrm{d}h_x\int_{-\pi/2}^{\pi/2}\mathrm{d}h_y\\ &\mapsto \frac{8}{2\pi^2}\int_0^{\pi/2}\mathrm{d}h_x\int_0^{\pi/2}\mathrm{d}h_y,\end{aligned} \tag{21}$$

where the last mapping holds because the cosines are symmetric in 0, and V'_{BZ} denotes the rescaled Brillouin Zone.

(e)At the strong coupling limit $U \gg t$, the Eq.(20) reads

$$\begin{aligned}\Omega &\approx \frac{2}{\pi^2}\int_0^{\pi/2}dh_x\int_0^{\pi/2}dh_y\left[1-\frac{8t^2}{U^2\Omega^2}\cos^2 h_x\cos^2 h_y\right]\\ &= \frac{1}{2}\left(1-2\frac{t^2}{U^2\Omega^2}\right)\ .\end{aligned} \tag{22}$$

Now try the solution $\Omega = \frac{1}{2} - \alpha\frac{t^2}{U^2}$, which leads to $\alpha = 4$ (this was stated wrongly to be 2 in the assignment).

Filling this in in the classical energy per site

$$E(\bar{n}, \Omega) = \frac{1}{N}\sum_{\mathbf{k}\in BZ}\omega_{\mathbf{k}}^{-}(\bar{n}, \Omega) + U(\Omega^2 - \bar{n}^2) \tag{23}$$

at the saddle point gives

$$E\left(\bar{n} = \frac{1}{2}, \Omega = \frac{1}{2}\right) = -4\frac{t^2}{U} \tag{24}$$

This already holds for the zeroth order $\Omega \approx \frac{1}{2}$, and requires some more work for the next order. The prefactor 4 is again the coordination number of the square lattice. Then the total classical energy at saddle point is given by

$$NE\left(\bar{n} = \frac{1}{2}, \Omega = \frac{1}{2}\right) = -4N\frac{t^2}{U} \ . \tag{25}$$

Since we limit ourselves to the configuration with the order parameter $\vec{S} = (0, 0, 1/2)$ for site A and $\vec{S} = (0, 0, -1/2)$ for site B, in the Heisenberg model, the first term

$$J\sum_{\mathbf{r}\boldsymbol{\delta}}\vec{S}_{\mathbf{r}}\cdot\vec{S}_{\mathbf{r}+\boldsymbol{\delta}} = -4NJ\times\frac{1}{4} \tag{26}$$

where 4 accounts for the number of nearest neighbors and N is the total number of sites. The last term in Heisenberg model

$$J\sum_{\mathbf{r}\boldsymbol{\delta}}\frac{1}{4} = JN \ . \tag{27}$$

In total, the Heisenberg Hamiltonian reduces to

$$J\sum_{\mathbf{r}\boldsymbol{\delta}}\left(\vec{S}_{\mathbf{r}}\cdot\vec{S}_{\mathbf{r}+\boldsymbol{\delta}} - \frac{1}{4}\right) \to -2NJ = -4N\frac{t^2}{U} \ , \tag{28}$$

which is the same as the classical energy at the saddle point in the large U limit.

(f)The average value of $\cos h_y$ over $[0, \pi/2]$ is given by

$$< h_y >= (\frac{\pi}{2})^{-1}\int_0^{\pi/2} dh_y \cos h_y = \frac{2}{\pi} \ . \tag{29}$$

Now we expand $\cos h_x$ around the Fermi surface $h_x = \frac{\pi}{2}$ introducing $h'_x = h_x - \frac{\pi}{2}$, i.e.,

$$\cos h_x \approx -h'_x \ . \tag{30}$$

Equation (20) is then modified as

$$\Omega \approx \frac{1}{\pi}\int_0^{h_0'} dh_x' \frac{1}{\sqrt{1+\left(\frac{8t}{U\pi\Omega}h_x'\right)^2}} = \frac{U\Omega}{8t}\text{arcsinh}\left(\frac{8t|h_0'|}{U\pi\Omega}\right) \tag{31}$$

which implies

$$\Omega = \frac{8t|h_0'|}{U\pi\sinh\left(\frac{8t}{U}\right)} \ . \tag{32}$$

At limit $t/U \gg 1$ one expects an exponential decay of the Neel order parameter

$$\Omega \approx \frac{16t|h_0'|}{U\pi}e^{-\frac{8t}{U}} \ , \tag{33}$$

which is still finite at large t/U.

(g)*In the present case only the nearest neighbors are counted, we see that the Fermi-surface coincides with the Brillouin zone boundary, and along everywhere on the Fermi-surface a gap opens for finite $U\Omega$. If we include the next-nearest-neighbor hopping, the Fermi-surface will more spherical than the case with only nearest neighbor hopping. As a consequence of such geometry, such Fermi-surface intersects with Brillouin zone only at certain points. Recall the saddle point equation for Neel order parameter

$$\Omega = \frac{2}{\pi^2}\int_0^{\pi/2} dh_x \int_0^{\pi/2} dh_y \frac{1}{\sqrt{1+\left(\frac{4t}{U\Omega}\cos h_x \cos h_y\right)^2}} \ , \tag{34}$$

or its equivalence reads

$$\frac{1}{U} = \frac{2}{\pi^2}\int_0^{\pi/2} dh_x \int_0^{\pi/2} dh_y \frac{1}{\sqrt{U^2\Omega^2+\left(4t\cos h_x \cos h_y\right)^2}} \ , \tag{35}$$

which implies a finite Ω for every finite U. When the next-nearest-neighbors are counted even for $\Omega = 0$, the integral could still be finite, but for infinitesimal U there is no condensation. So, for spin-ordering to occur, we need sufficiently large U.