Formalism to implement Renormalized Mean-Field Theory for $SU(N)$ fermions

Sumiran Pujari[1]

[1]*Dept. of Physics, University of Kentucky, Lexington, Kentucky, 40508, USA.*

In these notes we describe the generalization of Renormalized Mean-field theory for $SU(2)$ fermions to the case of general $SU(N)$ fermions. This brings in $N-1$ Gutzwiller variational parameters.

PACS numbers:

The first two sections deal with formalism and so can apply to other lattices and hopping terms as well. We use Bernal stack as an example to set up the discussions.

The $SU(N=2)$ Hamiltonian that can model Bernal stacked bilayer Graphene is

$$\begin{aligned} H &= T + V \\ T &= -t \sum_{\text{intra-layer}\{r,r'\},\sigma} c^\dagger_{r,\sigma} c_{r',\sigma} + \text{h.c.} \\ &\quad - t_p \sum_{\text{inter-layer}\{r,r'\},\sigma} c^\dagger_{r,\sigma} c_{r',\sigma} + \text{h.c.} \\ V &= \sum_r U_r \, n_{r,\uparrow} n_{r,\downarrow} \end{aligned} \tag{1}$$

Let us be at half-filling in the grand-canonical ensemble, i.e. $\mu = 0$. We would like to study $SU(N)$ for general N to compare to QMC numerics, for which the Hamiltonian be written as

$$\begin{aligned} H &= T + V \\ T &= -t \sum_{\text{intra-layer}\{r,r'\},\sigma} c^\dagger_{r,\sigma} c_{r',\sigma} + \text{h.c.} \\ &\quad - t_p \sum_{\text{inter-layer}\{r,r'\},\sigma} c^\dagger_{r,\sigma} c_{r',\sigma} + \text{h.c.} \\ V &= \sum_r \sum_{\{\mathcal{P}(\sigma_1,\sigma_2)\}} U_r \, n_{r,\sigma_1} n_{r,\sigma_2} \end{aligned} \tag{2}$$

where σ is a flavour index now which runs from 1 to N. $\{\mathcal{P}(\sigma_1,\sigma_2)\}$ denotes the set of unique permutation of two flavors. For $N=4$, they would be $\{(1,2),(1,3),(1,4),(2,3),(2,4),(3,4)\}$. The size of this permutation set is $(N,2) = N(N-1)/2$.

The non-interacting kinetic/hopping part of H in Eq. 1 or 2 hosts quadratic band touching for each spin or flavour species. The on-site interaction or Hubbard term is marginal from power counting in two dimensions. So a primary question is whether the quadratic band touching survives or is stable for weak but non-zero Hubbard term, or does a gap open up as soon as the Hubbard term becomes 0^+.

I. LARGE-N MEAN FIELD THEORY

To answer this question with mean-field theory, one would like to perform a mean-field theory for weak U. The usual mean-field approaches starting with Affleck, Marston in late 80s are designed instead for the strong or infinite U limit, where a t-J description can be supplemented and large-N MFT fruitfully applied. What does large-N MFT say for the weak U limit of Eq. 2 ?

Let us suppose a mean-field ansatz for decoupling the Hubbard term as a mean-field $\langle n_r, \sigma\rangle = a_{r,\sigma}$. Using this to decouple the Hubbard term, we get

$$U \sum_r \sum_\sigma n_{r,\sigma} \sum_{\sigma' \neq \sigma} \langle n_{r,\sigma'} \rangle \tag{3}$$

We do not consider the superconducting (presumed to be zero for weak repulsive interaction) and spin-flip type mean-field decouplings. To proceed, we use the half-filling constraint

$$\sum_\sigma \langle n_{r,\sigma} \rangle = \frac{N}{2} \tag{4}$$

to re-write the decoupled Hubbard term in Eq. 3 as

$$U \sum_r \sum_\sigma n_{r,\sigma} \left(\frac{N}{2} - \langle n_{r,\sigma} \rangle \right) \tag{5}$$

Since $\langle n_r, \sigma\rangle \in [0,1]$, therefore in the $N \to \infty$ limit, $N/2 - \langle n_r, \sigma\rangle \to N/2$. This is a trivial shift to the chemical potential for each flavour that is *equal* ($UN/2$) for all flavours. Thus, large-N MFT predicts no gap opening in the quadratic band touching for weak U. Of course, this prediction need not be correct for finite N. So we would like to have a MFT for fixed N.

For the other limit of strong U, we can expect a VBS type state for large-N MFT again through the lens of Heisenberg exchange physics.

II. UNRESTRICTED RENORMALIZED MEAN FIELD THEORY (RMFT)

A. Basic Formalism

In this section we generalize to any N the $SU(2)$ formulation of Gutzwiller projected type MFT by Wang *et al*[1] called RMFT , in order to do a fixed N MFT in the weak U. The approach can be applied to any U. This approach will actually be most useful in the strong U limit where the suppression of charge fluctuations due to interactions becomes especially significant. In the weak

U it will have smaller returns in terms of gain in total ground state energy for the MFT ansatz compared to RMFT ansatz. (We foresee presently that RMFT formulation might still be technically useful for stabilization of Dimer type orders which have modulation in the bond energies at weak-coupling.)

Eq. 3 of Wang *et al* gives a generalized projector for the $SU(2)$ to do the Gutzwiller projection

$$\mathcal{P}_r = F_{0,r} + y_r F_{1,r} + \eta_r y_r^2 F_{2,r} \tag{6}$$

where r is a lattice site index (we may suppress if it is not confusing in the following), $F_{n,r}$ are n^{th}-occupation projective operators (i.e. they project a ket/bra to the subspace of site occupation n *without* re-normalizing; also they act as identity on other sites). For spin-1/2 $SU(2)$, they are more explicitly $F_{0,r} = (1-n_{r,\uparrow})(1-n_{r,\downarrow})$ (called E_r in their notation), $F_{1,r} = \sum_\sigma n_{r,\sigma}(1-n_{r,-\sigma})$ (called Q_r (Q ??)) and $F_{2,r} = n_{r,\uparrow}n_{r,\downarrow}$ (called D_r). η_r is variational parameter, and y_r is like a fugacity parameter. $\mathcal{P}_r$ is Hermitian.

If $|\psi_0\rangle$ is an un-projected mean-field ansatz, then $|\psi\rangle = \prod_r \mathcal{P}_r|\psi_0\rangle$ is the (un-normalized) generalized Gutzwiller projected ansatz. The possibility of r/spatial dependence in the mean-field ansatz is referred to as "unrestricted" by Wang *et al*. For our purposes, we do not foresee the use of this "unrestricted" feature, but we retain the r index in this formalism section for completeness. The "restricted" version without spatial dependence is much older[2,3] motivated by Mott Insulator physics when the importance of disorder to the High Tc problem was likely not yet realized. Ref. 1 was precisely motivated by this issue of (impurity) disorder for Cuprates. Eq. 6 thus can be contrasted to the original Gutzwiller projection of the form $\prod_r(1-\alpha F_{2,r})|\psi_0\rangle$ where α is a spatially uniform variational parameter. The idea behind the fugacity parameter y_r is to ensure that the charge density is unchanged by the projection, i.e. $\langle\psi_0|\sum_\sigma n_{r,\sigma}|\psi_0\rangle = \langle\psi|\sum_\sigma n_{r,\sigma}|\psi\rangle/\langle\psi|\psi\rangle$ even as η_r parameter is variationally tuned. The motivation behind this maneuver is that it allows to directly view the projected ansatz $|\psi\rangle$ as a "renormalized" version of the un-projected ansatz $|\psi_0\rangle$, and thus to infer clearly the physics of $|\psi\rangle$ from that of $|\psi_0\rangle$ which is posited at the mean-field level, in the spirit of Fermi Liquid theory. This is a very appealing property of this scheme.

For $SU(N)$ with N-flavors of fermions at each site, we can generalize Eq. 6 naturally to

$$\begin{aligned}\mathcal{P}_r &= F_{0,r} + y_r F_{1,r} + f_{2,r} y_r^2 F_{2,r} + f_{3,r} y_r^3 F_{3,r} + \dots \\ &= \sum_{i=0}^{N} f_{i,r} y_r^i F_{i,r}\end{aligned} \tag{7}$$

where now we have $N-1$ variational parameters $\{f_i\}, i \in \{2,3,\dots,N\}$, and $f_{0,r} = f_{1,r} = 1$ are fixed constants. For the case of N flavors, the explicit forms for $F_{n,r}$ generalized from the $N=2$ case are

$$\begin{aligned}F_{0,r} &= \prod_\sigma (1-n_{r,\sigma}) \\ F_{1,r} &= \sum_\sigma \left(\prod_{\sigma'\neq\sigma}(1-n_{r,\sigma'})\right) n_{r,\sigma} \\ F_{2,r} &= \sum_{\sigma,\sigma'\neq\sigma} \left(\prod_{\sigma''\neq\{\sigma,\sigma'\}}(1-n_{r,\sigma'})\right) n_{r,\sigma}n_{r,\sigma'} \\ &\vdots \\ F_{N,r} &= \prod_\sigma n_{r,\sigma}\end{aligned} \tag{8}$$

where the σ flavour indices is understood to always run from 1 to N. A more compact way to write the same is

$$F_{i,r} \equiv \delta_{i,\sum_\sigma n_{r,\sigma}} \equiv \delta(i, \sum_\sigma n_{r,\sigma}) \tag{9}$$

keeping in mind the (projective) operator nature of the expression.

Notation : Let $|\psi_0\rangle$ be the normalized unprojected mean-field ansatz. $\langle\hat{O}\rangle_0 = \langle\psi_0|\hat{O}|\psi_0\rangle$, and $\langle\psi_0|\psi_0\rangle = 1$. Let $|\psi\rangle$ be projected un-normalized mean-field ansatz, i.e. $|\psi\rangle = \prod_r \mathcal{P}_r|\psi_0\rangle \equiv \mathcal{P}|\psi_0\rangle$. $\langle\hat{O}\rangle = \langle\psi|\hat{O}|\psi\rangle/\langle\psi|\psi\rangle = \langle\psi_0|\mathcal{P}\hat{O}\mathcal{P}|\psi_0\rangle/\langle\psi_0|\mathcal{P}^2|\psi_0\rangle = \langle\mathcal{P}\hat{O}\mathcal{P}\rangle_0/\langle\mathcal{P}^2\rangle_0$.

Gutzwiller approximation : While evaluating the expectation values of the projection operators, inter-site correlations are ignored. This is in-built by writing the variational parameter associated with a multi-site Gutzwiller projection in a factorizable form, i.e.

$$f^{\text{general}}_{i1,r1;i2,r2;\dots} F_{i1,r1}F_{i2,r2}\dots \equiv \left(f_{i1,r1}y_{r1}^{i1}F_{i1,r1}\right)\left(f_{i2,r2}y_{r2}^{i2}F_{i2,r2}\right)\dots \tag{10}$$

Given a mean-field ansatz $|\psi_0\rangle$, we can evaluate $\langle F_{i,r}\rangle_0$ ($N+1$ in number). Given variational parameters $\{f_{i,r}\}$, we would like to evaluate $\langle F_{i,r}\rangle$ (again $N+1$ in number). y_r is fixed by equaling projected and unprojected charge densities.

The first step by Wang *et al* is to eliminate the fugacity parameter y_r as follows : since $\mathcal{P}_r$ is linear combination of projection operators, therefore $\mathcal{P}_r^2 = \sum_{i=0}^N f_{i,r}^2 y_r^{2i} F_{i,r}$ as the cross-terms like $F_{i,r}F_{j,r}$ are zero at operator level

(and $F_{i,r}^2 = F_{i,r}$). We thus have

$$\begin{aligned}\langle \mathcal{P}^2 \rangle_0 &= \left\langle \left(\prod_r \mathcal{P}_r \right)^2 \right\rangle_0 \\ &= \left\langle \prod_r \mathcal{P}_r^2 \right\rangle_0 \\ &\to \text{Gutzwiller approximation} \\ &\to \prod_r \langle \mathcal{P}_r^2 \rangle_0 \end{aligned} \tag{11}$$

where $\langle \mathcal{P}_r^2 \rangle_0 = \sum_{i=0}^N f_{i,r}^2 y_r^{2i} \langle F_{i,r} \rangle_0$. Therefore,

$$\begin{aligned}\langle F_{i,r} \rangle &= \frac{\langle \mathcal{P} F_{i,r} \mathcal{P} \rangle_0}{\langle \mathcal{P}^2 \rangle_0} \\ &= \frac{\langle (\prod_{r1} \mathcal{P}_{r1}) F_{i,r} (\prod_{r2} \mathcal{P}_{r2}) \rangle_0}{\prod_{r1} \langle \mathcal{P}_{r1}^2 \rangle_0} \\ &\to \text{Gutzwiller approximation in numerator} \\ &\to \frac{\langle \mathcal{P}_r F_{i,r} \mathcal{P}_r \rangle_0 \prod_{r1 \neq r} \langle \mathcal{P}_{r1}^2 \rangle_0}{\prod_{r1} \langle \mathcal{P}_{r1}^2 \rangle_0} \\ &\implies \\ \langle F_{i,r} \rangle &= f_{i,r}^2 y_r^{2i} \frac{\langle F_{i,r} \rangle_0}{\langle \mathcal{P}_r^2 \rangle_0} \end{aligned} \tag{12}$$

where again in the numerator we have set the various cross-terms to zero. For $N = 2$, Wang *et al* reduce the $N + 1 = 3$ equations of Eq. 12 to get the following $N - 1 = 1$ equation,

$$\begin{aligned}\frac{\langle F_{i-1,r} \rangle \langle F_{i+1,r} \rangle}{\langle F_{i,r} \rangle^2} &= \frac{f_{i-1,r}^2 f_{i+1,r}^2}{f_{i,r}^4} \frac{\langle F_{i-1,r} \rangle_0 \langle F_{i+1,r} \rangle_0}{\langle F_{i,r} \rangle_0^2} \\ &\equiv c_{i,r} \end{aligned} \tag{13}$$

with $i = 1$ for $N = 2$, where the right hand side is now a number for each r given by our mean-field ansatz $|\psi_0\rangle$ and the unrestricted variational parameters $\{f_{i,r}\}$, in the process eliminating the fugacity parameters y_r. The two remaining equations are a) site occupation probabilities should sum to 1, or site r has either 0 or 1 or ... or N fermions

$$\sum_{i=0}^N \langle F_{i,r} \rangle = \sum_{i=0}^N \langle F_{i,r} \rangle_0 = 1 \tag{14}$$

and b) projected charge density equals unprojected charge density

$$\sum_{i=0}^N i \langle F_{i,r} \rangle = \sum_{i=0}^N i \langle F_{i,r} \rangle_0 \tag{15}$$

At half-filling, Eq. 15 will equal to $N/2$. Thus we are now equipped with $N+1$ equations to solve for the $N+1$ unknowns $\langle F_{i,r} \rangle$ for each r given a mean-field ansatz $|\psi_0\rangle$ and unrestricted variational parameters $f_{i,r}$. Since Eq. 13 is non-linear, the solution strategy is not evident for general N.

For $N = 2$ and assuming spatially uniform charge density, say at filling f, we have $\langle F_{0,r} \rangle = 1 - f + \langle F_{2,r} \rangle$ and $\langle F_{1,r} \rangle = f - 2\langle F_{2,r} \rangle$. $\langle F_{2,r} \rangle$ is given by the following quadratic equation :

$$\frac{\langle F_{2,r} \rangle^2}{(f - 2\langle F_{2,r} \rangle)^2} = f_{2,r}^2 \frac{\langle F_{2,r} \rangle_0^2}{(f - 2\langle F_{2,r} \rangle_0)^2} \tag{16}$$

which can be solved readily.

For general N, let us rather employ the following strategy : for each r a) find the fugacity parameter y_r by solving its governing equation (Eq. 17 below), b) Use Eq. 12 to evaluate the various $\langle F_{i,r} \rangle$ which are the only projected expectation values needed for RMFT. Firstly, Eq. 12 satisfies Eq. 14 by definition, so we do not have to worry about probabilities not summing to 1 which is good. Thus, with filling $f = \sum_{i=0}^N i \langle F_{i,r} \rangle_0$, plugging Eq. 12 into Eq. 15 to write

$$\sum_{i=0}^N (f - i) f_{i,r}^2 \langle F_{i,r} \rangle_0 x_r^i = 0 \tag{17}$$

where $x_r = y_r^2$ gives a N^{th} degree equation in x_r for each r. Having solved this (numerically for $N > 3$), we would choose that solution for $y_r = \sqrt{x_r}$ which respects $0 \leq \langle F_{i,r} \rangle \leq 1$ obtained through an application Eq. 12. This might generally be the smallest root greater than zero.

Assuming we have solved for $\langle F_{i,r} \rangle$ for each i,r, the next step is to rewrite the total energy $\langle H \rangle$ in terms of $\langle F_{i,r} \rangle$. For this, we need the following operator identities Eq. 18,19.

$$\begin{aligned}\mathcal{P}_r c_{r,\sigma}^\dagger \mathcal{P}_r &= \left(\sum_{i=0}^N f_{i,r} y_r^i F_{i,r} \right) c_{r,\sigma}^\dagger \left(\sum_{j=0}^N f_{j,r} y_r^j F_{j,r} \right) \\ &\to \text{only } i = j + 1 \text{ terms contribute} \\ &= \sum_{i=0}^{N-1} f_{i+1,r} f_{i,r} y_r^{2i+1} \times \\ &\quad \times \delta(i+1, \sum_{\sigma 1} n_{r,\sigma 1}) c_{r,\sigma}^\dagger \delta(i, \sum_{\sigma 2} n_{r,\sigma 2}) \\ &= \sum_{i=0}^{N-1} f_{i+1,r} f_{i,r} y_r^{2i+1} \times \\ &\quad \times c_{r,\sigma}^\dagger \delta(i, \sum_{\sigma 1 \neq \sigma} n_{r,\sigma 1}) \delta(0, n_{r,\sigma}) \\ &\Downarrow\!\Downarrow \text{ use } c_{r,\sigma}^\dagger \delta(0, n_{r,\sigma}) = c_{r,\sigma}^\dagger \\ \mathcal{P}_r c_{r,\sigma}^\dagger \mathcal{P}_r &= \left(\sum_{i=0}^{N-1} f_{i+1,r} f_{i,r} y_r^{2i+1} \delta(i, \sum_{\sigma 1 \neq \sigma} n_{r,\sigma 1}) \right) c_{r,\sigma}^\dagger \end{aligned} \tag{18}$$

Similarly,

$$\begin{aligned}
\mathcal{P}_r c_{r,\sigma}\mathcal{P}_r &= \left(\sum_{i=0}^{N} f_{i,r} y_r^i F_{i,r}\right) c_{r,\sigma} \left(\sum_{j=0}^{N} f_{j,r} y_r^j F_{j,r}\right) \\
&\to \text{only } i = j-1 \text{ terms contribute} \\
&= \sum_{i=1}^{N} f_{i-1,r} f_{i,r} y_r^{2i-1} \times \\
&\quad \times \delta(i-1, \sum_{\sigma 1} n_{r,\sigma 1}) c_{r,\sigma} \delta(i, \sum_{\sigma 2} n_{r,\sigma 2}) \\
&= \sum_{i=1}^{N} f_{i-1,r} f_{i,r} y_r^{2i-1} \times \\
&\quad \times c_{r,\sigma} \delta(i-1, \sum_{\sigma 1 \neq \sigma} n_{r,\sigma 1}) \delta(1, n_{r,\sigma}) \\
&\Downarrow \text{ use } c_{r,\sigma}\delta(1, n_{r,\sigma}) = c_{r,\sigma} \\
&= \left(\sum_{i=1}^{N} f_{i-1,r} f_{i,r} y_r^{2i-1} \delta(i-1, \sum_{\sigma 1 \neq \sigma} n_{r,\sigma 1})\right) c_{r,\sigma} \\
\mathcal{P}_r c_{r,\sigma}\mathcal{P}_r &= \left(\sum_{i=0}^{N-1} f_{i,r} f_{i+1,r} y_r^{2i+1} \delta(i, \sum_{\sigma 1 \neq \sigma} n_{r,\sigma 1})\right) c_{r,\sigma}
\end{aligned} \tag{19}$$

Eq. 18,19 reduce to Wang *et al* expressions upon $N = 2$ as expected. We also note that the parenthetical factors in Eq. 18,19 are same for both cases and can be thought of as "renormalization" factors which dress the fermions that comprise the unprojected state to the quasiparticles that comprise the projected state in analogy with Fermi Liquid theory.

For the kinetic energy we have

$$\begin{aligned}
\langle T \rangle &= \frac{\left\langle \mathcal{P}\left(\sum_{\{r,r'\},\sigma} t_{rr'} c^\dagger_{r,\sigma} c_{r',\sigma} + \text{h.c.}\right)\mathcal{P}\right\rangle_0}{\langle \mathcal{P}^2 \rangle_0} \\
&\to \text{Gutzwiller approximation} \\
&= \sum_{\{r,r'\},\sigma} t_{rr'} \frac{\left\langle (\mathcal{P}_r c^\dagger_{r,\sigma}\mathcal{P}_r)(\mathcal{P}_{r'} c_{r',\sigma}\mathcal{P}_{r'})\right\rangle_0}{\langle \mathcal{P}_r^2\rangle_0 \langle \mathcal{P}_{r'}^2\rangle_0} + \text{h.c.} \\
&\equiv \sum_{\{r,r'\},\sigma} t_{rr'} g^t_{r,\sigma} g^t_{r',\sigma} \left\langle c^\dagger_{r,\sigma} c_{r',\sigma}\right\rangle_0 + \text{h.c.}
\end{aligned} \tag{20}$$

where

$$\begin{aligned}
g^t_{r,\sigma} &= \sum_{i=0}^{N} \frac{f_{i+1,r} f_{i,r} y_r^{2i+1} \left\langle \delta(i, \sum_{\sigma 1 \neq \sigma} n_{r,\sigma 1})\right\rangle_0}{\langle \mathcal{P}_r^2\rangle_0} \\
&\to \text{use Eq. 12 for each } i \text{ to eliminate } \left\langle \mathcal{P}_r^2\right\rangle_0 \\
&= \sum_{i=0}^{N} \frac{f_{i+1,r} y_r \langle F_{i,r}\rangle}{f_{i,r}\langle F_{i,r}\rangle_0} \times \left\langle \delta(i, \sum_{\sigma 1 \neq \sigma} n_{r,\sigma 1})\right\rangle_0
\end{aligned} \tag{21}$$

is a renormalization factor for the quadratic hopping terms. In the above, we are anticipating no superconducting and spin-flip mean-fields which allows us to write

$$\begin{aligned}
\left\langle n_{r,\sigma 1} c^\dagger_{r,\sigma} c_{r',\sigma}\right\rangle_0 &\to \text{Wick decompose for } \sigma 1 \neq \sigma \\
&= \langle n_{r,\sigma 1}\rangle_0 \left\langle c^\dagger_{r,\sigma} c_{r',\sigma}\right\rangle_0
\end{aligned} \tag{22}$$

and thus

$$\begin{aligned}
&\left\langle f(n_{r,\sigma 1}, n_{r_\sigma 2}, \ldots) c^\dagger_{r,\sigma} g(n_{r',\sigma 3}, n_{r'_\sigma 4}, \ldots) c_{r',\sigma}\right\rangle_0 \\
&= \langle f(n_{r,\sigma 1}, n_{r_\sigma 2}, \ldots)\rangle_0 \left\langle g(n_{r',\sigma 3}, n_{r'_\sigma 4}, \ldots)\right\rangle_0 \left\langle c^\dagger_{r,\sigma} c_{r',\sigma}\right\rangle_0
\end{aligned} \tag{23}$$

where $\{\sigma 1, \sigma 2, \sigma 3, \sigma 4, \ldots\} \neq \sigma$. The functions f,g can be the projection operators of Eq. 20,21 for example. To make contact with the expressions by Wang *et al* we can remove y_r by the use of an implication of Eq. 12

$$y_r = \sqrt{\frac{\langle F_{i,r}\rangle_0}{\langle F_{i+1,r}\rangle_0} \frac{\langle F_{i+1,r}\rangle}{\langle F_{i,r}\rangle} \frac{f^2_{i,r}}{f^2_{i+1,r}}} \tag{24}$$

which leads to

$$g^t_{r,\sigma} = \sum_{i=0}^{N} \sqrt{\frac{\langle F_{i,r}\rangle}{\langle F_{i,r}\rangle_0} \frac{\langle F_{i+1,r}\rangle}{\langle F_{i+1,r}\rangle_0}} \times \left\langle \delta(i, \sum_{\sigma 1 \neq \sigma} n_{r,\sigma 1})\right\rangle_0 \tag{25}$$

This expression reduces to the expression of Wang *et al* (Eq. 11) for $N = 2$ as expected. In the above it is understood that we may have a non-zero chemical potential $\mu = t_{rr}$.

For the interaction energy we have

$$\begin{aligned}
\langle V \rangle &= \sum_{\{\mathcal{P}(\sigma 1,\sigma 2)\}}^{r} U_r \frac{\langle \mathcal{P} n_{r,\sigma 1} n_{r,\sigma 2}\mathcal{P}\rangle_0}{\langle \mathcal{P}^2\rangle_0} \\
&\to \text{Gutzwiller approximation} \\
&= \sum_{\{\mathcal{P}(\sigma 1,\sigma 2)\}}^{r} U_r \frac{\langle \mathcal{P}_r n_{r,\sigma 1} n_{r,\sigma 2}\mathcal{P}_r\rangle_0}{\langle \mathcal{P}_r^2\rangle_0} \\
&\to \text{terms commute freely} \\
&= \sum_{\{\mathcal{P}(\sigma 1,\sigma 2)\}}^{r} U_r \frac{\left\langle n_{r,\sigma 1} n_{r,\sigma 2}\mathcal{P}_r^2\right\rangle_0}{\langle \mathcal{P}_r^2\rangle_0} \\
&= \sum_{\{\mathcal{P}(\sigma 1,\sigma 2)\}}^{r} U_r \sum_{i=0}^{N} f^2_{i,r} y_r^{2i} \frac{\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{i,r}\rangle_0}{\langle \mathcal{P}_r^2\rangle_0} \\
&\to \text{use Eq. 12 for each } i \text{ to eliminate } \frac{f^2_{i,r} y_r^{2i}}{\langle \mathcal{P}_r^2\rangle_0} \\
\langle V \rangle &= \sum_{\{\mathcal{P}(\sigma 1,\sigma 2)\}}^{r} U_r \sum_{i=0}^{N} \frac{\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{i,r}\rangle_0}{\langle F_{i,r}\rangle_0} \langle F_{i,r}\rangle
\end{aligned} \tag{26}$$

The factors $\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{i,r}\rangle_0 / \langle F_{i,r}\rangle_0$ are understood as the ratio of probability for site r having $\sigma 1$ and $\sigma 2$ fermion conditioned on total occupation being i to the probability for site r having total occupation being i in the unprojected state $|\psi_0\rangle$. These are 0 obviously for

$i = 0$ or 1. For $N = 2$ Eq. 26 reduces to the expression of Wang *et al* $\sum_r U_r \langle F_{2,r}\rangle$ as expected.

By an application of Eq. 23, we can simplify $\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{i,r}\rangle_0$ as

$$\begin{aligned}
&\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{i,r}\rangle_0 \\
&= \left\langle n_{r,\sigma 1} n_{r,\sigma 2} \delta(i, \sum_\sigma n_{r,\sigma}) \right\rangle_0 \\
&= \left\langle n_{r,\sigma 1} n_{r,\sigma 2} \delta(i-2, \sum_{\sigma \neq \{\sigma 1,\sigma 2\}} n_{r,\sigma}) \right\rangle_0 \\
&= \langle n_{r,\sigma 1}\rangle_0 \langle n_{r,\sigma 2}\rangle_0 \left\langle \delta(i-2, \sum_{\sigma \neq \{\sigma 1,\sigma 2\}} n_{r,\sigma}) \right\rangle_0 \qquad (27)
\end{aligned}$$

Thus another way to write $\langle V\rangle$ is as

$$\langle V\rangle = \sum_{\{\mathcal{P}(\sigma 1,\sigma 2)\}}^{r} U_r \, g^U_{r,\sigma 1,\sigma 2} \langle n_{r,\sigma 1}\rangle_0 \langle n_{r,\sigma 2}\rangle_0 \qquad (28)$$

where

$$g^U_{i,r,\sigma 1,\sigma 2} = \sum_{i=0}^{N} \frac{\langle F_{i,r}\rangle}{\langle F_{i,r}\rangle_0} \times \left\langle \delta(i-2, \sum_{\sigma \neq \{\sigma 1,\sigma 2\}} n_{r,\sigma}) \right\rangle_0 \qquad (29)$$

is a renormalization factor for the quartic interaction terms.

If $SU(N)$ symmetry is unbroken, then we can evaluate the $\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{i,r}\rangle_0 / \langle F_{i,r}\rangle_0$ factors as they will become *independent* of precise value of $\sigma 1$ and $\sigma 2$ owing to the unbroken $SU(N)$ symmetry. They will be

$$\begin{aligned}
\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{0,r}\rangle_0 / \langle F_{0,r}\rangle_0 &= 0 \\
\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{1,r}\rangle_0 / \langle F_{1,r}\rangle_0 &= 0 \\
\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{2,r}\rangle_0 / \langle F_{2,r}\rangle_0 &= \frac{1}{(N,2)} \\
\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{3,r}\rangle_0 / \langle F_{3,r}\rangle_0 &= \frac{(N-2,1)}{(N,3)} \\
\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{4,r}\rangle_0 / \langle F_{4,r}\rangle_0 &= \frac{(N-2,2)}{(N,4)} \\
&\vdots \\
\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{i,r}\rangle_0 / \langle F_{i,r}\rangle_0 &= \frac{(N-2,i-2)}{(N,i)} \\
&\vdots \\
\langle n_{r,\sigma 1} n_{r,\sigma 2} F_{N,r}\rangle_0 / \langle F_{N,r}\rangle_0 &= \frac{(N-2,N-2)}{(N,N)} = 1 \qquad (30)
\end{aligned}$$

Therefore

$$\langle V\rangle = \sum_r U_r \sum_{i=2}^{N} \frac{(N,2)\,(N-2,i-2)}{(N,i)} \langle F_{i,r}\rangle \qquad (31)$$

if $SU(N)$ symmetry is unbroken. Can we make some inference about the large-N limit from the above structure in the combinatorial factors, perhaps by use of Stirling approximation ?

B. Implementation (also applicable to unprojected MFT)

So now it remains to find the mean-field ansatz $|\psi_0\rangle$ and variational parameters $f_{i,r}$ that minimizes $\langle H\rangle = \langle T\rangle + \langle V\rangle$. As is usual for mean-field theories, the structure of $\langle H\rangle \to (t_{rr'}\, g^t_r g^t_{r'} \left\langle c^\dagger_r c_{r'}\right\rangle_0 + \text{ h.c.}) + U_r\, g^U_r \langle n\rangle_0 \langle n\rangle_0$ can suggest a self-consistent iterative scheme to find the variational ground state as we learn in textbooks. Another way to do the variational procedure is to do an actual minimization of the total mean-field energy over the mean-field parameters ($|\psi_0\rangle and \{f_{i,r} w\}$). We describe the two approaches below. **In the following, if we neglect the steps involving the evaluation of the renormalization factors (g^t_r and g^U_r) and the variation of the parameters characterizing the Gutzwiller projection ($\{f_{i,r} w\}$), then we get an unprojected MFT scheme *without* any Gutzwiller projection.**

1. *Self-Consistent Eigenvalue Problem*

- 1) Start with an initial mean-field ansatz for the ground state $|\psi_0\rangle$ and initial variational parameters $\{f_{i,r}\}_0$ and their small variations written schematically as $\{df_{i,r}\}$.
- 2) Given a $|\psi_0\rangle$, we can evaluate $\left\langle c^\dagger_{r,\sigma} c_{r',\sigma}\right\rangle_0$, $\langle n_{r,\sigma}\rangle_0$ and $\langle F_{i,r}\rangle_0$. Given a set of $\{f_{i,r}\}_0$, we can evaluate y_r by solving Eq. 17. Thus we can compute the set of $\{\langle F_{i,r}\rangle\}$ by using Eq. 12. Thus we can compute the renormalization factors $g^t_{r,\sigma}$ and $g^U_{r,\sigma 1,\sigma 2}$ by using Eq. 25 and Eq. 29 respectively.
- 3) Solve the mean-field decoupled single-particle H_{MFT} for each flavor σ to construct a new many-body ground state $|\psi_1\rangle$ where

$$\begin{aligned}
H_{MFT} = &\sum_{\{r,r'\},\sigma} t_{rr'} g^t_{r,\sigma} g^t_{r',\sigma}\; c^\dagger_{r,\sigma} c_{r',\sigma} + \text{h.c.} \\
&+ \sum_{r,\sigma} U_r \left(\sum_{\sigma' \neq \sigma} g^U_{r,\sigma,\sigma'} \langle n_{r,\sigma'}\rangle_0 \right) n_{r,\sigma} \qquad (32)
\end{aligned}$$

- 4) For the new many-body ground state $|\psi_1\rangle$, we can evaluate $\langle H\rangle$ and the various $d\langle H\rangle/df_{i,r}$. Since we desire $d\langle H\rangle/df_{i,r} = 0$ and $\langle H\rangle$ to go towards the minimum, vary the variational parameters $\{f_{i,r}\}$ in direction of decreasing $\langle H\rangle$ by $\{df_{i,r}\}$ to get a new set of variational parameters $\{f_{i,r}\}_1$. This step

might require some computing finesse. We we can expect the landscape of $\langle H\rangle$ as a function of $\{f_{i,r}\}$ to be fairly simple (especially for r independent situations) since the Hamiltonian is not especially complicated from this minimization point of view. Essentially the $\{f_{i,r}\}$ are just serving to control the site occupations to account for the competition between the kinetic energy due to hopping terms and potential energy due to the interaction terms.

- 5) Redo from Step 2) with $|\psi_1\rangle$ and $\{f_{i,r}\}_1$. Iterate till convergence is achieved, i.e. $|\psi_1\rangle = |\psi_0\rangle$ and $\{f_{i,r}\}_0 = \{f_{i,r}\}_1$. $\mathcal{P}|\psi_0\rangle$ is the final variational ground state given by RMFT, where the projection is of course done with the converged set of variational parameters. $\mathcal{P} = \prod_r \mathcal{P}_r$ is given by Eq. 7.

2. *Minimization over all MFT parameters*

In the previous subsubsection, we only minimized over the variational parameters associated with the Gutzwiller projection $\{f_{i,r}\}$ and solved for $|\psi_0\rangle$ in a self-consistent way. In this subsubsection, we describe how to convert the later part also into a minimization procedure which is desirable from computer implementation point of view.

- 1) Start with an initial mean-field ansatz for the ground state $|\psi_0\rangle$ and initial variational parameters $\{f_{i,r}\}_0$. When we say a mean-field ansatz for the ground state $|\psi_0\rangle$, what we rather mean is a set of parameters like $\chi_{r,r',\sigma} \equiv \left\langle c^\dagger_{r,\sigma} c_{r',\sigma}\right\rangle_0$ which can include notationally on-site flavour density $n_{r,\sigma} \equiv \chi_{r,r,\sigma} \equiv \langle n_{r,\sigma}\rangle_0$, etc. (neglecting superconducting and spin-flip type of mean-fields for now) that give a set of single particle sets from which a many-body ground state (or thermal state) is constructed as a Slater determinant for our fermionic case of interest. We also have their small variations written schematically as $\{d\chi_{r,r',\sigma}\}$ and $\{df_{i,r}\}$.

- 2) Given a $|\psi_0\rangle$ characterized through a set of parameters $\{\chi_{r,r',\sigma}\}_0$, we can obtain $\left\langle c^\dagger_{r,\sigma} c_{r',\sigma}\right\rangle_0$, $\langle n_{r,\sigma}\rangle_0$ (trivially) and $\langle F_{i,r}\rangle_0$. Given a set of $\{f_{i,r}\}_0$, we can evaluate y_r by solving Eq. 17. Thus we can compute the set of $\{\langle F_{i,r}\rangle\}$ by using Eq. 12. Thus we can compute the renormalization factors $g^t_{r,\sigma}$ and $g^U_{r,\sigma 1,\sigma 2}$ by using Eq. 25 and Eq. 29 respectively.

- 3) Solve the mean-field decoupled single-particle H_{MFT} for each flavor σ to construct a new many-body ground state $|\psi_1\rangle$ where

$$H_{MFT} = \sum_{\{r,r'\},\sigma} t_{rr'} g^t_{r,\sigma} g^t_{r',\sigma}\ c^\dagger_{r,\sigma} c_{r',\sigma} + \text{h.c.} + \sum_{r,\sigma} U_r \left(\sum_{\sigma'\neq\sigma} g^U_{r,\sigma,\sigma'} \langle n_{r,\sigma'}\rangle_0 \right) n_{r,\sigma} \qquad (33)$$

- 4) For the new many-body ground state $|\psi_1\rangle$, we can now evaluate $\langle H\rangle$ simply by summing up the lowest energy levels up to the desired correct filling. Note this filling is same both at projected and unprojected levels. **Doing this sum is trivial from computer implementation point of view, since after evaluation of the single-particle eigenvalues from Step 3), it remains to just sort them and add up the lowest values up to the correct total filling.** Furthermore, this summation can be easily generalized to a finite-temperature situation involving Fermi-Dirac distributions. Thus we can evaluate the various $d\langle H\rangle/d\chi_{r,r',\sigma}$ and $d\langle H\rangle/df_{i,r}$. Since we desire $d\langle H\rangle/d\chi_{r,r',\sigma} = 0$ and $d\langle H\rangle/df_{i,r} = 0$ and $\langle H\rangle$ to go towards the minimum, vary the variational parameters $\{\chi_{r,r',\sigma}\}$ and $\{f_{i,r}\}$ in direction of decreasing $\langle H\rangle$ by $\{d\chi_{r,r',\sigma}\}$ and $\{df_{i,r}\}$ to get a new set of variational parameters $\{\chi_{r,r',\sigma}\}_1$ and $\{f_{i,r}\}_1$. This step might require some computing finesse. We can again expect the landscape of $\langle H\rangle$ as a function of $\{\chi_{r,r',\sigma}\}$ and $\{f_{i,r}\}$ to be not too extra complicated compared to the previous subsubsection (especially for situations with simple enough spatial dependence).

- 5) Redo from Step 2) with $\{\chi_{r,r',\sigma}\}_1$ and $|\psi_1\rangle$ and $\{f_{i,r}\}_1$. Iterate till convergence is achieved, i.e. $\{\chi_{r,r',\sigma}\}_1 = \{\chi_{r,r',\sigma}\}_0$ and $\{f_{i,r}\}_0 = \{f_{i,r}\}_1$. $\mathcal{P}|\psi_0\rangle$ is the final variational ground state given by RMFT, where the projection is of course done with the converged set of variational parameters. $\mathcal{P} = \prod_r \mathcal{P}_r$ is given by Eq. 7.

[1] Qiang-Hua Wang, Z. D. Wang, Yan Chen, and F. C. Zhang, Phys. Rev. B **73**, 092507 (2006).

[2] D. Vollhardt, Rev. Mod. Phys. **56**, 99 (1984).

[3] F.C. Zhang, C. Gros, T.M. Rice and H. Shiba, Supercond. Sci. Tech. **1** 36 (1988).