XYZ Quantum Heisenberg Models with $p$-Orbital bosons

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We demonstrate how the spin-1/2 XYZ quantum Heisenberg model can be realized with bosonic atoms loaded in the $p$ band of an optical lattice in the Mott regime. The combination of Bose statistics and the symmetry of the $p$-orbital wave functions leads to a non-integrable Heisenberg model with anti-ferromagnetic couplings. Moreover, the sign and relative strength of the couplings characterizing the model are shown to be experimentally tunable. We display the rich phase diagram in the one dimensional case, and discuss finite size effects relevant for trapped systems. Finally, experimental issues related to preparation, manipulation, detection, and imperfections are considered.

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Introduction.– Powerful tools developed recently to unravel the physics of many-body quantum systems offer an exciting new platform for understanding quantum magnetism. It is now possible to engineer different systems in the lab that mimic the physics of theoretically challenging spin models [1], thereby performing “quantum simulations” [2]. Along these lines, systems of trapped ions and of polar molecules are promising candidates. Trapped ions, for example, have already been employed to simulate both small [3] and large [4] numbers of spins. In these setups, however, sustaining control over the parameters becomes very difficult as the system size increases. Furthermore, due to trapping potentials realizations are limited to chains with up to 25 spins. It is also very difficult to construct paradigmatic spin models with short range interactions using systems of trapped ions. Similar limitations appear when using polar molecules, where the effective spin interactions [5, 6] are obtained from the intrinsic dipole-dipole interactions. Due to the character of the dipolar interaction, these systems give rise to emergent models that are inherently long range and the resulting couplings usually feature spatial anisotropies.

Short range spin models can instead be realized with cold atoms in optical lattices [1]. A bosonic system in a tilted lattice has recently been used to simulate the phase transition in a 1D Ising model [7]. Fermionic atoms were employed to study dynamical properties of quantum magnetism for spin systems [8, 9]. This idea, first introduced in Ref. [10], has also been applied to other configurations, and simulation of different types of spin models have been proposed [11]. However, due to the character of the atomic $s$-wave scattering among the different Zeeman levels, such mappings usually yield effective spin models supporting continuous symmetries like the XXZ model. But as the main goal of a quantum simulator is to realize systems that cannot be tackled via analytical and/or numerical approaches, it is important to explore alternative scenarios that yield low symmetry spin models with anisotropic couplings and external fields.

In this paper we propose such a scenario by demonstrating that bosonic atoms in the first excited band ($p$ band) of a two-dimensional (2D) optical lattice can realize the spin-1/2 XYZ quantum Heisenberg model in an external field. Systems of cold atoms in excited bands feature an additional orbital degree of freedom [12] that gives rise to novel physical properties [13], which include supersolids [14] and other types of novel phases [15], unconventional condensation [16], and frustration [17]. Also a condensate with a complex order parameter was recently observed experimentally [18, 19]. The dynamics of bosons in the $p$ band include anisotropic tunneling and orbital changing interactions, where two atoms in one orbital state scatter into two atoms in a different orbital state. This is the key mechanism leading to the anisotropy of the effective spin model obtained here: These processes reduce the continuous $U(1)$ symmetry characteristic of the XXZ model, which would effectively describe fermions in the $p$ band [20], into a set of discrete $Z_2$ symmetries characteristic of the XYZ model. In addition, due to the anomalous $p$-band dispersions the couplings of the resulting spin model can favor for anti-ferromagnetic order even in the bosonic case.

We also demonstrate how further control of both the strength and sign of the couplings is obtained by external driving. This means that one can realize a whole class of anisotropic XYZ models with ferromagnetic and/or anti-ferromagnetic correlations. To illustrate the rich physics that can be explored with this system we discuss the phase diagram of the 1D XYZ chain in an external field. This case exhibits ferromagnetic as well as anti-ferromagnetic phases, a magnetized/polarized phase, a spin-flop and a floating phase [21]. Finite size effects relevant for the trapped case are examined via exact diagonalization. This reveals the appearance of a devil’s
staircase manifested in the form of spin density waves. Finally, we discuss how to experimentally probe and manipulate the spin degrees of freedom.

**p-orbital Bose system.** We consider bosonic atoms of mass $m$ in a 2D optical lattice of the form $V(\mathbf{r}) = V_x \sin^2(k_x x) + V_y \sin^2(k_y y)$. Assuming that all atoms are in the first excited bands, the tight-binding Hamiltonian is

$$
\hat{H} = -\sum_{i,j} t_{ij} \hat{a}_{i}^{\dagger} \hat{a}_{j} + \sum_{\alpha} \left[ \frac{U_{\alpha}}{2} \hat{n}_{i,\alpha} (\hat{n}_{i,\alpha} - 1) + E_{\alpha} \hat{n}_{i,\alpha} \right] + \sum_{i,\alpha \neq \alpha'} \left( U_{\alpha\alpha'} \hat{n}_{i,\alpha} \hat{n}_{i,\alpha'} + \frac{U_{\alpha\alpha'}}{2} \hat{a}_{i,\alpha}^{\dagger} \hat{a}_{j,\alpha} \hat{a}_{i,\alpha'} \hat{a}_{j,\alpha'} \right). \tag{1}
$$

Here $\hat{a}_{i,\alpha}^{\dagger}$ creates a bosonic particle in the orbital $\alpha = p_x$, $p_y$ at site $i$, $\hat{n}_{i,\alpha} = \hat{a}_{i,\alpha}^{\dagger} \hat{a}_{i,\alpha}$, and the sum is over nearest neighbors $i, j$. The tunneling matrix elements are given by $t_{ij} = -\int d\mathbf{r} \hat{w}^{\alpha}(\mathbf{r})^* \left[ -\hbar^2 \nabla^2 / 2m + V(\mathbf{r}) \right] \hat{w}^{\alpha}(\mathbf{r})$ where $\hat{w}^{\alpha}(\mathbf{r})$ is the Wannier function of orbital $\alpha$ at site $i$. Note that $t_{ij}^{\alpha}$ is anisotropic. For instance, a boson in the $p_x$-orbital has a much larger tunneling rate in the $x$-direction than in the $y$-direction. The coupling constants are given by $U_{\alpha\alpha'} = U_0 \int d\mathbf{r} \left| \hat{w}^{\alpha}(\mathbf{r}) \right|^2 \left| \hat{w}^{\alpha'}(\mathbf{r}) \right|^2$, with $U_0 > 0$ the onsite interaction strength determined by the scattering length. The last term in Eq. (1) is the orbital changing term describing the flipping of a pair of atoms from the state $\alpha'$ to the state $\alpha$. Note that this term is absent in the case of fermionic atoms.

**Effective spin Hamiltonian.** We are interested in the physics of the Mott insulator phase with unit filling in the strongly repulsive limit $|t_{ij}^{\alpha}|^2 \ll U_{\alpha\alpha'}$. Projecting onto the Mott space of singly occupied sites with the operator $\hat{P}$, the Schrödinger equation becomes $\hat{H}_{\text{Mott}} \hat{P} |\psi\rangle = E \hat{P} |\psi\rangle$ with $\hat{H}_{\text{Mott}} = -\hat{P} \hat{H} (\hat{Q} - E) - E \hat{P} \hat{H}$. Here $Q = 1 - \hat{P}$ and $\hat{H} = \hat{Q} \hat{H} \hat{Q}$. Since $E \sim t^2 / U$, we can take $(\hat{Q} - E)^{-1} = \hat{Q}^{-1}$. The space of doubly occupied states of a given site $j$ is three-dimensional and spanned by $|p_x p_x\rangle = 2^{-1/2} \hat{a}_{j,\alpha}^{\dagger} \hat{a}_{j,\alpha}^{\dagger} |0\rangle$, $|p_y p_y\rangle = 2^{-1/2} \hat{a}_{j,\beta}^{\dagger} \hat{a}_{j,\beta}^{\dagger} |0\rangle$, and $|p_x p_y\rangle = \hat{a}_{j,\alpha}^{\dagger} \hat{a}_{j,\beta}^{\dagger} |0\rangle$. In this space, it is straightforward to find $\hat{H}_{Q}$ from Eq. (1), and subsequent inversion yields

$$
\hat{H}_{\text{Mott}}^{-1} = \begin{pmatrix}
U_{yy} / U^2 & -U_{xy} / U^2 & 0 \\
-U_{xy} / U^2 & U_{xx} / U^2 & 0 \\
0 & 0 & 1 / 2 U_{xy}
\end{pmatrix}
$$

with $U^2 = U_{xx} U_{yy} - U_{xy}^2$. In particular, the off-diagonal terms in $\hat{H}_{\text{Mott}}^{-1}$ derive from the orbital changing term. Using (2) we can now calculate all possible matrix elements of $\hat{H}_{\text{Mott}}$ in the Mott space,

$$
\hat{H}_{\text{Mott}} = -\sum_{i,j,\alpha} \left( \frac{2|t_{ij}^{\alpha}|^2 U_{\alpha}}{U^2} \hat{n}_{i,\alpha} \hat{n}_{j,\alpha} + \frac{|t_{ij}^{\alpha}|^2}{2U_{xy}} \hat{n}_{i,\alpha} \hat{n}_{j,\alpha} \right)
$$

$$
- \frac{2t_{ij}^{\alpha} t_{ji}^{\alpha}}{U^2} \hat{a}_{i,\alpha}^{\dagger} \hat{a}_{j,\alpha} \hat{a}_{j,\alpha}^{\dagger} \hat{a}_{i,\alpha} + \frac{t_{ij}^{\alpha} t_{ji}^{\alpha}}{2U_{xy}} \hat{a}_{i,\alpha}^{\dagger} \hat{a}_{j,\alpha} \hat{a}_{j,\alpha}^{\dagger} \hat{a}_{i,\alpha} \tag{3}
$$

where $\bar{x} = y$, and $\bar{y} = x$. By further employing the Schwinger angular momentum representation, $\hat{S}_{\bar{x}}^i = \frac{1}{2} (\hat{a}_{i,\alpha}^{\dagger} \hat{a}_{i,\alpha} - \hat{a}_{i,\alpha} \hat{a}_{i,\alpha}^{\dagger})$, $\hat{S}_{\bar{y}}^i = \hat{S}_{\bar{x}}^i + i \hat{S}_{\bar{y}}^i$, and $\hat{S}_{\bar{y}}^i = \hat{S}_{\bar{x}}^i - i \hat{S}_{\bar{y}}^i$, together with the constraint $\hat{a}_{i,\alpha}^{\dagger} \hat{a}_{i,\alpha} + \hat{a}_{i,\alpha} \hat{a}_{i,\alpha}^{\dagger} = 1$, we can (ignoring irrelevant constants) map (3) onto a spin-1/2 XYZ model in an external field [25]

$$
\hat{H}_{XYZ} = \sum_{ij} \left[ (1 + \gamma) \hat{S}_{\bar{x}}^i \hat{S}_{\bar{x}}^j + (1 - \gamma) \hat{S}_{\bar{y}}^i \hat{S}_{\bar{y}}^j \right]
$$

$$
+ \sum_i \Delta_i \hat{S}_{\bar{x}}^i \hat{S}_{\bar{y}}^i + h \sum_i \hat{S}_{\bar{x}}^i \tag{4}
$$

Here, $(i, j)$ means summing over each nearest neighbor pair $i, j$ only once. The couplings are given by $J_{ij} = -2t_{ij}^{\alpha} t_{ji}^{\alpha} / U_{xy}$, and $\Delta_i = -4(|t_{ij}^{\alpha}|^2 U_{yy} + |t_{ij}^{\alpha}|^2 U_{xx}) / U_{xy}^2 + (|t_{ij}^{\alpha}|^2 + |t_{ji}^{\alpha}|^2) / U_{xy}$. The magnetic field is $h = 4 \sum_{ij} (|t_{ij}^{\alpha}|^2 U_{xx} - |t_{ij}^{\alpha}|^2 U_{yy}) / U_{xy}^2 + E_p - E_p$, where $E_p$ is the onsite energy of the orbital $\alpha$.

Equation (4) is a main result of this paper. It demonstrates how $p$-orbital bosons in a 2D optical lattice can realize the XYZ quantum spin-1/2 Heisenberg model. Several interesting facts should be noted. First, $t_{ij}^{\alpha} t_{ji}^{\alpha} < 0$ due to the symmetry of the $p$-orbitals [12] and therefore $J_{ij} > 0$. Furthermore, since $|\gamma| < 1$ we have antiferromagnetic instead of the usual ferromagnetic couplings for bosons. Also, we obtain the XYZ model when $\gamma \neq 0$. The presence of $\gamma$ can be traced to the orbital changing term in Eq. (1), which reduces the continuous $U(1)$ symmetry of $\hat{S}_{\bar{x}}^i$ and $\hat{S}_{\bar{y}}^i$ to a set of $Z_2$ symmetries. The $Z_2$ symmetries reflect the ‘parity’ conservation in the original bosonic picture which classifies the many-body states according to total even or odd number of atoms in the $p_x$ and $p_y$ orbitals. Since the orbital changing term is absent for fermions, the XYZ model with anisotropic coupling is a peculiar feature of bosons in the $p$ band. We emphasize that the above derivation makes no assumptions regarding the geometry of the 2D lattice - i.e. it can be square, hexagonal etc.

**1D XYZ phase diagram.** To illustrate the rich physics of the XYZ model, we now focus on the case of a 1D lattice where where quantum fluctuations are especially pronounced. Note that by increasing both the lattice amplitude and spacing in the $y$ direction keeping $V_y k_y^2 \approx V_x k_x^2$, one can exponentially suppress tunneling in the $y$ direction to obtain a 1D model, while the $p_x$ and $p_y$
spins align along the orientation of the field in the $z$ direction. These three phases also characterize the phase diagram of the XXZ model in a longitudinal field [27]. However, for non-zero anisotropy $\gamma$, a gapless floating phase (FP) emerges between the SF and the AFM phases which is characterized by power-law decay of the correlations [21, 28, 29]. The transition from the AFM to the FP is of the commensurate-incommensurate (C-IC) type whereas the transition between the FP and SF phases is of the Berezinsky-Kosterlitz-Thouless (BKT) type. For $\Delta < -(1 + |\gamma|)$ there is a first order transition at $h = 0$ between the two polarized phases. Finally, there is an Ising transition between the PP and the SF phases.

The experimental realization of the Heisenberg model will inevitably involve finite size effects due to the harmonic trapping potential. Within the local density approximation, the trap renormalizes the couplings so that they become spatially dependent [30], but this effect can be negligible if the orbitals are small compared to the length scale of the trap. In the regime of strong repulsion, the main effect of the trap is instead that it gives rise to "welding cake" structures with Mott regions of integer filling. This effect was observed in the lowest band Bose-Hubbard model [1], and predicted theoretically to occur for anti-ferromagnetic systems [31]. To examine finite size effects, we have performed exact diagonalization in a chain with 18 spins with open boundary conditions. Figure 1 (b) displays the resulting finite size 'phase diagram'. The colors correspond to different values of the total magnetization $M = \sum_i \langle \hat{S}_i^z \rangle$ of the ground state. While the PP phase and the AMF phase are both clearly visible, the numerical results reveal a step like structure between the two phases. We attribute these steps in $M$ to a devil’s staircase structure of spin-density-waves (SDW). As we see from Fig. 1 (b), it is only possible to give a numerical result for the PP-SF Ising transition. In particular, the C-IC and BKT transitions are overshadowed by the transitions between SDW. In the thermodynamic limit the staircase becomes complete and the changes in $M$ become smooth. One then recovers the phase diagram of Fig. 1 (a). These transitions, between different SDW, are more pronounced for moderate systems sizes. For a typical experimental system with $\sim 50$ sites, for example, we estimate $\sim 15$ different SDW between the AFM and PP phases.

Measurements and manipulations.— While time-of-flight measurements can reveal some of the phases [19], single-site addressing techniques [33] will be much more powerful when extracting correlation functions. To address single orbital states or even perform spin rotations, one may borrow techniques developed for trapped ions [R]. Making use of the symmetries of the $p_x$ and $p_y$ orbitals, stimulated Raman transitions can drive both sideband and carrier transitions for the chosen orbitals in the Lamb-Dicke regime. These transitions can be made so short that the system is essentially frozen during the
measure the spin at any site in any direction \cite{3,23}. With the above mentioned rotations makes it possible to carrier transition acts as measuring†. The frequencies and ∆σp
Hamiltonian\hat{x}\sigma with \Delta \sigma\text{ps}
\hat{\sigma}x the \gamma
\text{and} \text{\Delta}\sigma\text{ps}
\hat{s}\alpha. This scheme, thus, realizes an effective spin Hamiltonian \hat{H}^{(i)}\sigma\text{xx}= (1 + \gamma), J_{yy} = (1 - \gamma), and J_{xz} = \Delta/J\text{ for} t_y/t_x = -0.1.

operation. Driving sideband transitions in this way, spin rotations may be implemented. For example, a spin rotation around \hat{x}\text{ is achieved by} driving the red-sidebands for both orbitals \cite{23}. As a result, the two \hat{p}\text{ orbitals are coupled to the } s \text{ orbital in a } V \text{ configuration and in the large detuned case an adiabatic elimination of the } s \text{ band gives an effective coupling between the } p_x \text{ and } p_y \text{ orbitals} \cite{6}. This scheme, thus, realizes an effective spin Hamiltonian \hat{H}^{(i)}\sigma\text{xx}=0, \hat{\Omega}_\alpha\text{ with } \Omega_\alpha \text{ the effective Rabi frequencies and } \Delta\sigma\text{ps}
\hat{\Omega}\text{ the detuning. Alternatively, Stark-shifting one of the } p \text{ orbitals results in a rotation around } s. \text{ Since the spin operators do not commute, any rotation can be realized from these two operations. Performing fluorescence on single orbital states by driving the carrier transition acts as measuring } \hat{S}_\sigma^z\text{. This combined with the above mentioned rotations makes it possible to measure the spin at any site in any direction} \cite{3,22}.

\text{Tuning of couplings.–} For a square optical lattice, we have \hat{U}_{xx} = \hat{U}_{yy}. Moreover, in the harmonic approximation \hat{U}_{xy} = \hat{U}_{yx}/3, from which it follows that \Delta < 0 \text{ and } \gamma = -1/2. \text{ This gives ferromagnetic couplings for the } z \text{ component of neighboring spins, while the interactions between } x \text{ and between the } y \text{ components have anti-ferromagnetic couplings. We now show how the relative strength and sign of the different couplings can be controlled by squeezing one of the orbital states. Such squeezing can be accomplished by again driving the carrier transition of either of the two orbitals, dispersively with a spatially dependent field} \cite{23}. The shape of the drive can be chosen such that the resulting Stark shift is weaker in the center of the sites, resulting in a narrowing of the orbital. To be specific, assume that the ratio \sigma of the harmonic length scales of the } p_x \text{ and } p_y \text{ orbitals in the } y \text{ direction is tuned. A straightforward cal-

ulation using harmonic oscillator functions yields } \alpha \equiv \hat{U}_{xx}/\hat{U}_{yy} = 2^{-3/2}3(1 + \sigma^2)^{3/2}/\alpha \text{ and } \beta \equiv \hat{U}_{xy}/\hat{U}_{yx} = 2^{-3/2}3(1 + \sigma^2)^{3/2}. \text{ The coupling constants now depend on } \sigma \text{ as } \Delta_\text{J} = 2t^2(\text{t}_0^{-1}\beta/(\alpha\beta - 1) + 2t^0(\text{t}_x^{-1}\alpha/(\alpha\beta - 1) - (\text{t}_x/\text{t}_0 + \text{t}_y/\text{t}_x)/2) and } \gamma = -4/(\alpha\beta - 1). \text{ The inset in Fig.5 displays the three coupling parameters as a function of } \sigma \text{ for } |\text{t}_x/\text{t}_0| = 0.1. \text{ We see that the relative size and even the sign of the couplings can be tuned by varying } \sigma. \text{ In particular, while } \hat{S}_y \text{ always has AFM couplings, they can be made both FM or AFM for } \hat{S}_x \text{ and } \hat{S}_y. \text{ In the main part of Fig.5 we sketch the different accessible models as a function of } \text{t}_y/\text{t}_x \text{ and } \sigma. \text{ This clearly demonstrates that one can realize a whole class of XYZ spin chains by using this method.}

\text{Experimental realization.–} In Ref. \cite{4}, the experimental realization of } p \text{-orbital bosons in an effective } 1D \text{ optical lattice with a life-time of several milliseconds was reported. With an average number of approximately two atoms per site, the atoms could tunnel hundreds of times in the } p \text{ band before decaying. Since the main decay mechanism stems from atom collisions} \cite{12,32}, \text{ an increase of up to a factor of 5 in the lifetime is expected when there is only one atom per site} \cite{4}. \text{ Typical values of the couplings can be estimated from the overlap integrals of neighboring Wannier functions. Considering } ^8\text{Rb atoms, } \lambda_{\text{lat}} = 843 \text{ nm and } \text{v}_x = 30 E_R, \text{ v}_y = 50 E_R \text{ and } \text{v}_z = 60 E_R, \text{ we obtain } J/E_R \sim 0.01 \text{ and the characteristic tunneling time } \tau = \hbar/J \sim 5 \text{ ms. This corresponds to a few dozens of times smaller than the expected lifetimes} \cite{4}, \text{ which should allow for experimental explorations of our results since relaxation typically occurs on a scale less than 10 tunneling times} \cite{30}. \text{ In addition, as pointed out in} \cite{23}, \text{ it is possible to increase the lifetimes even further with the use of external driving.}

\text{A major experimental challenge is to achieve a unit filling of the } p \text{ band. This could be achieved by having an excess number of atoms in the } p \text{ band and then adiabatically opening up the trap} \text{ such that the unit filling is reached. A minority of sites will be populated, however, by immobile } s \text{-orbital atoms. Since the interaction energy between } s \text{- and } p \text{-orbital atoms is higher than between two } p \text{-orbital atoms, processes involving } s \text{-orbital atoms will be suppressed. The presence of atoms in the } s \text{ band corresponds therefore to introducing static disorder in the system} \cite{23}. \text{ This may affect correlations} \cite{13}, \text{ but the qualitative physics will remain unchanged for concentrations close to a unit filling. A more detailed study of this interesting effect is beyond the scope of the present work.}

\text{As a final remark we note that the spin correlations discussed here will emerge at temperatures } k_B T \lesssim J \sim \text{t}_x/t^2/\hat{U} \cite{10}. \text{ In addition, we estimate the required entropy} \cite{38} \text{ by equating the critical temperature } T_c \text{ to the gap between the ground and first excited states in the anti-ferromagnetic phase. Using the energy spectrum obtained from exact diagonalization, } S = (E - F)/T_c \text{ yields}
the entropy per particle \( S/N = 0.06k_B \). Experimentally one has in fact already achieved \( S/N = 0.05k_B \) \cite{53}, which indicates that our results are within experimental reach.

**Conclusions.** We showed that the Mott regime of unit filling of bosonic atoms in the first excited bands of a 2D optical lattice realizes the spin-1/2 XYZ quantum Heisenberg model. We then illustrated the rich physics of this model by examining the phase diagram of the 1D case. Finite size effects relevant to the trapped systems were discussed in detail. We proposed a method to control the strength and relative size of the spin couplings thereby demonstrating how one can realize a whole class of XYZ models. We finally discussed experimental issues related to the realization of this model. We end by noting, that recent experiments reported a \( \sim 99\% \) loading fidelity of bosons into the \( d \)-band \cite{14}, which indeed opens possibilities to probe rich physics beyond spin-1/2 chains.

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SUPPLEMENTARY MATERIAL

DERIVATION OF THE EFFECTIVE SPIN MODEL

We are interested in the strong coupling regime where the system is deep in the Mott insulator phase with a unit filling $n = 1$ of the lattice sites. A natural way of analyzing this limit involves the use of projection operators that divide the Hilbert space of the associated eigenvalue problem in orthogonal subspaces according to site occupations. We define the $\hat{P}$ and $\hat{Q}$ operators that project, respectively, into the subspace of states with a unit occupation and into the perpendicular subspace. They decompose the eigenvalue equation $\hat{H}|\Psi\rangle = E|\Psi\rangle$, with $E$ its associated energy, in the form

$$\left(\hat{Q}\hat{H}\hat{P} + \hat{Q}\hat{H}\hat{P} + \hat{Q}\hat{H}\hat{P} \right)|\Psi\rangle = E\hat{Q}|\Psi\rangle$$

$$\left(\hat{P}\hat{H}\hat{Q} + \hat{P}\hat{H}\hat{Q} + \hat{P}\hat{H}\hat{Q} \right)|\Psi\rangle = E\hat{P}|\Psi\rangle,$$

where $\hat{H}_U$ is the interaction part of the Hamiltonian. Since $\hat{Q}\hat{H}\hat{Q}, \hat{Q}\hat{H}\hat{Q}, \hat{P}\hat{H}\hat{P}, \hat{P}\hat{H}\hat{P}$ and $\hat{P}\hat{H}\hat{P}$ all vanish, it follows that

$$\hat{Q}|\Psi\rangle = -\frac{1}{QHQ - E}\hat{Q}\hat{H}\hat{P}|\Psi\rangle.$$  \hspace{1cm} (7)

By further substitution of Eq. 7 in the eigenvalue equation, we are left with the Hamiltonian which describes the one particle Mott phase of $p$-orbital bosons

$$\hat{H}_{Mott} = -\hat{P}\hat{H}\hat{Q} \frac{1}{QHQ - E} \hat{Q}\hat{H}\hat{P}.$$  \hspace{1cm} (8)

So far this result is exact. It explicitly shows the role of the tunneling in the system, namely of coupling the subspace of states where the sites have unitary occupation with the states that have one site doubly occupied. First, a particle tunnels, say, from the site $j$ to $j + 1$, where it interacts with another particle according to what is described by $\hat{H}_U$. After interaction, one of the particles is brought back to the site $j$, and the final state is again characterized by lattice sites with a unit filling.

Equation 8 is the starting point in the derivation of the effective Hamiltonian describing the $n = 1$ Mott phase of $p$-orbital bosons. The procedure is developed here for an effective 1D system with dynamics along the $x$-axis, but generalization to the 2D lattice is straightforward. Realization of the 1D configuration relies on the adjustment of the lattice parameters, that should contain potential wells much deeper in the $y$ than in the $x$ axis, but in such a way that the quasi degeneracy between the different orbital states is still maintained. This means that $|t_{xy}|, |t_{yx}| \to 0$, and furthermore, due to the strong coupling regime condition, we also have that $U_{\alpha\beta} \gg |t_{xx}|, |t_{yy}|, \alpha, \beta = \{x, y\}$.

Under these assumptions, the operator $1/(\hat{Q}\hat{H}\hat{Q} - E)$ in Eq. 8 can be expanded to second order in $t/U_{\alpha\beta}$ ($\alpha, \beta = \{x, y\}$) in analogy to the customary procedure used for the Hubbard model at half filling. In the tight-binding regime considered here, it is enough to consider the 2-site problem. The basis spanning the subspace of states with unit filling is

$$\mathcal{H}_P = \{|x, x\}, |x, y\}, |y, x\}, |y, y\},$$

where $|\alpha, \beta\rangle$ represents the state with an $p_\alpha$-orbital atom in site $i$ and a $p_\beta$-orbital atom in site $j$. The relevant states for the doubly occupied sites is

$$\mathcal{H}_Q = \{|0, 2x\}, |0, 2y\rangle, |0, xy\rangle,$$

which span the intermediate states of the projection operation. We notice, however, that due to the possibility of transferring population between the different orbital states, the projection of the Hamiltonian in the $\mathcal{H}_Q$ subspace is not diagonal in this basis of intermediate states. This is a peculiarity of the present model and derives entirely from the orbital changing collisions. As a consequence, we compute $(\hat{H}_Q - E)^{-1}$, with $\hat{Q} = \hat{Q}\hat{H}\hat{Q}$ by calculating the projected Hamiltonian in the $\mathcal{H}_Q$ subspace and taking its corresponding inverse. Since $E \approx t^2/U_{\alpha\beta}$, it is justified to ignore $E$ and to consider $(\hat{H}_Q - E)^{-1} \approx \hat{H}_Q^{-1}$. Explicitly,

$$\hat{H}_Q = \begin{pmatrix} U_{xx} & U_{xy} & 0 \\ U_{yx} & U_{yy} & 0 \\ 0 & 0 & 2U_{xy} \end{pmatrix}$$

giving

$$\hat{H}_Q^{-1} = \begin{pmatrix} U_{yy}/U^2 & -U_{xy}/U^2 & 0 \\ -U_{yx}/U^2 & U_{xx}/U^2 & 0 \\ 0 & 0 & U_{xy}/2 \end{pmatrix},$$

where $U^2 \equiv U_{xx}U_{yy} - U_{xy}^2$.

We determine the final form of the effective Hamiltonian by computing the relevant matrix elements of Eq. 8. In the states of the $\mathcal{H}_P$ subspace yield non vanishing contribution.

From states of the type $|\alpha_i, \alpha_j\rangle$

$$\hat{a}_{\alpha_i, \hat{a}_{\alpha_i, \hat{a}_{\alpha_j}}^\dagger \hat{H}_Q^{-1} \hat{a}_{\alpha_i, \hat{a}_{\alpha_j}}^\dagger \hat{H}_Q^{-1} \sqrt{2}|0, 2\alpha_j\rangle$$

$$= \sqrt{2} \hat{a}_{\alpha_i, \hat{a}_{\alpha_j}}^\dagger \hat{H}_Q^{-1} \hat{a}_{\alpha_i, \hat{a}_{\alpha_j}}^\dagger \hat{H}_Q^{-1} \sqrt{2}|0, 2\alpha_j\rangle$$

$$= \frac{U_{\alpha\beta}}{U^2} \hat{a}_{\alpha_i, \hat{a}_{\alpha_j}}^\dagger \hat{H}_Q^{-1} \hat{a}_{\alpha_i, \hat{a}_{\alpha_j}}^\dagger \hat{H}_Q^{-1} \sqrt{2}|0, 2\alpha_j\rangle$$

the effective Hamiltonian acquires a term of the form

$$- \sum_{(i,j)} \sum_{\alpha} \frac{2U_{\alpha\beta}}{U^2} \hat{n}_{\alpha_i, \hat{n}_{\alpha_j}}^\dagger \hat{H}_Q^{-1} \hat{a}_{\alpha_i, \hat{a}_{\alpha_j}}^\dagger \hat{H}_Q^{-1} \sqrt{2}|0, 2\alpha_j\rangle.$$
In these and the following expressions, it is understood that $\beta \neq \alpha$. In the same way, from the states of the type $| \alpha_i, \beta_j \rangle$,
\[
\hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \hat{H}_Q^{-1} \hat{a}_{\beta,j}^\dagger \hat{a}_{\alpha,i} | \alpha_i, \beta_j \rangle = \hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \hat{H}_Q^{-1} | 0, \alpha_j, \beta_j \rangle
\]
\[
= \frac{1}{2U_{xy}} \hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} | 0, \alpha_j, \beta_j \rangle = \frac{1}{2U_{xy}} | \alpha_i, \beta_j \rangle,
\]
corresponding to the operator
\[
- \sum_{(i,j)} \sum_{\alpha} \frac{|t_{ij}|^2}{2U_{xy}} \hat{n}_{\alpha,i} \hat{n}_{\beta,j}.
\]
From the states of the type $| \beta_i, \alpha_j \rangle$ and the following process
\[
\hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \hat{H}_Q^{-1} \hat{a}_{\beta,j} \hat{a}_{\beta,i} | \beta_i, \alpha_j \rangle = \hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \hat{H}_Q^{-1} | 0, \alpha_j, \beta_j \rangle
\]
\[
= \frac{1}{2U_{xy}} \hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} | 0, \alpha_j, \beta_j \rangle = \frac{1}{2U_{xy}} | \alpha_i, \beta_j \rangle,
\]
the Hamiltonian gains a contribution as
\[
- \sum_{(i,j)} \sum_{\alpha} \frac{|t_{ij}|^2}{2U_{xy}} \hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \hat{a}_{\beta,i} \hat{a}_{\beta,j}
\]
Finally, we consider the states of the type $| \beta_i, \beta_j \rangle$,
\[
\hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \hat{H}_Q^{-1} \hat{a}_{\beta,j} \hat{a}_{\beta,i} | \beta_i, \beta_j \rangle = \hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \hat{H}_Q^{-1} \sqrt{2}| 0, 2\beta_j \rangle
\]
\[
= \sqrt{2} \hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \left( \frac{U_{xy}}{U^2} | 0, 2\beta_j \rangle - \frac{1}{2U_{xy}} | 0, 2\alpha_j \rangle \right) = - \frac{2U_{xy}}{U^2} | \alpha_i, \alpha_j \rangle,
\]
that contribute to the effective Hamiltonian with a term that changes the orbital states of the atoms in both sites
\[
\sum_{(i,j)} \sum_{\alpha, \alpha \neq \beta} \frac{2|t_{ij}|^2 U_{xy}}{U^2} \hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \hat{a}_{\beta,i} \hat{a}_{\beta,j}.
\]
The resulting expression for the effective Hamiltonian corresponds thus to
\[
\hat{H}_{\text{Mott}} = - \sum_{(i,j)} \sum_{\alpha} \left( \frac{2|t_{ij}|^2 U_{xy}}{U^2} \hat{n}_{\alpha,i} \hat{n}_{\alpha,j} + \frac{|t_{ij}|^2}{2U_{xy}} \hat{n}_{\alpha,i} \hat{n}_{\beta,j} - \frac{2t_{ij} U_{xy}}{U^2} \hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \hat{a}_{\beta,i} \hat{a}_{\beta,j} + \frac{t_{ij} U_{xy}}{2U^2} \hat{a}_{\alpha,i}^\dagger \hat{a}_{\alpha,j} \hat{a}_{\beta,i} \hat{a}_{\beta,j} \right).
\]
We now use the orbital states to define the Schwinger spin operators
\[
\hat{S}^z = \frac{1}{2} (\hat{a}_{\alpha}^\dagger \hat{a}_{\alpha} - \hat{a}_{\beta}^\dagger \hat{a}_{\beta})
\]
\[
\hat{S}^+ = \hat{S}^x + i\hat{S}^y = \hat{a}_{\alpha}^\dagger \hat{a}_{\beta}
\]
\[
\hat{S}^- = \hat{S}^x - i\hat{S}^y = \hat{a}_{\beta}^\dagger \hat{a}_{\alpha},
\]
and together with the constraint of unit occupation of the lattice sites in the $n = 1$ Mott phase, i.e. $\hat{n}_{x,i} + \hat{n}_{y,j} = 1$, we rewrite Eq. (9) as
\[
\hat{H}_{\text{Mott}} = - \sum_{(i,j)} (J^{zx} \hat{S}_i^z \hat{S}_j^z + J^{xx} \hat{S}_i^x \hat{S}_j^x + J^{yy} \hat{S}_i^y \hat{S}_j^y) - J^z \hat{S}_i^z.
\]
Thus, within the strong coupling regime, the physics of the $n = 1$ Mott insulator phase is equivalent to the spin-1/2 Heisenberg $XYZ$ model in an external field. In terms of the lattice parameters, the expressions for the various couplings follow
\[
J^{xx} = 2 \frac{t_{xy} U_{xy}}{U^2} (1 - 4 \frac{U_{xy}^2}{U^2})
\]
\[
J^{yy} = 2 \frac{t_{xy} U_{xy}}{U^2} (1 + 4 \frac{U_{xy}^2}{U^2})
\]
\[
J^{zz} = 4 \frac{|t_{xy}|^2 U_{xy}^2}{U^2} + 4 \frac{|t_{xy}|^2 U_{xy}}{U^2} - \frac{|t_{xy}|^2}{U_{xy}} - \frac{|t_{xy}|^2}{U_{xy}} + (E_{os}^x - E_{os}^y)
\]
In terms of Eq. (3) of the main text, we can identify $\Delta = -J^{zz}$, $h = -J^x$, and $\gamma = -4U_{xy}^2/U^2$.

**SINGLE SITE ADDRESSING OF ORBITAL STATES**

Single site addressing for the present setup implies selective detection/manipulation of the two orbitals. Since the spin is encoded in external spatial degrees of freedom rather than internal atomic electronic states, methods like those described in Refs. [2] would not work. To control the spatial state of the atoms at single sites we may instead apply methods borrowed from trapped ion physics [3]. Similar methods were already employed in the experiment [4] in order to load bosons from the $s$ band to the $p$ band. Müller et al. of Ref. [3] did not, however, consider single site addressing and more importantly they did not discuss control of the orbital degree of freedom.

Two internal atomic electronic states, e.g. an $F = 1$ and an $F = 2$ state for $^{87}$Rb atoms, are Raman coupled with two lasers. This transition is described by the matrix element $\Omega_{1,2} \langle F = 2 | e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}} | F = 1 \rangle / \delta$ where $\Omega_i$ and $\mathbf{k}_i$ are the laser amplitudes and wave vectors, respectively, and $\delta$ the detuning of the transitions relative to the ancilla electronic state. The spatial dependence of the lasers will induce couplings between vibrational states of the atom, i.e. different bands. The time duration for a $\pi/2$-pulse, for example, can be made very
short by making the effective Rabi frequency \( \Omega = \Omega_1 \Omega_2 / \delta \) large. In particular, this time can be made short on any other time scale in the system and one can approximately consider the system dynamics frozen during the applied pulse. Indeed, the same assumption applies to any single site addressing in optical lattices. Furthermore, by driving resonant two-photon transitions we do not need to worry about accidental degeneracies between other undesired states.

In the Mott insulator phase, as considered in this work, we can approximate single sites with two dimensional harmonic oscillators with frequencies \( \omega_\alpha = \sqrt{2 V_{\alpha} k_\alpha^2 / m} \). The Lamb-Dicke parameters \( \eta_\alpha = k_\alpha \sqrt{\hbar / 2 m \omega_\alpha} \), and within the Lamb-Dicke regime \( \eta_\alpha \ll 1 \) we can neglect multi-phonon transitions. Thus, in one dimension we have three possible transitions: (i) **Carrier transitions** - with no change in the vibrational state, (ii) **red sideband transitions** - which lower the vibrational state with one quantum, and (iii) **blue sideband transitions** - which raise the vibrational state with one quantum respectively, i.e. couple different orbital degree of freedom.

Since the different transitions are not degenerate, it is possible to select single transitions by carefully choosing the frequencies of the lasers. Moreover, considering for example \( k_1 - k_2 = k_x \), i.e. no component in the \( y \) direction, it is possible to only address the \( p_z \)-orbital. Thus, we have a method to singly address the different orbitals. Full control is achieved when every unitary \( \hat{R}_b(\varphi) = e^{-i S^b \varphi} \), where \( \beta = x, y, z \) and \( \varphi \) is an effective rotation angle, can be realized. To start with the simplest example, implementation of \( \hat{R}_z(\varphi) \), we first note that since we are considering the case with a single atom per site \( \hat{S}^z = \hat{S}^+ \hat{S}^- - 1 \) such that it is enough to realize the operation of \( \hat{S}^+ \hat{S}^- \). This is nothing but a phase shift of one of the orbitals. This is most easily done by driving the carrier transition off-resonantly for one of the two orbitals. Since the driving is largely detuned it only results in a Stark shift of the orbital.

The \( \hat{R}_x(\varphi) \) operation is preferably achieved by simultaneously driving off-resonantly the red sidebands of the two orbitals. The \( s \)-band will never get populated due to the large detuning while instead the transition between the two orbitals can be made resonant. More precisely, for the three involved states \( \{ x, 0, 0 \}, \{ 0, y, 0 \}, \{ 0, 0, s \} \) (with the last entry in the ket-vector being the \( s \)-orbital) the resulting coupling Hamiltonian in the rotating wave approximation has the form a \( V \)-coupled system:

\[
\hat{H}_V = \begin{bmatrix}
0 & 0 & \Omega_1 \\
0 & 0 & \Omega_2 \\
\Omega_1 & \Omega_2 & \delta
\end{bmatrix},
\]

where \( \Omega_1 \) and \( \Omega_2 \) have been taken real and for now spatially independent. For \( \delta \gg \Omega_1, \Omega_2 \) we adiabatically eliminate the state \( \{ 0, 0, s \} \) to obtain the desired Hamiltonian generating the rotation \( \hat{R}_x(\varphi) \), namely

\[
\hat{H}_x = \begin{bmatrix}
0 & \Omega \\
\Omega & 0
\end{bmatrix} = \Omega \hat{S}_x.
\]

Note that if the Raman transition between the two orbitals is not resonant, such an action performs a combination of an \( x \)- and \( z \)-rotation. To perform \( y \)-rotations, one could either adjust the phases of the lasers or simply note that \( \hat{R}_y(\varphi) = \hat{R}_z(\pi/4) \hat{R}_y(\varphi) \hat{R}_z(-\pi/4) \). With this at hand, any manipulation of single site spins can be performed. To measure the spin state in a given direction one should combine the rotations with single site resolved fluorescence (i.e. measuring \( \hat{S}_\gamma^\gamma \) \( \hat{S}_\alpha^\alpha \)). More precisely, since the drive laser can couple to the two orbitals individually, one orbital will be transparent to the laser while the other one will show fluorescence. In other words, one measures \( \hat{S}^\gamma \) on a single site. Other directions of the spin are measured in the same way, but after the correct rotation has been implemented to it. Furthermore, with the help of coincident detection it is possible to also extract correlators \( \langle \hat{S}_x^\alpha \hat{S}_z^\beta \rangle \). Since there is a single atom at every site, the “parity problem” \( \hat{S}_x \) of these techniques deriving from photon induced atom-atom collisions is avoided and thereby loss of atoms will not limit our measurement procedure. This summarizes how preparation, manipulations, and detection of single site spins can be performed.

Finally we note that the methods discussed above can be used in a broader context. For example, there is a transition between two \( p \)-orbital atoms (one \( p_x \) and one \( p_y \)-orbital atom) and one \( s \)- and the \( d_{xy} \)-orbital atom. This transition is resonant for any parameters \( V_x \) and \( V_y \) and could in principle cause rapid decay of the \( p \)-band state, or even Rabi-type oscillations between the bands. We note, however, that in the experiment of Ref. \( \hat{S}_x \) the collisional decay mechanism was surprisingly small despite this resonant transition. Nevertheless, one could suppress this resonant transition to increase the life-time even further with the technique described above: By
driving the red sideband for the two $p$-orbital states dispersive, the $s$ and $p$ bands will be repelled and thereby this breaks the resonance condition for $p_x + p_y \rightarrow s + dx_y$.

**EXTERNAL PARAMETER CONTROL**

The ideas of the previous section can also be utilized to change the system parameters. The simplest example is the application of $S^+ S^-$ which implements a shift in the external field $h$. Apart from the external field, it is also desirable to control the coupling in the $z$ component of the spin, $\Delta$, and especially to tune it from ferromagnetic into anti-ferromagnetic.

Using the fact that $|t_x| \gg |t_y|$ we have

$$\Delta \approx -|t_x|^2 \left( \frac{4}{U_{yy} U_{xx} U_{yy} - U_{xy}^2} - \frac{1}{U_{xy}} \right).$$  \hspace{1cm} (13)

This is most easily estimated in the harmonic approximation. Introducing the widths $\sigma_\alpha$ of the orbital wave functions for the spatial directions $\alpha = x, y, z$, in this limit

$$U_{xx} = U_{yy} = 3U_{xy} = \frac{u_0}{\sigma_x \sigma_y \sigma_z},$$  \hspace{1cm} (14)

where $u_0$ is an effective interaction strength (proportional to the $s$-wave scattering length). We notice that even though the use of lattice Wannier functions yields a different ratio between $U_{\alpha \alpha}$ and $U_{\alpha \beta}$ from what is obtained in the harmonic limit [10], it does not affect the qualitative picture of the results discussed here. Using [11] in the expression for $\Delta$ we find

$$\Delta = -|t_x|^2 \frac{3\sigma_x \sigma_y \sigma_z}{2u_0} < 0,$$  \hspace{1cm} (15)

which yields ferromagnetic couplings for the $z$-component of the spin in the harmonic approximation. This is also the case for $\Delta$ computed with numerically obtained Wannier functions for physically relevant parameters, i.e. within the tight-binding and single-band approximations and deep in the insulating phase.

The anti-ferromagnetic regime can be reached, however, again with techniques of trapped ion physics. Instead of changing $h$ by a constant amount in all sites we consider a Stark shift of one of the two orbitals that is spatially dependent. This is nothing but a potential that reshapes the lattice sites differently for the two orbitals. In particular we can imagine squeezing of one orbital in the $y$ direction. Thus, the two Wannier functions $w_x(\vec{r})$ and $w_y(\vec{r})$ have the same widths $\sigma_z$ but different widths $\sigma_y$. This would require driving the carrier transition with a field that has a spatially varying (on the length scale of the $y$ lattice spacing) mode profile. The squeezing in the $y$-direction of one orbital wave function will not affect the tunneling rates $t_x$ and $t_y$, but change both $U_{yy}$ and $U_{xy}$. We have numerically verified that by sufficiently strong squeezing, $\Delta$ becomes negative resulting in anti-ferromagnetic $z$-coupling (see Fig. 2 of the main text). The anti-ferromagnetic coupling can also be obtained by stretching one of the orbitals in the $y$ direction. We note that this manipulation also affects the anisotropy parameter $\gamma$ and therefore slightly shifts the phase boundaries of the phase diagram. However, the qualitative structure is not changed. As a summary, both $h$ and $\Delta$ can be controlled solely by external driving, i.e. without changing the lattice parameters.

**EFFECTIVE MODEL INCLUDING IMPERFECTIONS DUE TO $s$-ORBITAL ATOMS**

Transferring every atom from the $s$ band to the $p$ bands is experimentally challenging. Even though the possibility of loading atoms from the lowest band to the $d$ band with 97-99% fidelity was recently reported [11], in experiments involving the $p$ band approximately 20% of the atoms remain on the lowest band [4,12]. In the experiment reported in Ref. [4], the loading resulted in approximately two $p$-orbital atoms per site. Increasing the lattice amplitude and opening up the trap adiabatically will create an insulating state with unit filling. The $s$-orbital atoms can be considered immobile since the lattice amplitude will typically be around 20 recoil energies. Thus, random sites in the lattice will be populated by $s$-orbital atoms. Energetically it costs more energy to doubly occupy these states with one $s$- and one $p$-orbital atom than those with two $p$-orbital atoms, i.e. $U_{ps} > U_{\alpha \beta}$ where

$$U_{ps} = U_0 \int d\vec{r} |w_{is\alpha}^*(\vec{r})|^2 |w_{i\beta}^*(\vec{r})|^2$$  \hspace{1cm} (16)

and $w_{is\alpha}^*(\vec{r})$ is the $s$-orbital Wannier function at site $i$.

Repeated experimental realizations will prepare different random configurations as illustrated in Fig. 4. The various configurations are presumably equally probable. If a single realization is not determined from any measurement, the state will be a statistical average over all

![FIG. 4. (Color online) Schematic plot of three random experimental realization of the insulating state; yellow balls represent $s$-orbital atoms and blue ones $p$-orbital atoms.](image-url)
possible configurations. That is, we integrate out the
degrees of freedom of the $s$-band atoms (i.e. average over
all possible configurations constrained to a fixed ratio of
$s$-orbital atoms).

Let us consider two neighboring sites $i$ and $j$, one with
a $p$-orbital atom and one with an $s$-orbital atom. Since we
have neglected tunneling of $s$-orbital atoms, the only non-
vvanishing terms within second order perturbation theory
are
\[
\frac{-t^2}{U_{ps}} \hat{a}_{\alpha,i} \hat{a}_{\alpha,j} \hat{a}_{\alpha,i} \hat{a}_{s,j} = -\frac{t^2}{U_{ps}} \hat{n}_{\alpha,i},
\]  
(17)
where $\alpha = (x, y)$, $\hat{a}_{s,j}$ is the annihilation operator for an
$s$-orbital atom at site $j$ and we have used the fact that
$n_{s,j} = 1$. Now, since $t_x \neq t_y$ it follows that the presence
of an $s$-orbital shifts the external field $h = J_z$ locally.
Thus, the presence of $s$-orbital atoms will be manifest in
local fluctuations in the external field, i.e. we obtain an
XYZ chain with disorder.

\[
\hat{H}_{\text{Mott}}^{\text{(dis)}} = - \sum_{(i,j)} \left( J_{zz} \hat{S}_i^z \hat{S}_j^z + J_{xx} \hat{S}_i^x \hat{S}_j^x + J_{yy} \hat{S}_i^y \hat{S}_j^y \right) - \sum_i J_i \hat{S}_i^z.
\]

For few atoms on the lowest band, this effect should not
qualitatively change the results presented in this paper.
We expect then that the disorder is irrelevant [13]. For
a larger fraction of $s$-orbital atoms one could expect the
disorder to become relevant and localized phases to ap-
pear [13]. This interesting topic is, however, outside the
scope of the present paper.

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[1] F. Essler, H. Frahm, F. Gohmann, A. Klumper and V. E. Korepin, The One-Dimensional Hubbard Model, Cambridge University Press, Cambridge, (2005).
[2] C. Weitenberg et al., Nature 471, 319 (2011); T. Fukuhara et al, arXiv:1305.6559
[3] D. Leibfried et al., Rev. Mod. Phys. 75 281 (2003).
[4] T. Müller et al., Phys. Rev. Lett. 99, 200405 (2007).
[5] D. Wang et al., Phys. Rev. A 77, 053808 (2008).
[6] B. W. Shore, Manipulating Quantum Structures Using Laser Pulses, (Cambridge University Press, Cambridge, 2011).
[7] S. Haroche and J.-M. Raimond, Exploring the Quantum: Atoms, Cavities, and Photons, (Oxford University Press, Oxford, 2006).
[8] M. Knap et al., arXiv:1307.0006
[9] J. Pietraszewicz et. al, arXiv:1303.5223v2 (2013).
[10] A. Collin et al., Phys. Rev. A 81, 023605 (2010); T. Sowiński et al, arXiv:1304.6290
[11] Zhai, Yueyang et. al., arXiv:1306.3313 (2013).
[12] G. Wirth et al., Nature phys. 7, 147 (2011); P. Soltan-Panahi et al., Nature Phys. 8, 71 (2012).
[13] C. A. Doty and D. S. Fisher, Phys. Rev. B 45, 2167 (1992).