Mott insulators in plaquettes

J.-P. Martikainen

1 COMP Centre of Excellence, Department of Applied Physics, Aalto University, Fi-00076 Aalto, Finland
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We study small systems of strongly interacting ultracold atoms under the influence of gauge potentials and spin-orbit couplings. We use second order perturbation theory in tunneling, derive an effective theory for the strongly correlated insulating states with one atom per site, and solve it exactly. We find dramatic changes in the level structure and in the amount of degeneracies expected. We also demonstrate the dynamical behavior as the barriers between plaquettes are gradually removed and find potentially high overlap with the resonating valence bond (RVB) state of the larger system.

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I. INTRODUCTION

Weakly interacting gas of bosons can form a Bose-Einstein condensate at low enough temperatures. This condensate can be often well described by a classical theory where condensate atoms are described by a condensate wavefunction whose dynamics follows from the Gross-Pitaevskii equation [1]. In optical lattices potential barriers between sites suppress the movement of atoms and increase confinement which increases effective interaction strengths. Consequently optical lattices can push the weakly interacting quantum system into the regime a strongly correlated physics. Bose-Einstein condensation of weakly interacting systems gives way to Mott-insulator physics at high interactions and this transition was experimentally observed by Greiner et al. [2].

While the position of the transition (in higher dimensional systems) can be fairly accurately predicted with the Gutzwiller ansatz that is a product state of individual site quantum states, it predicts the physics of Mott insulators poorly since it does not take into account higher order tunneling processes. However these strongly correlated insulators can be studied in terms of different spin models and can have a very rich physics of quantum magnetism and criticality [3]. At a formal level spin models can be derived from the second order perturbation theory in kinetic (tunneling) energy of the lattice model [4, 5].

Recently there has been rapid experimental progress in creating artificial spin-orbit couplings [6] as well as gauge potentials [7, 8] in ultra cold quantum gases. Given this background even non-Abelian gauge fields [9, 10] have become feasible. (For a recent review see, for example, Dalibard et al. [11].) In addition to these advances, a three-dimensional array of independent plaquettes has also been demonstrated even to a level of being able to prepare specific quantum states in each plaquette [12].

The purpose of this article is to study insulating states in an optical lattice for small systems by exactly diagonalizing the effective Hamiltonian corresponding to the second order perturbation theory in tunneling. We will solve the system under quite general conditions so that tunneling coefficients can be spatially varying and artificial gauge potentials included easily. We demonstrate the level structure for few simple choices of phases and point out when, for example, the amount of degeneracies can vary with gauge potentials. Furthermore, we show some examples of dynamics in multi-plaquette systems and solve the problem of plaquettes with spin-orbit interactions exactly for 2- and 4-sites.

There are some interesting recent studies on the phase diagrams of Mott insulators with spin-orbit couplings [13, 14] that pointed out how the effective Hamiltonian becomes a combination of Heisenberg model, quantum compass model, and Dzyaloshinskii-Moriya interactions. The approach used in this paper is different in that our focus is on the full solution for small systems which naturally enable also the solution of time-dependent problems. This is relevant since in the experiment by Nascimb` ene et al. [12] resonating valence bond states were prepared in plaquettes of an optical lattice. In these experiments dynamics was an important ingredient and since the system was made out of independent plaquettes, exact diagonalization for small systems provides a natural theoretical framework.

The paper is organized as follows. We begin by outlining the theory relevant for our purposes in Sec. II. In Sec. III we exactly diagonalize the system with some simple gauge potentials both for the square as well as for the triangular plaquette. Then in Sec. IV we explore the dynamical behavior when barriers between plaquettes are removed and in Sec. V we exactly diagonalize the Mott insulating plaquette with spin-orbit interactions. We end with a few concluding remarks in Sec. VI.
II. FORMALISM

In each site $\mathbf{r}$ of the lattice the local physics for bosons is described by the interaction Hamiltonian [4, 5]

$$H_{I,\mathbf{r}} = \frac{U_{11}}{2} \hat{n}_{1,\mathbf{r}}(\hat{n}_{1,\mathbf{r}} - 1) + \frac{U_{22}}{2} \hat{n}_{2,\mathbf{r}}(\hat{n}_{2,\mathbf{r}} - 1) + U_{12} \hat{n}_{1,\mathbf{r}} \hat{n}_{2,\mathbf{r}},$$

(1)

where $\hat{n}_{\alpha,\mathbf{r}} = \hat{\psi}_{\alpha,\mathbf{r}} \hat{\psi}_{\alpha,\mathbf{r}}^\dagger (\alpha \in \{1, 2\})$ are the density operators for each component. Here the onsite eigenstates can be written in terms of occupation numbers as $|n_1, n_2\rangle$. The approach works equally well for fermions, but then $U_{11} = U_{22} = 0$ since $s$-wave interaction between identical fermions vanishes and Pauli exclusion principle must be enforced. Furthermore, this problem can be straightforwardly generalized to spinorial bosonic systems, multi-component fermionic systems [15], or Bose-Fermi mixtures [16, 17] by simply changing the term describing onsite interactions [18].

In this work tunneling processes are kept very general so that they can include position dependent tunnelings as well as, later in the text, spin-orbit couplings. In the absence of spin-orbit couplings the tunneling processes are described by

$$H_T = \sum_{\alpha, m} -t_{\alpha, m} \hat{\psi}_{\alpha, m+}^\dagger \hat{\psi}_{\alpha, m} - t_{\alpha, m}^* \hat{\psi}_{\alpha, m-}^\dagger \hat{\psi}_{\alpha, m+},$$

(2)

where $\alpha$ indicates the component index, $m$ indicates the bond, while $\hat{\psi}_{\alpha, m-}$ and $\hat{\psi}_{\alpha, m+}$ are the field operators for atoms of type $\alpha$ on either end of the bond $m$. Later we will introduce also spin-orbit couplings in which case the atom type can change in the tunneling process.

Throughout this paper we focus on the experimentally simplest case of having one atom per site. For all states having just one atom per site interaction energy vanishes so double (and higher) occupancy is energetically unfavorable. Adding tunneling terms into the model implies removing an atom from one site and adding it into another. If the initial state only had singly occupied sites, this implies that tunneling process creates a state where one site is doubly occupied. In the lowest order perturbation theory the tunneling term does not give rise to any energy shift since the state with double occupancy is orthogonal to initial state, but at second order there can be another tunneling process which brings the state back into the initial subspace of singly occupied sites. At this level tunneling terms do matter and they determine the energetics and dynamics of the various possible Mott insulating states.

When the tunneling processes are described by a Hamiltonian $H_T$ this second order perturbation theory gives rise to an effective Hamiltonian [14]

$$(H_{eff})_{\alpha\beta} = -\sum_{\gamma} \frac{(H_T)_{\alpha\gamma}(H_T)_{\gamma\beta}}{E_{\gamma} - (E_{\alpha} + E_{\beta})/2},$$

(3)

where $E_i$ are the eigenenergies of the interaction Hamiltonian, $\alpha$ and $\beta$ live in the manifold with one atom per site, while states labeled by $\gamma$ have one site with 2 atoms per site.

In the literature the this expression is typically written in terms of pseudo-spin operators. While this can formally be done in our cases as well, the expressions become ever more complex as tunneling properties in the system become more diverse. For this reason we choose not to rephrase the problem in terms of spin-operators, but construct the relevant Hamiltonians in the subspace with one atom per site with the computer. In this way all associated “spin”-models are included, but as an input one only needs the onsite interactions and tunneling coefficients. In principle, both interactions as well as tunnelings could be position dependent. The latter option is in fact important when we wish to study effects of gauge potentials in lattices and position dependence of atom-atom interactions can be important, for example, in bipartite lattices [19]. If we were to write results in terms of pseudo-spins, we would have to derive a separate spin-model for each variant of the problem.

Our procedure amounts to first constructing all eigenstates of $H_I = \sum_{\mathbf{r}} H_{I,\mathbf{r}}$ with (on average) unit filling and at maximum 2 atoms per site. From these states we construct the subspace with exactly one atom per site and then compute the elements $H_{eff}$ numerically. The resulting Hamiltonian can then be diagonalized and this solution (if so desired) can then be used to solve dynamical problems as well. In this paper we will focus on $2 \times 2$ or triangular plaquettes since the first system has been experimentally realized [12] and the latter one can be realized [20]. Furthermore, both can be solved fully without difficulty. We also solve dynamical problems in systems of two and three weakly coupled plaquettes.

III. MOTT INSULATOR IN GAUGE POTENTIALS

We show a schematic description of our system(s) elementary cells in Fig. 1. The various tunneling coefficients are given by $t_{\mathbf{r}}$, and they describe processes like (example for $t_1$) $-t_{\alpha,1} \hat{\psi}_{\alpha,2}^\dagger \hat{\psi}_{\alpha,1} - t_{\alpha,1}^* \hat{\psi}_{\alpha,1}^\dagger \hat{\psi}_{\alpha,2}$, for tunneling of $\alpha$ atoms between sites 1 and 2. Nascimbène et al. [12]
solved the eigenstates of this system in the case when \( t_2 = t_4 = t_y \) is different from \( t_1 = t_3 = t_x \). We wish to understand the role of gauge potentials in such a system and for this reason we allow for the possibility of complex and position dependent tunneling coefficients. In contrast to superfluid regime, if both components experience the same gauge potential, gauge potential does not affect the Mott insulator. For gauge potentials to play a role, we have to allow for the possibility of spin dependent gauge potential. To keep things as simple as possible we choose \( t_{1,1} = e^{i\phi}/2 \), all other tunneling coefficients as 1/2, and vary the phase \( \phi \). (Using Peirls substitution the phase could be related to gauge vector potential \( A \) through \( \phi = \int \mathbf{r} \cdot d\mathbf{r} \cdot \mathbf{A}/\hbar \). This gives rise to the Harper model in a plaquette \( \alpha \) and if the flux \( \alpha = \phi/2\pi = p/q \) is rational the ideal theory has a \( q \)-fold degenerate ground state.

In Fig. 2 (a) we show the eigenenergies as a function of \( \alpha \). At \( \alpha = 0 \) the result agrees with those reported in Ref. [12], but as gauge potential is turned on the 3-fold degeneracy of the first excited state is broken as the \( d \)-wave RVB state splits into a separate branch. As gauge potential becomes stronger the ground state becomes doubly degenerate at \( \alpha = 1/2 \) also in the interacting system. Furthermore, the gap separating the highest \( s \)-wave RVB state closes at \( \alpha = 1/2 \) and the eigenstate there becomes doubly degenerate.

One way to create gauge potentials in lattices is to shake the lattice \( \alpha \) appropriately and such tools have indeed been demonstrated experimentally \( \beta \). Some of the more simple methods of shaking cannot create a magnetic flux in a square lattice while they might do so in a triangular lattice. For this reason it is instructive to solve the problem also for a triangular plaquette. We show a typical the result in Fig. 2 (b). In a triangular plaquette with one atom per site the different component have necessarily different atom numbers. If \( N_1 = N_2 + 1 \) there are three eigensolutions. The excited state is doubly degenerate in the absence of gauge potential while its degeneracy is broken in the gauge potential. At \( \alpha = 1/2 \) the ground state is again doubly degenerate while the excited state is non-degenerate.

IV. FEW COUPLED PLAQUETTES

In the experiment by Nascimbé et al. [12] the plaquettes were not strongly coupled and they were able to create the \( s \)-wave RVB state in each plaquette. We can use our approach to also study systems with more than one plaquette. In this case it becomes possible to study how coupling between plaquette changes the system behavior. Since we have not made any assumptions about the magnitudes of tunneling strengths we can simply add tunneling terms between plaquettes without, for example, a need for a new perturbation theory in “small” inter-plaquette tunneling. One notable result from solving the problem for coupled plaquettes (for bosons) is that the ground state is degenerate in the limit of vanishing inter-plaquette tunneling and is separated from the first excited states by only a small gap as inter-plaquette tunneling is introduced.

In sharp contrast to this, the most excited state corresponding to the product state of plaquette \( s \)-wave RVB states is gapped in the limit of vanishing inter-plaquette tunneling and the gap remains quite large even as the inter-plaquette tunneling approaches the in-plaquette tunneling. More quantitatively, when all coupling strengths are the same, \( U_{11} = U_{22} = U_{12} = U \), and in-plaquette tunneling is taken as \( t = 1/2 \) the gap \( \Delta E = 1/U \) when inter-plaquette tunneling is zero. When inter-plaquette tunneling equals in-plaquette tunneling the gap is reduced to \( \Delta E \approx 0.77/U \) for two plaquettes and \( \Delta E \approx 0.65/U \) for three. This separation of the (experimentally relevant) most excited state might simplify studies where Hamiltonian is changed as a function of time, since unwanted transitions to other states can be suppressed.

To understand coupled plaquettes better, let us then demonstrate the dynamical behavior for two coupled plaquettes. We take the initial state to be the most excited state for uncoupled plaquettes. This state corresponds to the product state of plaquette \( s \)-wave RVB states. We then either increase the inter-plaquette tunneling \( t_b \) by linearly ramping it to the same value as the in-plaquette tunneling \( t \) or by turning it on instantaneously. In Fig. 3 we show how overlaps with the initial state and the RVB-state over all 8 sites (equal superposition of all possible ways to cover the lattice with singlet bonds between nearest neighbors) behave. As can be seen, the initial state has a substantial overlap with the resonating valence bond state in the 8-site system and this overlap increases further as the inter-plaquette tunneling approaches the in-plaquette tunneling and bonds start forming also between plaquettes. In this example, the maximum overlap is around 97%. The overlap with the initial product state remains large, but is substantially smaller than the overlap with the RVB-state. Incidentally the overlap

![FIG. 2. (a) Eigenenergies of $2 \times 2$ plaquette when another component experiences a gauge potential and $N_1 = N_2$. The uppermost state at $\alpha = 0$ is the s-wave RVB state and the first excited state is the d-wave RVB state as discussed in Ref. [12]. We choose $|t_1| = 1/2$ and $U_{11} = U_{22} = U_{12} = 1$. (b) Eigenenergies in a triangular plaquette when another component experiences a gauge potential and $N_1 = N_2 + 1$.](image-url)
V. PLAQUETTES WITH SPIN-ORBIT COUPLING

Recently it has become possible to create spin-orbit couplings in ultracold atomic gases [13]. This exciting development has opened up entirely new possibilities and motivated a rapidly expanding literature on various aspects of spin-orbit coupled systems using cold gases. The presence of spin-orbit coupling (SOC) changes our previous discussion in that it becomes possible for atoms to change type as they tunnel between sites. The tight binding model for a spin-orbit coupled two-component gas is given by ($i,j \in \{1,2\}$)

$$H_T = - \sum_{r \in g} \sum_{\gamma=x,y} \left( T^{(i,j)}_{\gamma} \hat{\psi}^\dagger_{r,i} \hat{\psi}_{r+\eta_{r,j}} + H.c. \right),$$

where $\hat{\psi}^\dagger_{r,i}$ creates an atom of type $i$ in the lattice site $r$ and $\eta_{r} = a \gamma$ is the vector to the nearest neighbor of $r$ along the direction $\gamma$ ($a$ is lattice spacing). $T^{(i,j)}_{\gamma}$ are the tunneling matrices, but note that (as in previous section) since tunneling coefficients in the plaquette can be made to vary, we have kept the possibility of position dependence in them. In our notation we mostly follow Radic et al. [14].

The free spin-orbit coupled system can be expressed in terms of a vector potential $A$ with a Hamiltonian $H_0 = (p - A)^2/2m$, where $m$ is the atomic mass. We choose the vector potential to be position independent and given by

$$A = (-ma\hat{\sigma}_x, -m\beta\hat{\sigma}_y),$$

where $\hat{\sigma}_\gamma$ ($\gamma \in \{x, y, z\}$) are the Pauli matrices. Peirls substitution

$$T_\gamma = t_\gamma e^{-iaA_\gamma} = t_\gamma e^{-i\theta_\gamma \hat{\sigma}_\gamma}$$

can then be used to relate tunneling coefficient $t_\gamma$ in the absence of SOC (i.e. $\theta_x = \theta_y = 0$) to those with SOC. This substitution is not exact and can be improved, but it is reasonably accurate over wide range of parameters and where its accuracy is somewhat worse it is still qualitatively useful [14]. Inaccuracies can become more serious in and closer to the superfluid regime.

When the expressions for tunneling elements in SOC system are expanded we find

$$T_x = t_x \left( \cos \theta_x \frac{i \sin \theta_x}{\sin \theta_x} \cos \theta_x \right)$$

and

$$T_y = t_y \left( \cos \theta_y \sin \theta_y \cos \theta_y \right).$$

In Fig. 3(b) we show the eigenenergies of the spin-orbit coupled system with only 2-sites. The basis is spanned by 4 states and without spin-orbit coupling the ground state in 3-fold degenerate. Spin-orbit coupling breaks this degeneracy so that ground state remains 2-fold degenerate. These ground states do not change with spin-orbit coupling, but the 2 excited state energies do depend in the strength of SO coupling. The eigenstates are however always such that the lower one is of type $|\psi\rangle = (|10\rangle_1 |10\rangle_2 - |01\rangle_1 |01\rangle_2)/\sqrt{2}$ while the upper one is of type $|\psi\rangle = (|10\rangle_1 |01\rangle_2 - |01\rangle_1 |10\rangle_2)/\sqrt{2}$.

In a two-dimensional system situation is more complex. In Fig. 4 we show the eigenenergies of the spin-orbit coupled plaquette as a function of $\theta_x$ and $\theta_y$. As SO coupling is turned on the initial three-fold degeneracy of the first excited state is broken and all states are non-degenerate. However, remarkably as one approaches $\theta_x = \theta_y = \pi/2$ all states become degenerate. (For non-interacting system one has at this point three-fold degenerate states with energies $E_{\pm} = \pm \sqrt{t_x^2 + t_y^2}$.) This suggests that close to this point the perturbative approach we have used might be breaking down and more accurate theory might...
FIG. 4. (Color online) 2-site system with spin-orbit coupling. The lowest level is doubly degenerate. We choose $t_x = 1/2$ and $U_{11} = U_{22} = U_{12} = 1$.

FIG. 5. (Color online) Eigenenergies for a $2 \times 2$ system with spin-orbit coupling as a function of $\theta_x$ and $\theta_y$. The inset in (a) shows the solutions at $\theta_y = 0$. We choose $U_{11} = U_{22} = U_{12} = 1$ and $t_x = t_y = 0.5$. All states are degenerate at $\theta_x = \theta_y = \pi/2$.

be required to properly resolve the eigenstates. Also, this high dimensionality of the ground state manifold might have interesting consequences for the dynamics as well as on how the system responds to experimental probes.

VI. CONCLUSIONS

In this article we have explored the physics of small insulating plaquettes under the influence of gauge potentials and spin-orbit couplings. Computations were done for bosonic systems, but in the simplest cases two-component fermionic problem amounts to sign change in the eigenenergies. For example, the highest excited state for bosons can become the ground state for fermions. At the formal level our approach does not distinguish between bosons and fermions since the only inputs into the solver are the various onsite interactions strengths and tunneling coefficients. For this reason the approach used here is also easy to apply to the study of fermionic multi-flavor systems [15] or Bose-Fermi mixtures. Since atoms could also be prepared on the excited bands of the lattice [26], it would be of interest to also explore the Mott insulating plaquettes in bipartite systems [19] and in excited bands.

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[1] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 71, 463 (1999).
[2] M. Greiner, O. Mandel, T. Esslinger, T. W. Häschen, and I. Bloch, Nature 415, 39 (2002).
[3] S. Sachdev, Nature Physics 4, 173 (2008).
[4] A. B. Kuklov and B. V. Svistunov, Phys. Rev. Lett. 90, 100401 (2003).
[5] E. Altman, W. Hofstetter, E. Demler, and M. D. Lukin, New J. Phys. 5, 113 (2003).
[6] Y.-J. Lin, K. Jimenez-Garca, and I. B. Spielman, Nature 471, 83 (2011).
[7] J. Struck, C. Ölschläger, R. Le Targat, P. Soltan-Panahi, A. Eckardt, M. Lewenstein, P. Windpassinger, and K. Sengstock, Science 333, 996 (2011).
[8] J. Struck, C. Ölschläger, M. Weinberg, P. Hauke, J. Simonet, A. Eckardt, M. Lewenstein, K. Sengstock, and P. Windpassinger, Phys. Rev. Lett. 108, 225304 (2012).
[9] J. Ruseckas, G. Juzeliunas, P. Öhberg, and M. Fleischhauer, Phys. Rev. Lett. 95, 010404 (2005).
[10] P. Hauke, O. Tielemann, A. Celi, C. Ölschläger, J. Simonet, J. Struck, M. Weinberg, P. Windpassinger, K. Sengstock, M. Lewenstein, et al., arXiv:1205.1398 (2012).
[11] J. Dalibard, F. Gerbier, G. Juzeliunas, and P. Öhberg, Rev. Mod. Phys. 83, 1523 (2011).
[12] S. Nascimbène, Y. Chen, M. Atala, M. Aidelsburger, S. Trotzky, B. Paredes, and I. Bloch, arXiv:1202.6361 (2012).
[13] W. S. Cole, S. Zhang, A. Paramekanti, and N. Trivedi, arXiv:1205.2319 (2012).
[14] J. Radic, A. Di Ciolo, K. Sun, and V. Galitski, arXiv:1205.2110 (2012).
[15] J. S. Krauser, J. Heinze, N. Fläschner, S. Götze, C. Becker, and K. Sengstock, arXiv:1203.0948 (2012).
[16] T. Best, S. Will, U. Schneider, L. Hackermüller, D. van Oosten, I. Bloch, and D.-S. Lühmann, Phys. Rev. Lett. 102, 030408 (2009).
[17] Y.-I. Shin, A. Schirotzek, C. H. Schunck, and W. Ketterle, Phys. Rev. Lett. 101, 070404 (2008).
[18] In spinorial systems or in higher bands there can be collisions that change the atom number of a component. In these cases simple Fock states are not the eigenstates of the system with more than one atom per site and the intermediate states created by the tunneling operator should be expanded in terms of the eigenstates of the interaction Hamiltonian. However, in this paper this distinction does not matter.
[19] J.-P. Martikainen and J. Larson, arXiv:1203.4402 (2012).
[20] A. Eckardt, P. Hauke, P. Soltan-Panahi, C. Becker, K. Sengstock, and M. Lewenstein, Europhysics Letters 89, 10010 (2010).
[21] F. Gerbier and J. Dalibard, New Journal of Physics 12, 033007 (2010).
[22] K. Sacha, K. Targoszka, and J. Zakrzewski, Phys. Rev. A 85, 053613 (2012).
[23] H. Lignier, C. Sias, D. Ciampini, Y. Singh, A. Zenesini, O. Morsch, and E. Arimondo, Phys. Rev. Lett. 99, 220403 (2007).
[24] Y.-A. Chen, S. Nascimbeni, M. Aidelsburger, M. Atala, S. Trotzky, and I. Bloch, Phys. Rev. Lett. 107, 210405 (2011).
[25] R. Ma, M. E. Tai, P. M. Preiss, W. S. Bakr, J. Simon, and M. Greiner, Phys. Rev. Lett. 107, 095301 (2011).
[26] G. Wirth, M. Ölschläger, and A. Hemmerich, Nature Physics 7, 147 (2011).