Mott insulators in a fully frustrated Bose–Hubbard model on the honeycomb lattice

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**Abstract.** We examine the effects of quantum fluctuations on a classical spin liquid state in the fully frustrated honeycomb lattice Bose–Hubbard model in the hard-core limit using quantum Monte Carlo simulations. Frustration is induced explicitly in the model by modulating the sign of the nearest-neighbor interaction spatially around each lattice hexagon. A superfluid-to-Mott insulating quantum phase transition can be induced by varying the relative strength of the classical interaction and quantum hopping. In the cases where the interaction has a regular spatial modulation, hopping promotes a phase transition to a symmetry-broken half-filled valence-bond solid state. When the interaction is forced to have no regular pattern, the insulating state is found to be random and gapped, suggesting the existence of a Mott glass phase.

**Contents**

1. Introduction ........................................ 2
2. The fully frustrated honeycomb lattice Bose–Hubbard model ........................................ 2
3. Quantum order by disorder ........................................ 10
4. Discussion ........................................ 12
Acknowledgments ........................................ 15
References ........................................ 15

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1. Introduction

A concentrated effort is currently under way to build exotic states of quantum matter in ultracold atomic systems [1]–[5]. These atomic systems are destined to become ‘quantum simulators’ of condensed matter Hamiltonians, allowing us to extend our reach to new models, phases and phase transitions inaccessible to traditional condensed matter theory or experiment [4, 6]. Although efforts to construct complex Bose or Fermi Hubbard Hamiltonians are still in their infancy, experimental progress has been rapid, motivating theorists to study increasingly realistic models that may some day be built and used in the search for exotic quantum phenomena.

Concomitant with this revolution, there has been resurgent interest in frustrated systems recently, due to the possibility that when frustration suppresses the ordering tendencies of a system, more subtle exotic phenomena will be observed. Particularly successful would be the stabilization of a quantum spin liquid [7]–[10]—a featureless Mott insulating (MI) phase with emergent gauge symmetry that harbors fractional excitations—in a cold atom system. Spin liquids are projected to occur in several two-dimensional (2D) Bose–Hubbard models [11, 12]; however, the typical feature shared by these Hamiltonians is that the range of the kinetic hopping (tunneling) and interactions are multi-particle, long-range or otherwise prohibitively complicated for realization in real experimental setups. They are also known to occur in the large \( N \) limit of SU(\( N \)) Heisenberg models [13], but this limit is similarly difficult from an experimental standpoint.

In this paper, we attempt to construct a featureless MI phase from a Bose–Hubbard Hamiltonian with only nearest-neighbor interactions. The model is motivated by the resonating valence-bond (RVB) [7, 8] phase contained in the triangular lattice quantum dimer model [14]. The quantum dimer model motivates our model through a mapping between frustrated boson interactions on the honeycomb lattice, and dimers on the (dual) triangular lattice. Our model is equivalent to a spin-1/2 XXZ model constructed by adding quantum XY (hopping) perturbations on top of a fully frustrated Ising model on the honeycomb lattice. We find that the hopping term lifts the degeneracy of the classical Ising model ground state, promoting various valence-bond solid (VBS) phases with coexisting charge-density wave (CDW) order, depending on the spatial distribution of the lattice frustration. When the spatial position of the frustration is made random, breaking all lattice symmetries, we find an incompressible (gapped) disordered Mott insulator, very similar to the results of Sengupta and Haas [15] for a phase described as a Mott glass.

2. The fully frustrated honeycomb lattice Bose–Hubbard model

In a recent breakthrough, Becker et al [16] constructed a versatile experimental setup for loading ultracold atoms into a triangular optical lattice, demonstrating for the first time a superfluid–MI transition in this 2D system. Their experimental realization involves creating a periodic potential constructed from three laser beams in the XY-plane. A rotation of the polarization of the three lasers in the XY-plane configures the potential minima in the geometry of a honeycomb lattice. In the typical unfrustrated case, this bipartite lattice is expected to induce antiferromagnetic ordering for atoms [17]. However, Becker et al’s demonstration that the sign of the tunneling matrix element can be reversed may suggest the possibility of inducing frustrated or anisotropic tunneling. It may therefore be possible in the future to introduce
frustration into otherwise geometrically unfrustrated models. We explore this scenario by examining the possible phases of the simplest fully frustrated honeycomb lattice Bose–Hubbard model with nearest-neighbor interactions using large-scale quantum Monte Carlo (QMC) simulations.

We consider very generally the simplest model for hard-core bosons on the honeycomb lattice,

\[ H = \sum_{\langle ij \rangle} (J_{ij} (n_i - 1/2)(n_j - 1/2)) - t/2 \sum_{\langle ij \rangle} (b_i^\dagger b_j + b_j b_i^\dagger), \]  

employing only nearest-neighbor hopping (\(b_i^\dagger\) and \(b_j\) are the boson creation and annihilation operators) and density–density interactions (\(n_i = 0\) or \(1\)). Here, the density–density interaction is written in such a way that it allows for exact mapping to the quantum spin-1/2 XXZ Hamiltonian,

\[ H = \sum_{\langle ij \rangle} (J_{ij} S_i^x S_j^x) - t \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_j^+ S_i^-), \]

via \(S_i^+ \rightarrow b_i^\dagger\), \(S_i^- \rightarrow b_i\) and \(n_i \rightarrow S_i^z + 1/2\). Considering first the limit when \(t = 0\), one has the classical Ising model, where frustration may be induced by ensuring that the sign of \(J_{ij}\) is modulated in such a way that nearest-neighbor interactions cannot be fully satisfied around a hexagonal plaquette. In the extreme limit where each hexagon on the lattice is frustrated (i.e. the model is ‘fully frustrated’) the low-temperature phase is an extensively degenerate manifold of equal-energy states—a type of classical spin liquid [18]. Each configuration in the degenerate manifold of states can be mapped to a close-packed hard-core dimer configuration on the dual triangular lattice [19]. It is well known that the quantum version of the triangular lattice dimer model contains an RVB liquid in its phase diagram [14]. Although an exact mapping from the quantum dimer model to a quantum spin model is not available, one may consider the \(t = 0\) classical fully frustrated Ising model ground state as a starting point, and ask whether quantum perturbations in the \(t \neq 0\) model contain the spin counterpart to the RVB phase [7, 8], i.e. a \(Z_2\) quantum spin liquid phase [14].

Our Hamiltonian (1) has a distinct advantage over some other frustrated spin models since it may be simulated without the sign problem using stochastic series expansion (SSE) QMC [20]–[23] at finite temperature. Imposing the fully frustrated constraint but keeping the magnitude of the interaction isotropic on the lattice, one can rewrite the model

\[ H = J \sum_{\langle ij \rangle} (-1)^{A_{ij}} (n_i - 1/2)(n_j - 1/2) - t/2 \sum_{\langle ij \rangle} (b_i^\dagger b_j + b_j b_i^\dagger), \]

where \(A_{ij}\) takes the value of zero or one on each bond, subject to the constraint that the sum over each hexagon, \(\sum_{\partial \text{o}} A_{ij}\), is odd. When \(t \neq 0\) the model is not fully gauge-invariant [24], and modulating the sign of the hopping \(t\) would introduce a sign problem; we nonetheless refer to the choice of \(A_{ij}\) subject to the constraint as a gauge choice.

In the classical limit, the choice of the gauge \(A_{ij}\) does not affect the nature of the ground state manifold, owing to the one-to-one mapping to the classical hard-core dimer tiling, which retains a residual entropy of \(S = 0.214\) per site [19]. In this paper, we examine three different gauge choices (each with \(J\) positive and negative) to study the effect of quantum hopping (\(t\)-term) on the classically degenerate manifold (see figure 1). The first choice of gauge we refer to as the discrete translationally symmetric (DTS) gauge, where the pattern of bonds where \(A_{ij} = 1\) reduces the symmetry of the lattice such that only a discrete translational symmetry remains.
We also study a gauge that we call the discrete rotationally symmetric (DRS) gauge, where the \( A_{ij} \) variables leave the system with a nontrivial rotational symmetry and reduced translational symmetry. The third gauge is one in which we use a classical Monte Carlo to generate an unbiased random pattern of \( A_{ij} \) that satisfies the fully frustrated requirement \( \sum_O A_{ij} = 1 \), and this is called the ‘random’ gauge. Here, by ‘unbiased’ we mean that each unique configuration that satisfies the fully frustrated requirement is equally likely when we generate a random instance. Figure 1 illustrates the three gauges with their unit cells outlined (where a unit cell exists).

We now examine the results of QMC simulations on the models defined in the previous section. We fix \( t = 1 \) in all the results to follow. Note first that when \( J/t = 0 \) the sign of \( J \) on the bonds is irrelevant, and the model becomes an \( XY \)-superfluid for all gauge choices, characterized by a nonzero superfluid density (or spin stiffness) of \( \rho_s = 0.292(1) \). This is the limit where the SSE QMC simulation with directed loops works most efficiently; hence we approach the transition to MI behavior by increasing \( J/t \) from zero in the simulations. We begin by examining the superfluid density (measured via the winding number [25]) at a fixed low temperature, \( T = 0.1t \), as a function of increasing \( J/t \). The results are illustrated in figure 2 for the three gauges. We observe that quantum phase transitions between a superfluid and various
insulating states occur when the interaction $|J/t| \approx 2$. In the unfrustrated honeycomb model, this phase transition occurs at $|J/t| = 2$ [17], between a superfluid and a crystal state. The specific value of the critical $J_c$ is similar but not strictly identical for different gauges or for opposite signs of $J/t$ in a fixed gauge.

Using the three different gauge choices, we now have access to six different insulating states (including $\pm J$). In order to determine the ordering nature of the ground state, if any, we first examine the $q$-space sublattice structure factors at a fixed $J$ and temperature $T$. $|J| = 3$ was chosen to be well in the insulating phase, but of sufficiently small interaction to ensure algorithmic ergodicity. The $T$ dependence of most observables was examined to find the approximate low-$T$ convergence: $T = 0.1t$ was chosen in most of the data given below (except for the random gauge when $J = 3$, in which case $T = 0.033t$ was used to ensure that we are below the single particle gap). Also, although the SSE QMC simulation is, in general, very efficient at finding the ground state of a system, it is also capable of becoming stuck in a local minimum in configuration space, similar to classical Monte Carlo algorithms. An example of such a local minimum would be a screw dislocation if the ground state pattern is broken into a set of layers. The energy cost of such a defect would be finite and although translating the defect should be possible, fixing it requires passing through intermediate states of even higher energy. In order to overcome this problem we use the technique of thermal annealing. We used an annealing schedule of $10^5$ equilibration steps and $10^5$ Monte Carlo steps at each temperature, starting at $\beta = 4$ and increasing $\beta$ by 1 until reaching $\beta = 25$. This schedule was sufficient to remove screw dislocations in the DTS gauge when $J/t = -3$ for a $24 \times 24$ lattice.

Figure 3 illustrates the density–density sublattice structure factor, calculated as

$$S(q) = \frac{1}{N} \sum_{ij} e^{-iqr_{ij}} ((n_i - 1/2)(n_j - 1/2)), \quad (4)$$

where $r_{ij}$ is the vector connecting the unit cell containing site $i$ to the unit cell containing site $j$ on a honeycomb lattice and $N$ is the number of unit cells, and the sum runs over all sites of a particular sublattice. We use the vectors between unit cells and a sublattice decomposition so that all the necessary information is contained in the familiar Brillouin zone of the triangular lattice. Figure 3 shows the density–density sublattice structure factors for both signs of $J$ for the three gauges of interest, where we restrict the sum over a set of $n_i$ that are on a particular sublattice or, in other words, we are showing the sublattice structure factor. In the case of the DTS and DRS gauges, sharp peaks occur at certain wavevectors $q_i$ in the $q$-dependent sublattice structure factor. A peak will represent long-range order if $S(q_i)/N$ survives in the thermodynamic limit. In figure 4, we examine the finite-size scaling of the various peaks, which demonstrates that in the case of the DTS and DRS gauges, there is indeed long-range order in the particle density.

We also measure the sublattice structure factor of the bond–bond correlation function to search for VBS order. This structure factor is defined as

$$S(q) = \frac{1}{N} \sum_{ab} e^{-iqr_{ab}} \langle B_a B_b \rangle, \quad (5)$$

$$B_a = b_i^\dagger b_j + b_i b_j^\dagger, \quad (6)$$

where $a$ labels the bond connecting the sites $i$ and $j$, and $r_{ab}$ is the vector connecting the unit cells containing bonds $a$ and $b$. A VBS phase will have Bragg peaks in this structure factor, which survive the thermodynamic limit as discussed above. Figure 5 shows the sublattice
Figure 3. The sublattice structure factor of the density–density correlation function for the six cases studied in this paper. The peaks in (a)–(d) are Bragg peaks that scale with the size of the system (see figure 4) indicating long-range order, while those in (e) and (f) are not. $T = 0.1t$ (except for (f), which was done at $T = 0.033t$), $J/t = 3$ and the lattice contains $24 \times 24$ unit cells for each sublattice structure factor (1152 sites).

structure factor of the bond–bond correlation function for all the cases studied in this paper. Crystalline long-range ordered structures in the sites and bonds are visible when the system is found in a particular symmetry-broken state at low temperatures; these are the respective VBS phases.
Next, we generate real-space images of the lattice in order to help us visualize the various ground state particle and bond patterns. In order to visualize quantum order in the (2+1)D QMC simulation cell, we essentially ‘project’ the SSE basis configurations and operator list back into the 2D plane—effectively averaging the simulation cell over the entire Monte Carlo simulation. One then can imagine plotting averaged basis variables by associating a color with the expectation value of each site: red for \( \langle n_i \rangle = 0 \), blue for \( \langle n_i \rangle = 1 \), and mixed (shades of purple) for \( 0 < \langle n_i \rangle < 1 \) (figure 6). Similarly, we average the expectation value of the kinetic energy operator \( B_a \), defined in equation (6), over the imaginary time expansion, and associate a thickness of the bond proportional to \( \langle B_a \rangle \).

The corresponding images of each gauge are presented in figure 6. Figures 6(a)–(d) show clear long-range order in the sites and bonds, matching with the structure factors presented in figures 3 and 5. The lack of order in the structure factors for the random gauges is now clarified by the real-space images. In the case when \( J = -3 \), the system appears to be made up of random domains of filled and empty sites, consistent with the lack of long-range order. In the case when \( J = 3 \), we find a similar picture, except that in this case the domains are half-filled (because most of the bonds are repulsive) and the regions of disordered sites with no dominant filling tend to be larger, while the whole system lacks long-range order.

In all six cases the average filling is half (corresponding to zero magnetization in the spin language) even though our simulations are grand canonical. The low-temperature boson compressibility (uniform spin susceptibility) gives information about the density fluctuations in the ground state: if the susceptibility goes to zero, the phase is a gapped (Mott) insulating state. The temperature at which it turns off then gives us information about the gap to single

Figure 4. Scaling of the peaks of the density–density sublattice structure factor for the four ordered cases and one disordered case (‘random’ gauge with \( J = 3 \)). Bragg peaks are signified by the function approaching a constant in the limit of \( 1/L \to 0 \), where \( L = \sqrt{N/2} \) is the length of the system. Fluctuations in the scaling of the DRS gauges reflect the fact that the system has multiple ground states with distinct ordering wave vectors that must be searched. In the random gauge the fluctuations occur due to a finite size effect, where small systems are unstable to short-range CDW (antiferromagnetic) order. In the thermodynamic limit such clusters may result in short-range order, but do not give rise to long-range CDW (antiferromagnetic) order.
Figure 5. The sublattice structure factor of the bond–bond correlation function for the six cases studied in this paper. The peaks in (a)–(d) are Bragg peaks that scale with the size of the system indicating long-range order, whereas those in (e) and (f) are not. The $q = (0, 0)$ peaks exist because every bond sublattice has a nonzero expectation value of the hopping operator. This does not imply a long-range ordered phase, only a finite density of kinetic bonds.

particle excitations. In figure 7, susceptibility data for the DTS and DRS gauges for both signs of $J$, as well as detailed data collected when $J = 3$ for the random gauge, are shown. For the $J = 3$ random gauge, it is clear that at low temperatures, susceptibility is zero; at high
temperatures ($T \approx 0.1$), the value of susceptibility is higher than that for other gauge choices. This is partly because there is no long-range ordered pattern that needs to be broken in order to insert a particle. Indeed, the lack of ordering in the structure factors and real-space picture, combined with the fact that at low temperatures the phase is incompressible, suggests that the state is a disordered MI state—a possible ‘Mott glass’ [15].
Figure 7. The low-temperature susceptibility of the MI in all gauges (except random $J = -3$) with $|J| = 3$. For all cases the susceptibility approaches zero at a finite temperature, with the smallest gap in the case of the random gauge where $J = 3$.

3. Quantum order by disorder

The results of QMC simulations show a superfluid–MI phase transition in each of the cases studied, where the Mott insulator is a symmetry-broken crystalline state whenever the gauge choice is repeating and a disordered state when the gauge is random. Keeping in mind that the $t$ term of the Hamiltonian is off-diagonal in the density-basis choice, we can understand the crystalline phases in the limit of large $J/t$. Namely, treating $t$ as a perturbation on top of the classical Ising model degenerate ground state, one can ask: which local $t$ operations can lower the kinetic energy (maximize hopping) without costing energy proportional to $J$? In all cases we can see that the crystalline (VBS) states discovered by the QMC satisfy these two criteria. The simplest case comes from the DTS gauge where $J = -3$. Hopping tends to occur on satisfied repulsive bonds—that is where energy is minimized when a particle is next to a hole. The two hopping sites are also connected to two frustrated bonds before and after exchanging their positions, as shown in figure 8. The real-space figure of the ground state shows a mixing of the two states in figure 8, suggesting that such a superposition is also energetically favorable in the simulation.

In the case when $J = -3$ in the manifold of states that satisfy the classical part of the Hamiltonian, the hopping operator will act only on those bonds that prefer holes next to particles. This is because swapping such sites is the only way to remain in the set of states that satisfies the classical part of the Hamiltonian. The only scenario in which the hopping operator can act on an attractive bond is if it is frustrated. Looking at figure 8 again, all the bonds connected to the two swapped sites, except the bond between them, switch from frustrated to unfrustrated and vice versa when the sites are swapped. Figure 9 shows the exhaustive set of possibilities for attractive bond hopping, and shows how there is no configuration possible that would allow a hopping on an attractive bond to be a part of the ground state.
Figure 8. The left state is taken to the right state by the action of the $b_i^\dagger b_j$ element of the Hamiltonian. If the left state satisfies the classical ($J$) part of the Hamiltonian, so will the right state. In this way, the superposition of these two (local) states reduces the energy of the quantum ($t$) Hamiltonian without increasing the energy in the classical part of the Hamiltonian. Blue (red) circles represent particles (holes), while the green zigzags represent frustrated bonds. The overall sign of $J$ here is negative, while $A_{ij} = 0$ for solid bonds and 1 for dashed bonds.

Figure 9. The exhaustive set of cases of hopping on a frustrated attractive bond. When the central bond is a frustrated attractive bond, every action of the hopping operator has a state that costs an energy of order $J$ (denoted by an ‘X’) as either the state before and/or after hopping. Blue (red) circles represent particles (holes), while the green zigzags represent frustrated bonds. The overall sign of $J$ here is negative.

By eliminating the possibility that the attractive bonds fluctuate to lower the system’s energy we find that only the repulsive bonds will fluctuate, and the numerical simulations confirm this result. The ground state can now be described as the superposition of states that allows each repulsive bond to fluctuate as much as possible. If we extend this simple idea to all the gauges and signs of $J$, we can check to see if the highly fluctuating bonds in each case correspond to local configurations that satisfy configurations similar to figure 8. Figure 10 shows the local structure around each of the highly fluctuating bonds from the DTS and DRS gauges, and in each case the local configuration satisfies what we expect from the perturbation theory approach.
Figure 10. A comparison of the local structures around highly fluctuating bonds from all gauges. In each case, the central bond is the highly fluctuating bond. In the top row of images $J = -3$, so dashed bonds represent repulsive bonds. In the bottom row, $J = 3$, so dashed bonds represent attractive bonds. Blue (red) circles represent particles (holes), while the green zigzags represent frustrated bonds. As both gauges are presented, attractive bonds have been noted in purple. The top layer shows the (a) DTS gauge and two (c,e) local configurations of the DRS gauge, all with $J = -3$. The bottom layer shows the (b) DTS gauge and again two (d,f) local configurations of the DRS gauge, all with $J = 3$.

To further cement our understanding of the fluctuations, we can use the information extracted from QMC measurements of the bond–bond correlation function, $\langle B_a B_b \rangle$, to see whether it matches these expectations. We will use the simplest case to build our intuition, the DTS gauge with $J = -3$. In this case, when looking at a layer of highly fluctuating bonds in their dominant configuration, any of them may hop to reduce energy. Once one of them hops, however, neighbors on the same layer that were able to hop before are no longer able to do so. Comparing this with numerical results, we find that this nearest-neighbor behavior is reproduced. Figure 11 shows the real-space image of the ground state generated using the bond–bond correlation function. The bond–bond correlation function (represented by thickness of bonds) is weaker for nearest neighbours than for bonds two unit cells apart. The graph in figure 12 plots the thickness as a function of position along the chain and clearly shows that adjacent bonds are anticorrelated when compared with well-separated bonds.

4. Discussion

From our QMC data we have demonstrated that a superfluid–Mott insulator phase transition can exist in the nearest-neighbor Bose–Hubbard model on the honeycomb lattice where the interactions are constrained to be fully frustrating around each hexagon, subject to a gauge choice. We are able to classify the MI phases in each case where the gauge is a repeating pattern as a symmetry-broken crystal with coexisting charge-density wave and valence-bond order (i.e. a CDW–VBS [26]). Bragg peaks in the density–density and bond–bond correlations
Figure 11. A real-space picture of the lattice generated using the bond–bond and density–density correlation function, with the red bond and black site as the reference bond. Note the subtle oscillation in bond thickness of the striped bonds for those bonds on the same layer as the reference.

Figure 12. Numerical version of the data presented in figure 11, with \( a = 3 \), showing the thickness of the striped bonds in reference to the red bond. Here the oscillation in the correlation function is very clear, with anticorrelation of nearest neighbors in the same layer.

functions confirm the long-range order that we have illustrated using a real-space averaging of the QMC simulation cell. One could describe the MI phases as occurring by an order-by-disorder mechanism, where the degeneracy of the classical manifold of states for \( t = 0 \) is lifted by quantum ‘perturbation’ or hopping. We have intuitively described this order-by-disorder mechanism by a simple perturbation theory picture to first order in the hopping, subject to the constraint that each hopping process costs no energy in the (classical) interaction.
When the gauge choice of the interaction frustration is not a repeating pattern, we find that the order-by-disorder mechanism is destroyed. In this case, QMC finds a superfluid–MI transition, where the Mott insulator is a disordered phase, featureless on long length scales. Both the $q$-space structure factors and the real-space simulation cell pictures confirm that the ground state configurations have no long-range order. For $J = -3$, repeated simulations using different gauge choices show that the configuration of the ground state consists of domains of filled or empty sites. In this way, the random gauge with $J = -3$ can be considered a disordered solid in the density and valence-bond sectors. Since most of the hopping dynamics take place on the interface between domains, excitations of this gauge should be similar to those in the DTS gauge when $J = -3$.

The random gauge with $J = 3$ is the most interesting case, lacking in long-range order and displaying the largest number of per-site fluctuations while remaining globally gapped to change in the particle number. Real-space pictures show the existence of disconnected islands of clusters, within which we find short-range CDW (antiferromagnetic) order manifest in a density–density correlation function. This correlation decays to zero within disordered clusters or between different clusters. Like all the other gauges, the random gauge also has gap to single particle excitations, as can be seen from the fact that the susceptibility reduces to zero at low temperatures. As is apparent from figure 6, this phase has a non-vanishing local density Edwards–Anderson (EA) order parameter (a measurement very similar to the local susceptibility [15]); however, it is not described as a typical ‘Bose glass’, since it is gapped. In addition to the distribution of the EA order parameter there is a distribution of bond strength that is induced due to the local choice of frustrating interactions.

The existence of a local density EA order parameter suggests that this MI does not fit the typical description of a quantum spin liquid, which should break no lattice symmetry (and have an emergent gauge symmetry). It may be more accurately described as a Mott glass state [15]. From the discussion above we can examine the type of excitations expected to occur out of this ground state. In the limit of $t = 0$, the only excitations in our model correspond to inserting a single particle and raising the energy of the system by $J$. In the limit of small $t/J$, different superpositions of classically allowed states will have different expectations of energy, but finding eigenstates other than the ground state is difficult in SSE QMC. Since the total particle number commutes with the Hamiltonian, we can use it as a quantum number to label different sets of states. If we can change the total filling of our ground state without violating the classical constraint, the new state we have can only be different in energy by a certain function of $t$, or it may have zero energy difference. The earlier discussion of hopping taken with attractive bonds leads us to one method of constructing such a state.

Let us imagine a situation similar to figure 8, except that the central bond is considered to be a satisfied attractive bond. In this scenario if we insert or remove two particles the number of frustrated bonds does not change, but we are taken to a new eigenstate of the quantum Hamiltonian. Using QMC simulations with an applied chemical potential we were able to explore the excited state with two extra particles, compared to a half-filled system. The evolution of the simulation suggests a large barrier between the half-filled state and the state with two extra particles, as the state with one extra particle must have an energy penalty of order $J$, consistent with our earlier discussion. Repeated simulations from random initial configurations reveal that states away from half-filling must have some energy penalty, as the simulation always finds those states at half-filling at low temperatures to be the lowest-energy states. This implies that there is an energy difference between the ground state and the state with two extra particles, and the difference between these states is not of order $J$, but some function of $t$.

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In conclusion, we have studied a fully frustrated Bose–Hubbard model on the honeycomb lattice, where the frustration is induced by explicitly modulating the sign of the interaction around each hexagon to preclude a satisfied interaction. This choice of (classical) gauge can induce order-by-disorder when perturbed by the quantum hopping term, in the case when the gauge choice has a regular spatial pattern. In the case when the gauge choice is explicitly chosen to break all lattice symmetries, a disordered Mott insulator or Mott glass state is induced. Although no clear candidate quantum spin liquid state exists in the gauge choices studied here, there exist novel ordered states generated from the disordered classical manifold and a novel Mott glass phase extending over a large region of phase space. The identification of novel phases in Bose–Hubbard Hamiltonians with only nearest-neighbor interactions is an important step towards the creation of such phases in cold atomic systems in optical lattices.

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