Journal of the Nigerian Association of Mathematical Physics
Volume **20 (March, 2012), pp 227 – 230**
© J. of NAMP

Gutzwiller Renormalization Factors for the t-J model

Aiyohuyin E. O. and Amen Oni-Ojo

Department of Physics,
University of Benin, Benin City, Nigeria

Abstract

The Gutzwiller factors are derived using Hilbert space counting techniques. The results compare favourably well to other results in the literature. The results are particularly simple for a homogenous wavefunctions with fixed particle number.

1.0 Introduction

The t-J model is obtained from the Hubbard model in the limit of large ratios of u/t. The Hilbert space of the t-J model excludes all configurations containing doubly occupied sites [1]. The Hamiltonian is expanded thus [2]

$$H^{(eff)} \;=\; e^{is}\; H\; e^{-is} \tag{1}$$

where H is the Hubbard Hamiltonian, where e^{is} is a unitary transformation.
The choice made for s is [2]

$$S = -\,i \sum_{\langle ij\rangle\sigma} \frac{t_{ij}}{u}\left(a^{+}_{i\sigma} d_{j\sigma} + a^{+}_{j\sigma} d_{i\sigma} - hc\right) \tag{2}$$

To restrict the system to the subspace of no double occupancies the t-J Hamiltonian is written

$$H_{t-J} = P_G\; H^{eff}\; P_G \tag{3}$$

where $P_G = \sum_i \left(1 - n_{i\uparrow} n_{i\downarrow}\right)$ (4)

is the Gutzwiller projection operator.
The t-J model Hamiltonian becomes [1]

$$H_{t-J} = -\,t \sum_{\langle ij\rangle} \left(\hat{a}^{+}_{i\sigma}\hat{a}_{j\sigma} + a^{+}_{j\sigma} a_{i\sigma}\right) + \; J \sum_{\langle ij\rangle} \left(\vec{S}_i . \vec{S}_j - \hat{n}_i \hat{n}_j / 4\right) \tag{5}$$

This model describes the low energy subspace compared to the Hubbard model Hamiltonian.
The projected BCS wave functions are assumed to be the solution of the t-J model [3]

$$\left|\psi\right\rangle = P_N P_G \left|BCS\right\rangle \tag{6}$$

where P_G projects out double occupancies and P_N fixes the particle number to N. These projected wave functions have been used to study Mott-Hubbard metal insulation transition [4].

To calculate the variational energy of a projected state, the expectation value of the form [2]

$$\frac{\left\langle \psi_o \right| P_G\; H\; P_G \left| \psi_o \right\rangle}{\left\langle \psi_o \right| P_G\; P_G \left| \psi_o \right\rangle} \tag{7}$$

must be considered, where $\left|\psi_o\right\rangle$ is any wave function with no restriction in the number of double occupancies. To evaluate the expectation value in (7) approximate analytical calculations can be performed based on the Gutzwiller approximation.

Corresponding author: ***Aiyohuyin E. O.,*** E-mail: -, Tel. +2348023381237

2.0 Gutzwiller Approximation

The Hilbert space counting arguments are used in this technique. This Gutzwiller factor is approximated thus

$$g_o \approx \frac{\langle \hat{0} \rangle \psi}{\langle \hat{0} \rangle \psi_o}$$

where $|\psi\rangle = P_G |\psi_o\rangle$. The ratio in (8) is determined by calculating the probability of occupancy at site i. Thus one calculates the probabilities for a site to be empty, singly occupied with spin σ and doubly occupied respectively. The Hilbert space restrictions are shown in Table 1 [2].

Table 1: Probability for different occupancies on site *i* in $|\psi\rangle$ *and* $|\psi_o\rangle$

Occupancy on site *i*	Probabilities	
	$\|\psi\rangle$	$\|\psi_o\rangle$
$\langle (1-\hat{n}_{i\downarrow})(1-\hat{n}_{i\uparrow}) \rangle$	$1-n_i$	$(1-n^\circ{}_{i\downarrow})(1-n^\circ{}_{i\uparrow})$
$\langle (\hat{n}_{i\downarrow})(1-\hat{n}_{i\uparrow}) \rangle$	$n_{i\downarrow}$	$n^\circ{}_{i\downarrow}(1-n^\circ{}_{i\uparrow})$
$\langle (\hat{n}_{i\uparrow})(1-\hat{n}_{i\downarrow}) \rangle$	$n_{i\downarrow}$	$n^\circ{}_{i\uparrow}(1-n^\circ{}_{i\downarrow})$
$\langle \hat{n}_{i\downarrow} n_{i\uparrow} \rangle$	0	$n^\circ{}_{i\downarrow} n^\circ{}_{i\uparrow}$

3.0 Evaluation of the Gutzwiller factors for the t-J Hamiltonian

The t-J Hamiltonian is [1]

$$H_{t-J} = -\sum_{\langle ij \rangle \sigma} t_{ij} \left(c^+_{i\sigma} c_{j\sigma} + c^+_{i\sigma'} c_{j\sigma'} \right) + \sum_{\langle ij \rangle} J_{ij} \left(\vec{S}_i . \vec{S}_j - \frac{1}{4} n_i n_j \right) \tag{9}$$

where $J = 4t^2/u$, $\langle ij \rangle$ are pairs of neighbour sites. This low energy model of the Hubbard Hamiltonian does not allow for double occupancies on a site. When the filling is half, each site has only one electron and the hopping of electrons is frozen because hopping will result in double occupancies of sites. Due to this, the kinetic energy term disappears and the t-J model reduces to the antiferromangnetic Heisenberg model [5]

For the first term of the t-J model, the Gutzwiller factor is

$$\tilde{g}_t \approx \frac{\langle c^+_{i\sigma} c_{j\sigma} \rangle \psi}{\langle c^+_{i\sigma} c_{j\sigma} \rangle \psi_o} \tag{10}$$

To obtain equation (11), projected operators $(1-\hat{n}_{i-\sigma})$ and $(1-\hat{n}_{j-\sigma}) c_{j\sigma}$ are used.

$$\tilde{g}_t \approx \frac{\langle (1-\hat{n}_{i-\sigma}) c^+_{i\sigma} (1-\hat{n}_{j-\sigma}) c_{j\sigma} \rangle \psi}{\langle (1-\hat{n}_{i-\sigma}) c^+_{i\sigma} (1-\hat{n}_{j-\sigma}) c_{j\sigma} \rangle \psi_o} \tag{11}$$

To obtain equation (12) from equation (11), table 1 is used. The probability for $(1-\hat{n}_{i-\sigma}) c^+_{i\sigma} (1-\hat{n}_{j-\sigma}) c_{j\sigma}$ in the states $|\psi\rangle$ *and* $|\psi_o\rangle$ are considered.

$$= \frac{\left(n_{i\sigma} (1-n_j) n_{j\sigma} (1-n_i) \right)^{1/2}}{\left(n^\circ{}_{i\sigma} (1-n^\circ{}_{j\sigma}) (1-n^\circ{}_{i-\sigma}) (1-n^\circ{}_{j-\sigma}) n^\circ{}_{j\sigma} (1-n^\circ{}_{j-\sigma}) (1-n^\circ{}_{i\sigma}) (1-n^\circ{}_{i-\sigma}) \right)^{1/2}} \tag{12}$$

Now $\langle c^+_{i\sigma} c_{j\sigma} \rangle \psi$

$$= \langle (1-n_{i-\sigma}) c^+_{i\sigma} (1-n_{j-\sigma}) c_{j\sigma} \rangle \psi$$

$$\approx \tilde{g}_t \langle (1-n_{i-\sigma}) c^+_{i\sigma} (1-n_{j-\sigma}) c_{j\sigma} \rangle \psi_o = \tilde{g}_t (1-n^\circ{}_{i-\sigma})(1-n^\circ{}_{j-\sigma}) \langle c^+_{i\sigma} c_{j\sigma} \rangle \psi_o$$

Hence

$$g_t = \frac{\left(n_{i\sigma}\left(1-n_j\right)n_{j\sigma}\left(1-n_i\right)\right)^{1/2}}{\left(n^\circ{}_{i\sigma}\left(1-n^\circ{}_{j\sigma}\right)n^\circ{}_{j\sigma}\left(1-n^\circ{}_{i\sigma}\right)\right)^{1/2}}$$

For a homogenous wavefunctions with fixed particle number and spin symmetry [2],

$$n^\circ{}_{i\sigma} = n^\circ{}_{i-\sigma} = n^\circ{}_{i/2} = n/_2$$

Then $n_{i\sigma} = n_{i-\sigma} = n_{i/2} = n/_2$

$$\therefore\ g_t = \frac{1-n}{1-n/_2}$$

For the magnetic case

$$n_{i\sigma} = n^\circ{}_{i\sigma}\left(1-n^\circ{}_{i-\sigma}\right) = \frac{n}{n-2n^\circ{}_{i\uparrow}n^\circ{}_{i\downarrow}}$$

and $\quad g_t = \dfrac{1-n}{1-2n^\circ{}_\uparrow n^\circ{}_\downarrow/n}$, where $n^\circ{}_\uparrow$ *and* $n^\circ{}_\downarrow$ are from the same site.

Similarly, the Gutzwiller factors for the operator $\left\langle c^+_{j\sigma}\, c_{j\sigma}\right\rangle$ are identical to that of the operator $\left\langle c^+_{i\sigma}\, c_{j\sigma}\right\rangle$. The next term in the t-J model is the operator (super exchange interaction)

$$\left\langle \vec{S}_i\ \vec{S}_j\right\rangle$$

$$\left\langle \vec{S}_i\ \vec{S}_j\right\rangle\psi = g_s\left\langle \vec{S}_i\ \vec{S}_j\right\rangle\psi_o$$

In the magnetic limit [2]

$$g_s = \frac{1}{\left(1-n^\circ{}_\uparrow n^\circ{}_\downarrow/n\right)^2}$$

In the non-magnetic limit $n^\circ{}_\sigma = n/2$ and $g_s = \dfrac{1}{(1-n/2)^2}$.

The last term in the t-J model is the operator

$$\sum_{\langle ij\rangle} -J\ \hat{n}_i\ \hat{n}_j/4$$

The Gutzwiller factor is defined by

$$\left\langle \hat{n}_i\ \hat{n}_j\right\rangle\psi\ =\ g\left\langle \hat{n}_i\ \hat{n}_j\right\rangle\psi_o$$

The process $\hat{n}_i\ \hat{n}_j$ requires a spin on site *i* and a spin on site *j*. In the state $\left|\psi\right\rangle$, the probability of occupancy is:

$$\left(n^\circ{}_{i\uparrow}\, n^\circ{}_{i\downarrow}\left(n^\circ{}_{j\uparrow}\, n^\circ{}_{j\downarrow}\ n^\circ{}_{j\downarrow}n^\circ{}_{j\uparrow}n^\circ{}_{i\uparrow}\, n^\circ{}_{i\downarrow}\right)\right)^{1/2}$$

In the state $\left|\psi\right\rangle$, the probability of occupancy is $\left(n_{i\sigma}n_{j\sigma}\ n_{j\sigma}n_{i\sigma}\right)^{1/2}\left(n_{j-\sigma}n_{i-\sigma}\right)^{1/2}$

Inserting $n_{i\sigma} = n^\circ{}_{i\sigma}\left(1-n^\circ{}_{i-\sigma}\right) = \dfrac{n}{n-2n^\circ{}_{i\uparrow}n^\circ{}_{i\downarrow}}$

in the numerator of the ratio below

$$g\ = \frac{\left(n_{i\uparrow}\, n_{j\downarrow}\ n_{j\downarrow}n_{j\uparrow}n_{i\uparrow}\, n_{i\downarrow}\right)^{1/2}}{\left(n^\circ{}_{i\uparrow}\, n^\circ{}_{i\downarrow}\ n^\circ{}_{j\uparrow}\, n^\circ{}_{j\downarrow}\ n^\circ{}_{j\uparrow}n^\circ{}_{j\downarrow}n^\circ{}_{i\uparrow}\, n^\circ{}_{i\downarrow}\right)^{1/2}} = \frac{\left(1-n^\circ_{i\downarrow}\right)n^3\left(1-n^\circ_{j\downarrow}\right)\left(1-n^\circ_{j\uparrow}\right)^{1/2}\left(1-n^\circ_{i\uparrow}\right)^{1/2}}{\left(n-2n^\circ_{i\uparrow}n^\circ_{i\downarrow}\right)^{3/2}\left(n-2n^\circ_{j\uparrow}n^\circ_{j\downarrow}\right)^{3/2}\left(n^\circ_{i\downarrow}n^\circ_{j\downarrow}\right)^{1/2}}$$

In the non-magnetic limit $n^\circ_\sigma =\ n/2$

$$\therefore\ g = \frac{\left(1 - n/_2\right)\ \left(1 - n/_2\right)\left(1 - n/_2\right)n^3}{\left(n - 2n^2/4\right)^{3/2}\ \left(n - 2n^2/4\right)^{3/2}\ \left(n/_2\right)}$$

$$g = \frac{\left(1 - n/_2\right)^3\ n^2}{\left(n - 2n^2/_4\right)^3} = \frac{2n^2\ \left(1 - n/_2\right)^3}{\left(n - n^2/_2\right)^3} = \frac{2n^2\ \left(1 - n/_2\right)^3}{\left(n - n^2/_2\right)^2} = \frac{2n^2\ \left(1 - n/_2\right)^3}{\left(n - n^2/_2\right)\left(n - n^2/_2\right)^2}$$

$$g = \frac{2}{n}$$

4.0 Discussion and Conclusion

In this paper, we have obtain the following "Gultzwiller renormalization factors for the t – J, model:

For the term $a^+_{i\sigma}a_{j\sigma}$, the Gultzwiller renormalization factor for the non-magnetic case is $\frac{1-n}{1-n/_2}$ where n is the particle density, and the Gultzwiller renormalization factor for the magnetic case is $\frac{1-n}{1-2n^o_\uparrow\, n^o_\downarrow/n}$, where $n^o_\uparrow$ *and* $n^o_\downarrow$ are from the same site, n is the particle density after projection and n^o is particle density before projection. Similar results hold for the Hermitian conjugate.

For the term $\vec{S}_i\vec{S}_j$ (superexchange interaction), the Gutzwiller renormalization factors are

$\frac{1}{\left(1 - n^o_\uparrow\, n^o_\downarrow/n\right)^2}$ *and* $\frac{1}{\left(1 - n/2\right)^2}$ for the magnetic and non magnetic cases respectively. n is the particle density after projection and n^o is the particle density before projection.

Finally, the term $\hat{n}_i\,\hat{n}_j/4$ has the Gutzwiller factors

$\frac{\left(1 - n^o_{i\downarrow}\right)\left(1 - n^o_{j\downarrow}\right)\left(1 - n^o_{i\uparrow}\right)^{1/2}\ \left(1 - n^o_{j\uparrow}\right)^{1/2} n^3}{\left(n - 2n^o_{i\uparrow}n^o_{i\downarrow}\right)^{1/2}\ \left(n - 2n^o_{j\uparrow}n^o_{j\downarrow}\right)^{3/2}\left(n^o_{i\downarrow}n^o_{j\downarrow}\right)^{1/2}}$ *and* $\frac{2\left(1 - n/2\right)^3 n^2}{\left(n - 2\,n^2/4\right)}$ for magnetic and non magnetic cases respectively. n is the particle density after projection and n^o is the particle density before projection.

In [6], the results obtained for the t-J model are similar. The Gutzwiller factors depend on the densities at the sites *i* and *j*. However, the intersite coulomb interaction is not renormalized in [6]. These results are also in agreement with the results in [7] and [8]. The results in the paper are also in considerable agreement with results in [9]. As pointed out in [9], the Gutzwiller renormalization factors may change considerably in the case of inhomogeneous charge distribution as the local density may change before and after projection.

The result obtained here, are in exact agreement with [10]. The use of Gutzwiller rormalization factors can lead to the estimation of the energies of the t-J model in the projected states. The Gutzwiller approximation is used to relate the expectation values of the kinetic energies in the projected state to the corresponding expectation values in the unprojected state.

The use of Gutzwiller factors is an alternative approach to solution of the projected wavefunctions. The technique compares favourably to the use of Variational Monte Carlo [11, 12, 13] and renormalized field theory [7].

REFERENCES

[1] Peter Fulde, Electron Correlations in Molecules and Solids (Springer, Berlin, 1995).
[2] B. Edegger, V.N. Muthukumar and C. Gros, Advances in Physics 56, 972 (2007).
[3] P.W. Anderson Science 235, 1196 (1987)
[4] W.F. Brinkman and T.M. Rice, Phys. Rev. B2, 4302 (1970)
[5] M.R. Norman and C. Pepin, Rep. Prog. Phys. 66, 1547 (2003)
[6] Huai – Xiang Huang, You-Quan Li, and Fu-Chun Zhang, Phys. Rev. B71, 184514 (2005)
[7] F.C. Zhang, C. Gros, T.M. Rice and H. Shiba, Supercond. Sci. Technol. 1,36 (1988)
[8] D. Vollhardt, Rev. Mod. Phys. 56, 99(1984)
[9] M. Raczkowski, Acta Physica Polonica A 114, 107 (2008).
[10] Noboru Fukushima, B. Edegger, C. Gros and V.N. Muthukumar Phys. Rev. B72, 144505 (2005).
[11] Q Chen, J. Stajic, S. Tan and K. Levin Phys. Rep 412, 1 (2005).
[12] S. Chakraverty, B.I. Halperium and D.R. Nelton, Phys. Rev. B37, 7444 (1988).
[13] S. Liang, B. Doucot and P.W. Anderson Phys. Rev. Lett. 61, 365, (1988).