Inducing spin-dependent tunneling to probe magnetic correlations in optical lattices

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We suggest a simple experimental method for probing antiferromagnetic spin correlations of two-component Fermi gases in optical lattices. The method relies on a spin-selective Raman transition to excite atoms of one spin species to their first excited vibrational mode where the tunneling is large. The resulting difference in the tunneling dynamics of the two spin species can then be exploited, to reveal the spin correlations by measuring the number of doubly occupied lattice sites at a later time. We perform quantum Monte Carlo simulations of the spin system and solve the optical lattice dynamics numerically to show how the timed probe can be used to identify antiferromagnetic spin correlations in optical lattices.

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I. INTRODUCTION

Atoms in optical lattices provide a powerful test bed for probing the properties of quantum systems in periodic potentials. Several fundamental results have been reported including the observation of Mott physics [1], fermionic pairing [2], and the fermionization of bosons in one dimension [3]. Promising new research directions are emerging with the creation of Dirac points in honeycomb lattices [4] and the achievement of single site resolution for probing and manipulating two dimensional (2D) lattices [5, 6]. A major objective in the study of atoms in optical lattices is to unravel the physics of quantum magnetism, and for this purpose it is crucial to be able to measure the spin correlations of the atoms efficiently. Several methods have been suggested including Bragg scattering [7], time-of-flight measurements [8–10], and light polarization experiments [11]. A complication for these methods is, however, that the experimental signal is small, and that one has to average over many experimental realizations.

To address this, we recently suggested a superlattice method which yields large macroscopic signatures of the spin correlations and allows for the detection of both short- and long-range correlations [12]. It is based on spin-dependent transport using a spin-selective Raman transition followed by the application of an additional moving superlattice potential. The spin-correlations can then be extracted by measuring the number of doubly occupied lattice sites.

In this paper we propose a similar but experimentally simpler method, which replaces the moving superlattice by a precisely timed period of free tunneling dynamics of the atoms followed by a measurement of the double occupancy. We analyze the spin dependence of the tunneling dynamics and show how this can be used to reveal the spin correlations in the initial state. The main result of our paper is the demonstration that timed measurements of the probability for double occupancy of the lattice sites yields distinct signatures of the magnetic correlations.

Importantly, the method we propose here does not require any spin dependence of the lattice potential and only utilizes only the optical lattice potential which is already present. This is a major advantage from an experimental perspective.

II. MODEL AND METHOD

We consider a gas of fermionic atoms in an optical lattice with equal populations in two internal states |σ⟩ (σ = ↑, ↓), which we refer to as spin in the following. For strong repulsion and half-filling, the gas is in the Mott phase at low temperature T which is well described by the Heisenberg model [13]

\[ \hat{H} = J \sum_{\langle l,m \rangle} \left[ \hat{s}_l^x \hat{s}_m^x + \hat{s}_l^y \hat{s}_m^y + (1 + \Delta) \hat{s}_l^z \hat{s}_m^z \right]. \]

Here, \( \hat{s}_l \) is the spin-1/2 operator for atoms at site \( l \), and \( \langle l,m \rangle \) denotes neighboring pairs. The interaction strength J can exhibit a small anisotropy, quantified by the anisotropy parameter Δ. A major incentive for studying atoms in optical lattices is to observe the phase transition to an antiferromagnetic (AF) ordered state which occurs at \( T = T_N \approx 0.945J \) in 3D for the isotropic (Δ = 0) Heisenberg model [14]. To achieve this, one needs a sensitive experimental probe of the spin correlations.

The key idea of the present paper is to access the spin correlation functions by inducing a difference in the tunneling dynamics of the two different spin states |↑⟩ and |↓⟩ as shown in the sketch of Figure 1a. To this end, we excite all |↑⟩ atoms to their first excited vibrational state in the lattice sites while the |↓⟩ atoms remain in the ground state [14]. This can be done experimentally by set of spin-selective Raman transitions on the vibrational sideband of an auxiliary state. Then we simply allow the system to evolve for some time and subsequently measure the number of sites which are doubly occupied \( N_d \). Since the tunneling to neighboring sites is larger...
for the first excited state than for the ground state, the $|\downarrow\rangle$ atoms essentially remains at the initial lattice site as shown in Figure 1(a). In practice, the number of doubly occupied sites can be counted by merging two atoms residing on the same lattice site to a molecule by application of a photo-association pulse or via a Feshbach resonance.[11][15]

In our theoretical modeling the lattice potential is held constant during the procedure and we assume that the interaction is tuned to a sufficiently weak value, for instance by using a Feshbach resonance [10], so that the system can be considered non-interacting during the tunneling dynamics. The three spatial components of the atomic wave function then evolve independently. Assuming the motion in the $y$- and $z$-directions to be frozen by strong lattice potentials, it is sufficient to consider the dynamics along the $x$-direction, where the atoms are trapped by a periodic potential $A(x,t) = A \sin^2(\pi x/d)$ with $d$ the lattice constant. With this potential the single particle Bloch eigenenergies $E_k$ and corresponding eigenfunctions $|\psi_k^\prime\rangle$ are indexed by a vibrational state label $l = 0, 1, 2, \ldots$ and a Bloch wavevector $k$. The initial states are taken to be the Wannier functions given by $|W_j^n\rangle = \frac{1}{\sqrt{N}} \sum_k e^{-iE_k l} |\psi_k^\prime\rangle$, which describe a localized state of the $n$th vibrational mode centered around lattice site $j$.[17]

Because the Wannier functions are not eigenfunctions of the non-interacting lattice Hamiltonian, they evolve over time. To describe this we introduce the transition matrix $U(t) = e^{-iHt} = \sum_{ij} U_{ij}^{(n)}(t) \tilde{a}^\dagger_i a_j$, where $\tilde{a}^\dagger_i$ is the creation operator for the Wannier state $|W_j^n\rangle$ and we use units for which $\hbar = 1$. The time evolution operator $U(t)$ is quadratic in $\tilde{a}$ and $\tilde{a}^\dagger$ and diagonal in the vibrational quantum number $n$ since we assume the system to be non-interacting during the evolution. The matrix elements of this transition matrix read

$$U_{ij}^{(n)}(t) = \langle W_j^n | W_i^n(t) \rangle = \frac{1}{N} \sum_k e^{ik(j-i)l} e^{-iE_k t},$$  \hspace{1cm} (2)$$

where $|W_i^n(t)\rangle$ represents the initial Wannier function $|W_i^n\rangle$ evolved for a time $t$. We are mainly interested in the probability for a site $i$ to be doubly occupied $P_d(i) = \langle \tilde{n}_{i\uparrow}(t) \tilde{n}_{i\downarrow}(t) \rangle$. Our proposed scheme is based on the fact that this probability can be expressed in terms of spin correlation functions of the initial state and the overlap matrix elements $U_{ij}^{(n)}[12]$. Since the $|\downarrow\rangle$ atoms remain in the vibrational ground state $n = 0$ while the $|\uparrow\rangle$ atoms are transferred to the first excited state $n = 1$, we write $U_{ij}^{(1)} = U_{ij}^\dagger$ and $U_{ij}^{(0)} = U_{ij}$. Then we obtain

$$P_d(i) = \sum_{j,t} |U_{ij}^\dagger(t)|^2 |U_{ji}^\dagger(t)|^2 \left( \frac{1}{4} - \langle \hat{s}_j^z \hat{s}_i^z \rangle \right)$$

$$- \sum_{j,t} U_{ij}^\dagger U_{ji}^\dagger U_{ij} U_{ji} \langle \hat{s}_j^z \hat{s}_i^z \rangle.$$ \hspace{1cm} (3)$$

In the limit where the $|\downarrow\rangle$ atoms do not move $|U_{ii}^\dagger|^2 \approx \delta_{i,i}$, Eq. (3) reduces to

$$P_d(i) = \frac{1}{4} - \sum_{j \neq i} \left| U_{ij}^\dagger(t) \right|^2 \langle \hat{s}_j^z \hat{s}_i^z \rangle.$$ \hspace{1cm} (4)$$

Equations (3) and (4) demonstrate the direct link between the observed double occupancy and the spin correlation function $\langle \hat{s}_j^z \hat{s}_i^z \rangle$ describing AF ordering in the initial state.

III. RESULTS

We now present our numerical results. The spin correlation functions $\langle \hat{s}_i \cdot \hat{s}_j \rangle$ for the initial state determined by the 3D Heisenberg model [4] are obtained from full quantum Monte Carlo (QMC) simulations using the stochastic series expansion method [18] with directed-loop updates [19]. The subsequent time evolution after the $|\uparrow\rangle$ atoms are excited to the first vibrational state is then calculated by numerical diagonalization of the non-interacting Hamiltonian taking the motion to be along a single direction. As an example, we will here present results for a 1D lattice with $N = 32$ sites and a lattice height $A = 10E_R$ where $E_R = h^2\pi^2/2Md^2$ is the recoil energy with $M$ the atom mass. The numerical diagonalization is performed using a lattice unit cell consisting of 1028 real-space points.

A. Single atom dynamics

We first consider the time evolution of a single atom. Figure 1(b) and 1(c) depicts the probability $|U_{00}^\dagger(t)|^2$ of a $|\sigma\rangle$ atom which starts at $t = 0$ at site $i = 0$, to be at site $j$ at time $t$. We see that for the parameters chosen, the $|\downarrow\rangle$ atoms do not move but remain at their initial position (Fig. 1(b)) whereas the $|\uparrow\rangle$ atoms move (Fig. 1(c)). This makes this tunneling dynamics well suited for measuring AF ordering. Note that at certain times the wavefunction of the $|\uparrow\rangle$ atoms mostly samples either even or odd lattice sites in a way similar to a random walk in 1D. In Fig. 2(b) we plot the tunneling time of the $|\uparrow\rangle$ atoms, $t^\dagger$, defined as the first zero of $\partial_t |U_{00}^\dagger(t)|^2$, as a function of the lattice depth. According to the WKB approximation this time depends exponentially on the lattice height, and we indeed find $t^\dagger \propto \exp(0.4A/E_R)$ for deep lattices. Thus, by adjusting the lattice depth one can tune the time scale of the probe. It is, however, important that the lattice depth is sufficiently deep so that only the $|\uparrow\rangle$ atoms move. This is illustrated in Fig. 2(right) where we plot $P_{\text{error}} = 1 - |U_{ii}^{(1)}(t^\dagger)|^2$, which represents the probability that a $|\downarrow\rangle$ has moved after the $|\uparrow\rangle$ tunneling time $t^\dagger$. As expected, the error decreases rapidly with increasing lattice depth.
FIG. 1: (a) A cartoon depicting the tunneling dynamics for the two spin species. (b–c) The actual tunneling dynamics for the two lowest lying vibrational Wannier states of a one-dimensional lattice with lattice height $A = 10 E_R$. We show the norm square of the wavefunction projected onto Wannier states centered around each lattice site. There is a clear difference in the tunneling dynamics between (b) the almost stationary vibrational ground state ($\uparrow$ atom) and (c) the first excited state ($\uparrow$ atom) which tunnels to its neighboring sites. The dashed line indicates the first minimum of the probability for the $\uparrow$ atom to remain at its initial position.

FIG. 2: (Color online) (a) the tunneling time versus lattice depth $A$ of the first excited vibrational state which sets the time scale of the probe. (b) the error probability as a function of lattice depth $A$.

B. Many-body dynamics and AF ordering

We now analyze the evolution of the double occupancy, $P_d$, starting from a correlated initial state determined by the 3D Heisenberg model. This is shown in Fig. 3.

We focus first on the non-interacting case corresponding to $T = \infty$ which is plotted as the solid line forming the boundary to the grey area. For this case, the spins are uncorrelated and $\langle \delta_{nm} \delta_{ij} \rangle = \frac{1}{A} \delta_{nm}$. Since the vibrational ground state is essentially immobile $|U_{ij}^1|^2 \approx \delta_{ij}$ for all the relevant times, we find $P_d \approx \frac{1}{4} (1 - |U_{ii}^1(t)|^2)$. Hence for a half-filled non-interacting system, $P_d$ cannot be larger than 1/4 and will in general be lower because of the non-vanishing probability that the $|\uparrow\rangle$ atoms return to their initial states. The oscillations in $P_d$ for uncorrelated atoms are therefore directly linked to the oscillations in $|U_{ij}^1(t)|^2$ which are shown in Fig. 1. Since the tunneling time $t^*$ gives the time for the first minimum of $|U_{ij}^1(t)|^2$, it corresponds to the first maximum of $P_d$. At this minimum, $|U_{ii}^1(t)|^2 \approx 0$ and the value of $P_d$ at the first maximum is therefore very close to 1/4, which is also the long time uncorrelated value.

We now turn to $P_d$ for finite temperature also plotted in Fig. 3. We have chosen a slightly anisotropic Heisenberg system with $\Delta = 0.01$, which forces the staggered magnetization to be along the z-axis. The AF correlations are clearly visible as increased oscillations of $P_d$ as a function of time which is the main result of the present paper. In particular, note that the probability $P_d$ is larger than 1/4 for certain times which is a clear sign of AF ordering. To analyze this effect further, we consider the high temperature regime $J/T \ll 1$ with $k_b = 1$, where

$$\langle \delta_i^\uparrow \delta_j^\uparrow \rangle = \frac{1}{4} \delta_{ij} - \frac{J}{16T} \delta_{i,j} + O(J^2/T^2) \quad (5)$$

with $\delta_{i,j}$ the Kronecker delta function connecting neighboring sites. Using this in Eq. 4 we get

$$P_d(i) = \frac{1}{4} (1 - |U_{ii}^1(t)|^2) + \frac{J}{8T} |U_{ii}^1(t)|^2 \quad (6)$$

for $J/T \ll 1$. Equation 6 clearly illustrates how AF correlations can increase $P_d$; for example as seen from Fig. 4 at $t = t^*$, we have that $|U_{ii}^1(t^*)|^2 \approx 0$ and $|U_{ii}^1(t^*)|^2 \approx 1/4$ such that $P_d(i) = \frac{1}{4} (1 + \frac{J}{4T})$. As the temperature is lowered, the oscillations of $P_d$ becomes larger reflecting the increasing AF correlations.

FIG. 3: (Color online) The double occupancy probability $P_d$ as a function time $t$ at different temperatures $T$ for the slightly anisotropic Heisenberg system ($\Delta = 1.01$) and a lattice depth $A = 10 E_R$. 
We see that for the oscillations at later times, the difference increases significantly for $T < T_N \approx 0.945J$ when long-range order sets in, although the absolute size of the difference is rather small. Note also the two dips at $t \approx 260h/E_R$ and $t \approx 500h/E_R$ which shows up as long-range correlations set in at $T = T_N$. From Fig. 4 one can also see that short-range correlations leave a signature at $T > T_N$, for example yielding an AF signal at $t \approx t^*$ of $\Delta P_d(T = 2J) = 0.0195 \approx 0.08P(T = \infty)$.

IV. CONCLUSIONS AND DISCUSSIONS

In summary, we have demonstrated how to detect antiferromagnetic spin correlations in optical lattices by utilizing the difference in the tunneling dynamics of the two lowest lying vibrational states of the atomic wavefunctions. Measurement of the number of doubly occupied sites yields a macroscopic signature of the magnetic correlations which is proportional to the number of lattice sites. Below the critical temperature $T_N$ the method has large signatures $\Delta P_d \approx 0.1$ as a result of the spin correlations.

The method presented here is particularly relevant for measuring short range correlations as it provides an easily accessible experimental method, which requires a minor change of the experimental setups already present. For measuring long range correlations the method is less suited as the spreading of the wave function for long times introduces an uncertainty in the correlation function measured. Such long correlation can thus be measured more precisely with different schemes, for instance relying on superlattice potentials [12].

Here we have mainly focussed on the detection of antiferromagnetic correlations, but the method may also be used to probe other spin ordered states. In Fig. 5 we show the $k$-space representation of $|U_{ij}^+|^2$ for three different selected times. As seen, by selecting appropriate times a magnetic ordering with periodicities of, for example, $k = \pi/2$ and $k = \pi/3$, can also be probed.

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[1] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature (London) 415, 39 (2002); R. Jördens, N. Strohmaier, K. Günter, H. Moritz, and T. Esslinger, ibid 455, 204 (2008); I. B. Spielman, W. D. Phillips, and J. V. Porto, Phys. Rev. Lett. 98, 080404 (2007); U. Schneider, L. Hackermüller, S. Will, Th. Best, I. Bloch, T. A. Costi,
R. W. Helmes, D. Rasch, and A. Rosch, Science 322, 1520 (2008).

[2] J. K. Chin, D. E. Miller, Y. Liu, C. Stan, W. Setiawan, C. Sanner, K. Xu, and W. Ketterle, Nature (London) 443, 961 (2006).

[3] B. Paredes, A. Widera, V. Murg, O. Mandel, S. Fölling, I. Cirac, G. V. Shlyapnikov, T. W. Hänsch, and I. Bloch, Nature (London) 429, 277 (2004); T. Kinoshita, T. Wenger, and D. S. Weiss, Science 305, 1125 (2004).

[4] L. Tarruell, D. Greif, T. Uehlinger, G. Jotzu, T. Esslinger, arXiv:1111.5020.

[5] J. F. Sherson, C. Weitenberg, M. Endres, M. Cheneau, I. Bloch, and S. Kuhr, Nature (London) 467, 68 (2010); W. S. Bakr, A. Peng, M. E. Tai, R. Ma, J. Simon, J. I. Gillen, S. Fölling, L. Pollet, and M. Greiner, Science 329, 547 (2010).

[6] C. Weitenberg, M. Endres, J. F. Sherson, M. Cheneau, P. Schauss, T. Fukuhara, I. Bloch, and S. Kuhr, Nature (London) 471, 319 (2011).

[7] T. A. Corcovilos, S. K. Baur, J. M. Hitchcock, E. J. Mueller, and R. G. Hulet, Phys. Rev. A 81, 013415 (2010).

[8] E. Altman, E. Demler, and M. D. Lukin, Phys. Rev. A 70, 013603 (2004).

[9] G. M. Bruun, O. F. Syljuåsen, K. G. L. Pedersen, B. M. Andersen, E. Demler, and A. S. Sørensen, Phys. Rev. A 80, 033622 (2009).

[10] B. M. Andersen and G. M. Bruun, Phys. Rev. A 76, 041602 (2007).

[11] G. M. Bruun, B. M. Andersen, E. Demler, and A. S. Sørensen, Phys. Rev. Lett. 102, 030401 (2009); K. Eckert, O. Romero-Isart, M. Rodriguez, M. Lewenstein, E. S. Polzik, and A. Sanpera, Nat. Phys. 4, 50 (2008).

[12] K. G. L. Pedersen, B. M. Andersen, G. M. Bruun, O. F. Syljuåsen, and A. S. Sørensen, Phys. Rev. A 84, 041603(R) (2011).

[13] L.-M. Duan, E. Demler, and M. D. Lukin, Phys. Rev. Lett. 91, 090402 (2003); A. B. Kuklov and B. V. Svetunov ibid 99, 100401 (2003).

[14] I. Bouchoule, H. Perrin, A. Kuhn, M. Morinaga and C. Salomon, Phys. Rev. A 59, R8 (1999).

[15] D. Greif, L. Tarruell, T. Uehlinger, R. Jordens, and T. Esslinger, Phys. Rev. Lett. 106, 145302 (2011).

[16] J. T. Stewart, J. P. Gaebler, T. E. Drake, and D. S. Jin, Phys. Rev. Lett. 104, 235301 (2010); M. Fattori, G. Roati, B. Deissler, C. D’Errico, M. Zaccanti, M. Jona-Lasinio, L. Santos, M. Inguscio, and G. Modugno, ibid 101, 190405 (2008).

[17] G. K. Brennen, C. M. Caves, P. S. Jessen, and I. H. Deutsch, Phys. Rev. Lett. 82, 1060 (1999); D. Jaksch, H.-J. Briegel, J. I. Cirac, C. W. Gardiner, and P. Zoller, ibid. 82, 1975 (1999).

[18] O. F. Syljuåsen and A. W. Sandvik, Phys. Rev. E 66, 046701 (2002).

[19] A. W. Sandvik and J. Kurki-Suonio, Phys. Rev. B 43, 5950 (1991).