Phase diagram of the Hubbard model on honeycomb lattice

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(Dated: October 28, 2010)

In this paper we generalized the slave-particle technique to study the phase diagram of the Hubbard model on honeycomb lattice which may contain charge fluctuations. For large $U$, we have antiferromagnetic order phase. As we decrease $U$ below $U_{c2} \simeq 3t$, the system undergoes a first order phase transition into a gapped spin rotation invariant phase. Under a semiclassical approximation of the slave-particle approach, we find that such phase breaks the translation symmetry, the parity and the lattice rotation symmetry. However, beyond the semiclassical approximation, a $Z_2$ spin liquid that does not break any lattice symmetry is also possible.

Introduction.— Hubbard model\[1, 2\] is believed to describe the physics of many strongly correlated systems e.g., Mott insulator\[3, 4\] and high temperature superconductors\[5–7\]. It is the simplest model one can write capturing the strong correlation physics. So far many theoretical\[8, 9\] and numerical techniques\[10–12\] have been developed to study this model. Among them is the slave particle\[13–16\] theory which was motivated by the RVB state first introduced by P.W. Anderson\[17\]. One of the interesting phases that have been studied and is strongly supported by the slave particle approach is the $Z_2$ spin liquid phase\[18–20\] which does not show any long range order down to zero temperature. Unfortunately QMC does not have sign problem on bipartite lattices at half filling so we can trust its results. For small $U$-limit they have reported the semi-metallic phase. At $U_{c1} \sim 3.5t$ they have seen a phase transition to the spin liquid with nonzero spin excitation gap (gapped spin liquid). At $U_{c2}$ the charge gap opens up and therefore this transition point is associated with the Mott metal-insulator transition. For a larger value of $U_{c2} \sim 4.3t$ they have obtained the anti-Ferromagnetic (AF) order in which the charge gap is still nonzero but the spin excitation is the gapless Goldstone mode.\[21\]

In this paper, we generalized the slave-particle technique to study the phase diagram of the Hubbard model on honeycomb lattice. We would like to point out that the slave-rotor method\[7, 12\] to capture charge fluctuations\[13–21\] to study the antiferromagnetic phase. It is the other method to include charge fluctuations,\[21\] that does not break any symmetry and has finite charge/spin gaps. All phase transitions are first order which agrees with experiments\[3\].

We would like to point out that the slave-rotor method is the other method to include charge fluctuations,\[21\] which give rise to a nodal spin liquid between $1.68t < U < 1.74t$. The slave-rotor method is more reliable for small $U/t$ and gives rise to the correct semi-metal phase. Our method is quite unreliable at small $U/t$ and gives rise to a (wrong) superconducting state.

In the large $U/t$ limit, the Hubbard model can be approximated by the Heisenberg model and we expect strong AF order in it. This model has been extensively studied by different methods\[22–28\]. Here we use a different approach to study the antiferromagnetic phase. It is shown that the spin/charge gapped phase has an instability towards antiferromagnetism.

The Hubbard model is defined as the following:

$$H = U \sum \langle i \rangle n_{i \uparrow} n_{i \downarrow} - t \sum_{\langle i,j \rangle, \sigma} C_{i \sigma}^\dagger C_{j \sigma} + h.c. \quad (1)$$

Here $\langle i, j \rangle$ means site $j$ is one of the nearest neighbors of site $i$. We know that Hilbert space
of Hubbard Hamiltonian has four sates per site. \( |0\rangle_i, |\uparrow\rangle_i, |\downarrow\rangle_i, |\uparrow\downarrow\rangle_i \). Let’s name each state as follows: \( \text{holon} \) \( h_i \), \( \text{spin up spinon} \) \( f_{i,\uparrow} \), \( \text{spin down spinon} \) \( f_{i,\downarrow} \), \( \text{doublon} \) \( d_i \). In which \( |\text{vac}\rangle_i \) is the vacuum, an unphysical state which contains no slave particles even holons. Using this picture we can rewrite the electron creation operator as: \( C_{i,\sigma}^\dagger = f_{i,\sigma}^\dagger h_i + \sigma d_{i,\sigma}^\dagger \).

It should be mentioned that the physical Hilbert space contains only four states: empty state (holon), one electron (spinon) and two electrons (doublon) on each site. So we always have one and only one slave particle on each site. So we conclude that we should put the local constraint \( n_{i,\uparrow}^f + n_{i,\downarrow}^f + n_{i,\uparrow}^d + n_{i,\downarrow}^d = 1 \), to get rid of redundant states. This is the physical constraint which should be satisfied on every site. We could also obtain this result by noting that the electron operators are fermion and should satisfy the anticommutation relations. From the definition of \( C_{i,\sigma}^\dagger \) it is obvious that it is invariant under U(1) gauge transformation (We require \( h_i \) and \( d_i \) to remain bosonic operators \( i.e. \), preserve their statistics after transformation, otherwise we would have SU(2) gauge invariance. However at \( U = \infty \) we have only fermions and only in that case we have SU(2) gauge symmetry). It is worth noting that all the slave particles carry the same charge under the internal U(1) gauge. Since the constraint as well as the Hubbard Hamiltonian are gauge invariant, so is the action of the Hubbard model.

In terms of new slave particles, the Hubbard Hamiltonian can be written as:

\[
H = \sum U d_i^\dagger d_i - t \sum_{\langle i,j \rangle} (\chi_{i,j}^f \chi_{j,i}^b + \Delta_{i,j}^f \Delta_{i,j}^b + h.c.)
\]

In which we have used these notations \( \chi_{i,j}^f = \sum_{\sigma} f_{i,\sigma}^\dagger f_{j,\sigma} \), \( \chi_{i,j}^b = h_i^\dagger h_j - d_i^\dagger d_j \), \( \Delta_{i,j}^f = \sum_{\sigma} \sigma f_{-\sigma,i}^\dagger f_{\sigma,j} \), \( \Delta_{i,j}^b = d_i^\dagger h_j + h_i^\dagger d_j \). To implement the constraint we appeal to the path integral and the Langegrange multiplier methods.

\[
S = \int Df^\dagger Df Dh^\dagger Dh Dd^\dagger Dd \ e^{-\frac{1}{\hbar} \int dt L}
\]

\[
L = f_{i,\sigma}^\dagger \frac{\partial}{\partial \tau} f_{i,\sigma} + d_{i,\sigma}^\dagger \frac{\partial}{\partial \tau} d_{i,\sigma} + h_i^\dagger \frac{\partial}{\partial \tau} h_i + i\lambda_i g_i + H
\]

\[
g_i = f_{i,\uparrow}^\dagger f_{i,\downarrow}^\dagger + f_{i,\downarrow}^\dagger f_{i,\uparrow} + h_i^\dagger h_i + d_{i,\uparrow}^\dagger d_{i,\downarrow}^\dagger - 1
\]

The above motivates us to define the effective Hamiltonian as \( H_{\text{eff}} = H + i \sum \lambda_i g_i \). Now by using the Hubbard-Stratonovic transformation we can decouple spinons from [hard-core] bosons at the mean field level. To do so we just replace \( \chi_{i,j} \) and other operators with their average. For translational invariant systems we have only fermions and doublons. Therefore, as long as \( \Delta_f \) is nonzero, the pairing between holons and doublons is nonzero, and they form bound state. Using the Bogoliubov transformation we can show that the ground-state wave-function of bosons is a paired state which is completely symmetric between holons and doublons. Therefore, as long as this state represents the ground state wave-function of bosons is a paired state which is completely symmetric between holons and doublons. Therefore, as long as this state represents the ground.

\[
\chi_b = \langle h_{k,\uparrow}^\dagger h_{k,\downarrow} - d_{k,\uparrow}^\dagger d_{k,\downarrow} \rangle = 0
\]

Spinons cannot hop in this case and the system is insulator. Self-consistent equations show that \( \chi_f = 0 \) as well and therefore the following Hamiltonians describe the low energy theory of this phase:

\[
H^A_{f} = \sum_k \begin{pmatrix} f_{k,A,\uparrow}^\dagger & f_{-k,B,\downarrow} \end{pmatrix} \begin{pmatrix} -\lambda_0 & -t\Delta_b^k \\ -t\Delta_b^k & +\lambda_0 \end{pmatrix} \begin{pmatrix} f_{k,A,\uparrow} \\ f_{-k,B,\downarrow} \end{pmatrix}
\]

\[
H^A_b = \sum_k \begin{pmatrix} d_{k,A}^\dagger & h_{-k,B} \end{pmatrix} \begin{pmatrix} U - \lambda_0 & -t\Delta_f^k \\ -t\Delta_f^k & -\lambda_0 \end{pmatrix} \begin{pmatrix} d_{k,A} \\ h_{-k,B} \end{pmatrix}
\]

where \( \Delta_f^k = \sum_{\delta} \Delta_\delta^k e^{i\vec{k} \cdot \vec{\delta}} \) and \( \vec{\delta} \) connects two nearest neighbors. We have similar equations for \( H^B_{f,A} \).
and $H^B.A$. Using the Bogoliubov transformation we can diagonalize the above Hamiltonians. The energy eigenvalues for spinons are $E_{b,k}^\pm = \sqrt{x_0^2 + (\pm t \Delta f)^2}$.

At half filling, in order to excite a charge we need to annihilate two spinons and create a pair of holon-doublon. So we can define the charge excitation gap as the sum of the excitation energy of a holon and a doublon. When the charge gap is nonzero then the paired holon-doublon state is stable because exciting quasi-particles on top of this state costs energy. For this state, the charge gap is $E_g^\pm = \min E_{b,k}^\pm = 2 \sqrt{(U - 6 \lambda_0)/2} - (3t \Delta f)^2$.

Therefore, as long as $U - 2 \lambda_0 > 6 t \Delta f$, charge gap is finite and we are in the insulating phase.

On the other hand, when the charge gap closes, the paired holon-doublon state becomes unstable and free holons and doublons proliferate. In this state, doublons and holons condense independently (single boson condensation) such that $(\delta_i A) = -(\delta_i B)$ and $(\delta_i A) = (\delta_i B)$, and therefore $\chi_b = 2 (\chi_i A)^2 = 2 \chi_i B \neq 0$, therefore spinons can hop freely and the ground state is no longer an insulator. Since doublons condense at sublattice $A$ and $B$ with opposite signs, we show that $\Delta_b = 0$ and as a result $\Delta_f = 0$, we relate the onset of single boson condensation, i.e. the critical point below which charge gap closes, to the Mott transition. It should be mentioned that $\chi_f \neq 0$ as well as $\Delta_b, \Delta_f$ jump at this point, so we obtain a first order phase transition in this way, which is consistent with experiments. We like to point out that since $d^i h$ operator that carries $2e$ electric charge, condenses in this state, we indeed obtain a superconducting state instead of a semi-metallic phase.

**Phase diagram.**— In the following sections we discuss the three phases that we have obtained from the slave particle method.

**Superconducting phase.**— Now let us approach the Mott transition point from below i.e. from superconducting side. In this phase both $\Delta_f$ and $\Delta_b$ are zero and therefore the charge excitation gap as well as the spin excitation gap vanishes. Gapless charge excitation implies $\min E_{b,k}^\pm = \max E_{d,k}^\pm = U - 2 \lambda_0 - 6 \chi_f = 0$. This condition can be satisfied up to $U_{c1} = 2 \lambda_0 + 6 \chi_f t = 2.2 t$.

At this point the Mott transition happens. In terms of physical electrons, we obtain an s-wave superconducting state with gapless charge and spin excitations. The pairing order parameter changes sign under parity and 60 degrees rotation and transforms trivially under all other symmetry transformations. It should be mentioned that at small $U$ limit, the Bose gas of holons and doublons becomes very dense and there is strong interaction between them. So the mean-field results are unreliable in this regime and the superconducting state is a fake result. However, our method captures two important right features of the system below the phase transition, because we obtain zero spin excitation energy as well as zero charge excitation energy.

**Charge/spin gapped phase.**— For $U > U_{c1}$ we have $\chi_b = 0$. So the quasi-particle weight of spinons are zero and they cannot hop since for any $i$ and $j$ arbitrary sites: $\langle f_{j,\sigma}^\dagger f_{i,\sigma} \rangle = 0$. Therefore this state is like a superconductor with infinite carrier’s mass $m \sim \frac{1}{t} \to \infty$. Now let us find $U_{c1}$. To do so we assume that $\Delta_f \sim \Delta_b \sim \Delta_f, \Delta_b \sim \eta (\tilde{k})$, where $\eta (\tilde{k}) = e^{i k_y} + 2e^{-i \frac{\phi}{2}} \cos \frac{\sqrt{3}}{2} x_0 k_x$ and therefore the energy spectrum of spinons and bosons are $E_g^\pm = \sqrt{\lambda^2 + (t \Delta_b(k))^2}$ and $\pm U/2 + \sqrt{(U/2 - \lambda^2)^2 - (t \Delta_f(k))^2}$ respectively. From the energy dispersion of bosons, one can read that the charge gap closes when $U_{c1} = 2 \lambda_0 + 6 \Delta_f t$. Our numerical results show that near the phase transition, $\Delta_f \sim 0.5$ and $\lambda \sim -0.4$ and the Mott transition occurs at $U_{c1}/t = 2.2$. For large $U/t$ limit: $\Delta_f \to 0.53$, $\Delta_b \sim \frac{1}{t}, \lambda \sim (\frac{1}{t})^3 \ln \frac{1}{t}$ and $m_b \sim \frac{\eta_b}{\eta_0} \sim (\frac{1}{t})^2$. It is clear from the energy spectrum of spinons that in the spin liquid phase, there is a gap in their spectrum equal to: $E_g^\pm = |\lambda|$. Note that in the spin-charge separation picture, the physics of spin is determined by that of spinons. Therefore the spin excitation gap is also $E_g^\pm = |\lambda|$.

Now let us focus on the gauge theory of this phase. In this phase the effective action of spinons is of the following form:

$$H_{\lambda} = \lambda \sum_{i,\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} - t \sum_{<i,j>_{\sigma,\tau}} \Delta_b (i, j, \sigma) f_{i,\sigma}^\dagger f_{j,\sigma} + h.c.$$  \hspace{1cm} (6)

Now if we transform operators as: $f_{i,\sigma} \to e^{i \alpha} f_{i,\sigma}$ and $f_{i,\sigma} \to e^{-i \alpha} f_{i,\sigma}$ for any arbitrary phase $\alpha$, i.e. assuming a staggered global gauge transformation, then the effective Hamiltonian does not change. Therefore the invariant gauge group (IGG) of the Hamiltonian is the staggered $U(1)$. The reason is that there is no hopping term due to the nonzero charge gap and the gauge transformation of two neighboring sites have opposite phases, the total phase change of the pairing term becomes zero and therefore gauge fluctuations are described by staggered compact $U(1)$ instead of compact $U(1)$ gauge theory. This is equivalent to assuming positive unit charge on sublattice A and negative unit charge on sublattice B for slave particles under the internal gauge transformation.

So, at mean field level, the charge/spin gapped phase has a neutral spinless $U(1)$ gapless mode as its only low energy excitations. However, it is well known that $U(1)$ theory in $2+1D$ is confined due to instanton effects. So let us assume that the $U(1)$ fluctuations are weak and use the semiclassical approach to study the $U(1)$ confined phase where the $U(1)$ mode is gapped. We find that these instanton operators, $e^{i \theta}$ (in the dual XY model), carry a non-trivial crystal momentum. Also, under 60 degree lattice rotation and parity, an instanton is changed...
to an anti-instanton, $e^{i\theta} \rightarrow e^{-i\theta}$. The instantons carry trivial quantum numbers for other symmetries. However, a triple instanton operator $\cos(3\theta)$ carries trivial quantum numbers for all symmetries. This allows us to conclude that the neutral spinless $U(1)$ mode is described by $L = \frac{1}{2g}(\partial\theta)^2 + K \cos(3\theta)$. In the semiclassical limit (the small $g$ limit), $\langle e^{i\theta}\rangle \neq 0$ and we obtain a phase that breaks the translation, the parity and the $60^\circ$ rotation symmetries, but not spin rotation symmetry.

We like to point out that in the presence of second neighbor hopping in the Hubbard model the charge/spin gapped phase can be spin liquid that do not break translation, parity, $60^\circ$ degree lattice rotation, and spin rotation symmetries. It is because we can break the staggered compact $U(1)$ gauge symmetry down to a $Z_2$ one by Anderson-Higgs mechanism. If we add second neighbor hopping to the Hubbard model, within slave particle approach, this term generates pairing terms of the form $f_{i,-\sigma}^\dagger f_{j,\sigma}^\dagger f_{j,\sigma^*} f_{i,-\sigma^*}$, i.e. it induces the same sublattice pairing and the Hamiltonian is no longer invariant under the staggered global $U(1)$ gauge transformation. In this case the staggered compact $U(1)$ gauge symmetry is broken down to a $Z_2$ gauge symmetry. The $U(1)$ gauge fluctuations are gapped and thus our mean field state is stable and we can trust our meanfield results. Therefore we obtain a spin liquid phase.

$\textbf{Antiferromagnetic phase.}$.— In this part we show that the charge/spin gapped phase is unstable towards antiferromagnetic order above $U_{c2} = 3t$. To obtain Neel order in the t-J model we simply assume that $\langle S_{z,A} \rangle = -\langle S_{z,B} \rangle = m$. But how can one implement this idea in the Hubbard model within slave particle approach? In the Neel order phase, translation symmetry is broken and there is an asymmetric situation between sublattices $A$ and $B$. For example we can obtain an antiferromagnetic phase by assuming $\Delta_{1,f} = \langle f_{j,B,\uparrow} f_{i,A,\downarrow} \rangle \neq \langle f_{j,A,\downarrow} f_{i,B,\uparrow} \rangle = \Delta_{2,f}$. This assumption simply means that the chance of finding a spin-up spinon on sublattice $A$ and another spin-down spinon on sublattice $B$ is more than finding the opposite one, so this method introduces staggered sublattice magnetization and leads to the Neel order. If there is a Neel order in the system then the chance of creating one holon-doublon pair from annihilating a spin-up spinon on sublattice $A$ and a spin-down spinon on sublattice $B$ is more than the other process. Therefore the excitation energy of spinons for up-spin on $A$ and down-spin on $B$ is $E_1^f(k) = \sqrt{\lambda^2 + |t\Delta_{1,f}(k)|^2}$ while for down-spin on $A$ and up-spin on $B$ is $E_2^f(k) = \sqrt{\lambda^2 + |t\Delta_{2,f}(k)|^2}$. On the other hand, since we are not interested in CDW, we need a symmetric situation between sublattices $A$ and $B$ for the charge sector. So the energy excitation of bosons is $E_b(k) = \sqrt{(U/2 - \lambda)^2 - |\Delta_f(k)|^2}$. Using these assumptions we lead to the following self-consistency equations:

\[ \Delta_{1,f} = \frac{t}{N_s} \sum_k |\eta(k)|^2 \Delta_{1,b} / E_{1,f}(k) \]  
\[ \Delta_{2,f} = \frac{t}{N_s} \sum_k |\eta(k)|^2 \Delta_{2,b} / E_{2,f}(k) \]  
\[ \Delta_f = \Delta_{1,f} + \Delta_{2,f} \]  
\[ \frac{\Delta_{1,b}\Delta_{1,f} + \Delta_{2,b}\Delta_{2,f}}{\Delta_{1,b} + \Delta_{2,f}} = \frac{t}{N_s} \sum_k |\eta(k)|^2 \Delta_f / E_b(k) \]  

By solving the above equations we find that above $U_{c2} = 3t$, $m \neq 0$. So we conclude that for $U > U_{c2}$ we obtain AF order. It is interesting that in this phase, the gap of spinons is very small and negligible (for example at $U=4$, it is $-2 \times 10^{-7}$). So in this phase we can assume that spinons are massless quasi-particles.

In conclusion, we have used a generalized slave particle method to derive the phase diagram of the Hubbard model at half filling on the honeycomb lattice. Within the mean field approximation we can decouple fermions from bosons to achieve the effective Hamiltonian that describes the low energy physics of the system. The physics of the Mott transition is discussed and it turns out to be a first order phase transition. It is shown that the phase transition occurs when the charge gap opens up. Above the critical point, within meanfield theory we obtain a spin liquid phase. But after including gauge fluctuations of the emergent spin liquid and investigating the instanton effect, we argue that this phase is unstable and we finally obtain a spin/charge gapped phase that breaks the translation symmetry. For large $U$ limit, a new approach to study antiferromagnetic phase within the slave particle picture has been developed. It is shown that the gapped spin liquid phase has an instability towards antiferromagnetism.

$\textbf{Acknowledgement}.$.— We thank B. Swingle, T. Senthil, P.A. Lee, M. Barkeshli and T. Grover for their useful comments and helpful discussions. This research is partially supported by NSF Grant No. DMR-1005541.
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