# $\langle M^2 \rangle$ DQMC Derivation

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# 1 Introduction

Discussion of calculating $\langle M^2 \rangle$ in DQMC for the Fermi-Hubbard model.

## 1.1 Single Site

The magnetization at site $i$ is given as follows:

$$M = n_{i\uparrow} - n_{i\downarrow} \tag{1}$$

We can square this to get the local (onsite) contribution of the magnetization squared

$$M^2 = (n_{i\uparrow} - n_{i\downarrow})^2 \tag{2}$$

$$M^2 = (n_{i\uparrow} - n_{i\downarrow})(n_{i\uparrow} - n_{i\downarrow}) \tag{3}$$

$$M^2 = n_{i\uparrow}^2 + n_{i\downarrow}^2 - 2n_{i\uparrow}n_{i\downarrow} \tag{4}$$

Note that $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ Then

$$n_{i\sigma}^2 = (c_{i\sigma}^\dagger c_{i\sigma})(c_{i\sigma}^\dagger c_{i\sigma}) \tag{5}$$

$$n_{i\sigma}^2 = c_{i\sigma}^\dagger c_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} \tag{6}$$

If we use the relation $\{c_{i\sigma}, c_{i\sigma}^\dagger\} = 1$ where $\{c_{i\sigma}, c_{i\sigma}^\dagger\} = c_{i\sigma}c_{i\sigma}^\dagger + c_{i\sigma}^\dagger c_{i\sigma}$ then we can get $c_{i\sigma}c_{i\sigma}^\dagger = 1 - c_{i\sigma}^\dagger c_{i\sigma}$
Substitute that in:

$$n_{i\sigma}^2 = c_{i\sigma}^\dagger (1 - c_{i\sigma}^\dagger c_{i\sigma}) c_{i\sigma} \tag{7}$$

$$n_{i\sigma}^2 = c_{i\sigma}^\dagger c_{i\sigma} - c_{i\sigma}^\dagger c_{i\sigma}^\dagger c_{i\sigma} c_{i\sigma} \tag{8}$$

Because we're working with fermions, we can only create one particle per state, so $c_{i\sigma}^\dagger c_{i\sigma}^\dagger = 0$
Thus

$$n_{i\sigma}^2 = c_{i\sigma}^\dagger c_{i\sigma} - 0 \tag{9}$$

$$n_{i\sigma}^2 = c_{i\sigma}^\dagger c_{i\sigma} \tag{10}$$

And previously we stated that $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$
Thus

$$n_{i\sigma}^2 = n_{i\sigma} \tag{11}$$

Now if we go back to our equation for $M^2$ we can replace $n_{i\sigma}^2 \to n_{i\sigma}$:

$$M^2 = n_{i\uparrow} + n_{i\downarrow} - 2n_{i\uparrow}n_{i\downarrow} \tag{12}$$

Where the density is given by $N = n_{i\uparrow} + n_{i\downarrow}$ and the double occupancy is given by $D = n_{i\uparrow}n_{i\downarrow}$

$$M_{\text{onsite}}^2 = N - 2D \tag{13}$$

This gives us $M^2$ in terms of the density and double occupancy. This is the onsite contribution.

### 1.1.1 Expressing density in terms of Green's Functions

The greens function is given as follows:

$$G_{ij\sigma} = \langle c_{i\sigma} c_{j\sigma}^\dagger \rangle \tag{14}$$

If we use the anticommutation relation $\{c_{i\sigma}, c_{j\sigma}^\dagger\} = c_{i\sigma}c_{j\sigma}^\dagger + c_{j\sigma}^\dagger c_{i\sigma} = \delta_{ij}$
then we can make a substitution to get $\langle n_{i\sigma} \rangle$ in terms of $G_{ij\sigma}$

$$\langle n_{i\sigma} \rangle = \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle = \langle 1 - c_{i\sigma} c_i^\dagger \rangle = 1 - G_{ii\sigma} \tag{15}$$

We can now express $M_{\text{onsite}}^2$ in terms of the Green's function using this.
Where $N = (1 - G_{\uparrow,ii}) + (1 - G_{\downarrow,ii})$ and $D = (1 - G_{\uparrow,ii})(1 - G_{\downarrow,ii})$

$$M_{\text{onsite}}^2 = N - 2D \tag{16}$$

$$M_{\text{onsite}}^2 = ((1 - G_{\uparrow,ii}) + (1 - G_{\downarrow,ii})) - (2(1 - G_{\uparrow,ii})(1 - G_{\downarrow,ii})) \tag{17}$$

$$M^2_{\text{onsite}} = 2 - G_{\uparrow,ii} - G_{\downarrow,ii} - 2(1 - G_{\downarrow,ii} - G_{\uparrow,ii} + G_{\uparrow,ii}G_{\downarrow,ii}) \tag{18}$$

$$M^2_{\text{onsite}} = 2 - G_{\uparrow,ii} - G_{\downarrow,ii} - 2 + 2G_{\downarrow,ii} + 2G_{\uparrow,ii} - 2G_{\uparrow,ii}G_{\downarrow,ii} \tag{19}$$

$$\boxed{M^2_{\text{onsite}} = G_{\uparrow,ii} + G_{\downarrow,ii} - 2G_{\uparrow,ii}G_{\downarrow,ii}} \tag{20}$$

## 1.2 Multiple Sites

when we expand this to multiple sites, we end up with:

$$M^2 = \left(\sum_i (n_{i\uparrow} - n_{i\downarrow})\right)^2 = \sum_{i,j} (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \tag{21}$$

$$M^2 = \sum_{i,j} [n_{i\uparrow}n_{j\uparrow} + n_{i\downarrow}n_{j\downarrow} - n_{i\uparrow}n_{j\downarrow} - n_{i\downarrow}n_{j\uparrow}] \tag{22}$$

Which gives us two cases: $i = j$ and $i \neq j$.
For $i = j$ we get the diagonal result:

$$M^2_{\text{diagonal}} = \sum_{i \text{ where } i=j} n_{i\uparrow}n_{i\uparrow} + n_{i\downarrow}n_{i\downarrow} - 2n_{i\uparrow}n_{i\downarrow} \tag{23}$$

$$M^2_{\text{diagonal}} = \sum_{i \text{ where } i=j} G_{\uparrow,ii} + G_{\downarrow,ii} - 2G_{\uparrow,ii}G_{\downarrow,ii} \tag{24}$$

For $i \neq j$ we get a different result:

$$M^2_{\text{off diagonal}} = \sum_{i,j \text{ where } i\neq j} [n_{i\uparrow}n_{j\uparrow} + n_{i\downarrow}n_{j\downarrow} - n_{i\uparrow}n_{j\downarrow} - n_{i\downarrow}n_{j\uparrow}] \tag{25}$$

## 1.3 Wick's Theorem

We already calculated the diagonal terms above, but now we need to calculate the off diagonal terms. We can use Wick's theorem for this.

$$M^2 = M^2_{\text{diagonal}} + M^2_{\text{off diagonal}} \tag{26}$$

$$M^2 = G_{\uparrow,ii} + G_{\downarrow,ii} - 2G_{\uparrow,ii}G_{\downarrow,ii} + M^2_{\text{off diagonal}} \tag{27}$$

Now we have to figure out what $M^2_{\text{off diagonal}}$ is. Our off diagonal equation is copied from above:

$$M^2_{\text{off diagonal}} = \sum_{i,j \text{ where } i\neq j} [n_{i\uparrow}n_{j\uparrow} + n_{i\downarrow}n_{j\downarrow} - n_{i\uparrow}n_{j\downarrow} - n_{i\downarrow}n_{j\uparrow}] \tag{28}$$

Wick's theorem states:

$$\langle c^\dagger_{i\sigma}c_{j\sigma}c^\dagger_{k\sigma'}c_{l\sigma'}\rangle = \langle c^\dagger_{i\sigma}c_{j\sigma}\rangle\langle c^\dagger_{k\sigma'}c_{l\sigma'}\rangle - \langle c^\dagger_{i\sigma}c_{l\sigma'}\rangle\langle c^\dagger_{k\sigma'}c_{j\sigma}\rangle \tag{29}$$

where $G_{\sigma,ij} = \langle c_{i\sigma}c^\dagger_{j\sigma}\rangle$
We can go term by term to calculate what $M^2_{\text{off diagonal}}$ should be
**First Term:** $n_{i\uparrow}n_{j\uparrow}$

$$\langle n_{i\uparrow}n_{j\uparrow}\rangle = \langle c^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{j\uparrow}c_{j\uparrow}\rangle \tag{30}$$

$$= \langle c^\dagger_{i\uparrow}c_{i\uparrow}\rangle\langle c^\dagger_{j\uparrow}c_{j\uparrow}\rangle - \langle c^\dagger_{i\uparrow}c_{j\uparrow}\rangle\langle c^\dagger_{j\uparrow}c_{i\uparrow}\rangle \tag{31}$$

Note here that because we have different indices in the two right terms, and we already said that $i \neq j$, the anticommutation relation $\{c_{i\sigma}, c^\dagger_{j\sigma}\} = c_{i\sigma}c^\dagger_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma} = \delta_{ij}$ gives us a 0 instead of a 1.

$$= (1 - G_{\uparrow,ii}) \cdot (1 - G_{\uparrow,jj}) - (0 - G_{\uparrow,ij}) \cdot (0 - G_{\uparrow,ji}) \tag{32}$$

$$\boxed{1 - G_{\uparrow,ii} - G_{\uparrow,jj} + G_{\uparrow,ii}G_{\uparrow,jj} - G_{\uparrow,ij}G_{\uparrow,ji}} \tag{33}$$

**Second Term:** $n_{i\downarrow}n_{j\downarrow}$

$$\langle n_{i\downarrow}n_{j\downarrow}\rangle = \langle c^\dagger_{i\downarrow}c_{i\downarrow}c^\dagger_{j\downarrow}c_{j\downarrow}\rangle \tag{34}$$

$$= \langle c^\dagger_{i\downarrow}c_{i\downarrow}\rangle\langle c^\dagger_{j\downarrow}c_{j\downarrow}\rangle - \langle c^\dagger_{i\downarrow}c_{j\downarrow}\rangle\langle c^\dagger_{j\downarrow}c_{i\downarrow}\rangle \tag{35}$$

$$= (1 - G_{\downarrow,ii}) \cdot (1 - G_{\downarrow,jj}) - (0 - G_{\downarrow,ij}) \cdot (0 - G_{\downarrow,ji}) \tag{36}$$

$$\boxed{1 - G_{\downarrow,ii} - G_{\downarrow,jj} + G_{\downarrow,ii}G_{\downarrow,jj} - G_{\downarrow,ij}G_{\downarrow,ji}} \tag{37}$$

**Third Term:** $n_{i\uparrow}n_{j\downarrow}$

$$\langle n_{i\uparrow}n_{j\downarrow}\rangle = \langle c^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{j\downarrow}c_{j\downarrow}\rangle \tag{38}$$

These operators are commutable because of the different $\sigma =\uparrow, \downarrow$.

$$= \langle c^\dagger_{i\uparrow}c_{i\uparrow}\rangle\langle c^\dagger_{j\downarrow}c_{j\downarrow}\rangle \tag{39}$$

$$= (1 - G_{\uparrow,ii}) \cdot (1 - G_{\downarrow,jj}) \tag{40}$$

$$\boxed{\langle n_{i\uparrow} n_{j\downarrow} \rangle = 1 - G_{\uparrow,ii} - G_{\downarrow,jj} + G_{\uparrow,ii} G_{\downarrow,jj}} \tag{41}$$

**Fourth Term:** $n_{i\downarrow} n_{j\uparrow}$

$$\langle n_{i\downarrow} n_{j\uparrow} \rangle = \langle c^\dagger_{i\downarrow} c_{i\downarrow} c^\dagger_{j\uparrow} c_{j\uparrow} \rangle \tag{42}$$

These operators are commutable because of the different $\sigma = \downarrow, \uparrow$.

$$= \langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle \langle c^\dagger_{j\uparrow} c_{j\uparrow} \rangle \tag{43}$$

$$= (1 - G_{\downarrow,ii}) \cdot (1 - G_{\uparrow,jj}) \tag{44}$$

$$\boxed{\langle n_{i\downarrow} n_{j\uparrow} \rangle = 1 - G_{\downarrow,ii} - G_{\uparrow,jj} + G_{\downarrow,ii} G_{\uparrow,jj}} \tag{45}$$

## 1.4 Final Result:

We can now combine all of these terms to get our final result:

$$\langle M^2 \rangle = \langle M^2_{\text{diagonal}} \rangle + \langle M^2_{\text{off diagonal}} \rangle \tag{46}$$

$$\langle M^2_{\text{diagonal}} \rangle = \sum_{i \text{ where } i=j} n_{i\uparrow} n_{i\uparrow} + n_{i\downarrow} n_{i\downarrow} - 2 n_{i\uparrow} n_{i\downarrow} \tag{47}$$

$$\langle M^2_{\text{diagonal}} \rangle = \sum_{i \text{ where } i=j} G_{\uparrow,ii} + G_{\downarrow,ii} - 2 G_{\uparrow,ii} G_{\downarrow,ii} \tag{48}$$

$$\langle M^2_{\text{off diagonal}} \rangle = \sum_{i,j \text{ where } i \neq j} n_{i\uparrow} n_{j\uparrow} + n_{i\downarrow} n_{j\downarrow} - n_{i\uparrow} n_{j\downarrow} - n_{i\downarrow} n_{j\uparrow} \tag{49}$$

$$\begin{aligned} \langle M^2_{\text{off diagonal}} \rangle = \sum_{i,j \text{ where } i \neq j} \Big[ & (1 - G_{\uparrow,ii} - G_{\uparrow,jj} + G_{\uparrow,ii} G_{\uparrow,jj} - G_{\uparrow,ij} G_{\uparrow,ji}) \\ & + (1 - G_{\downarrow,ii} - G_{\downarrow,jj} + G_{\downarrow,ii} G_{\downarrow,jj} - G_{\downarrow,ij} G_{\downarrow,ji}) \\ & - (1 - G_{\uparrow,ii} - G_{\downarrow,jj} + G_{\uparrow,ii} G_{\downarrow,jj}) \\ & - (1 - G_{\downarrow,ii} - G_{\uparrow,jj} + G_{\downarrow,ii} G_{\uparrow,jj}) \Big] \end{aligned} \tag{50}$$

$$\langle M^2_{\text{off diagonal}} \rangle = \sum_{i,j \text{ where } i \neq j} G_{\uparrow,ii} G_{\uparrow,jj} + G_{\downarrow,ii} G_{\downarrow,jj} - G_{\uparrow,ii} G_{\downarrow,jj} - G_{\downarrow,ii} G_{\uparrow,jj} - G_{\uparrow,ij} G_{\uparrow,ji} - G_{\downarrow,ij} G_{\downarrow,ji} \tag{51}$$

Example Julia code:

```
M_Zsqrd = 0
for i in 1:N, j in 1:N
    if i == j
        term = real(Gdn[i,i] + Gup[i,i] - 2*Gdn[i,i]*Gup[i,i])
    else
        term = real(Gup[i,i]*Gup[j,j] - Gup[i,j]*Gup[j,i] +
                    Gdn[i,i]*Gdn[j,j] - Gdn[i,j]*Gdn[j,i] -
                    Gup[i,i]*Gdn[j,j] - Gdn[i,i]*Gup[j,j])
    end
    M_Zsqrd += term
end
```