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Perspectives of optical lattices with state-dependent tunneling in approaching quantum magnetism in the presence of the external harmonic trapping potential

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ABSTRACT

We study theoretically potential advantages of two-component mixtures in optical lattices with state-dependent tunneling for approaching long-range-order phases and detecting easy-axis antiferromagnetic correlations. While we do not find additional advantages of mixtures with large hopping imbalance for approaching quantum magnetism in a harmonic trap, it is shown that a nonzero difference in hopping amplitudes remains highly important for a proper symmetry breaking in the pseudospin space for the single-site-resolution imaging and can be advantageously used for a significant increase of the signal-to-noise ratio and thus detecting long-range easy-axis antiferromagnetic correlations in the corresponding experiments.

1. Introduction

Due to a recent experimental realization of state-dependent optical lattices for two-component mixtures of ultracold ^{40}K atoms with the magnetic-field-gradient technique and low heating rate [1] it is now much easier to access and study asymmetric lattice models without a necessity of using heteronuclear fermionic mixtures (e.g., ^{6}Li–^{40}K) or long-living metastable electronic states of the same fermionic isotope (e.g., $3P_0$ state of ^{173}Yb). Among potential applications of this technique one can suggest approaching long-range magnetically-ordered states [2]. It is known that quantum magnetism in ultracold fermionic mixtures is one of major experimental challenges nowadays and a significant progress already has been made in this direction. In particular, short-range antiferromagnetic (AFM) correlations were effectively measured [3,4] and their unique dynamics in the presence of the tunable lattice geometry was observed recently [5].

Considering two-component fermionic mixtures from the point of view of theoretical models and spin symmetries, optical lattices with state-dependent (i.e., spin-dependent) hopping amplitudes effectively break the initial continuous SU(2) symmetry of the system described by the Hubbard model towards $\mathrm{U}(1)\times\mathbb{Z}_2$, where $\mathbb{Z}_2$ is a discrete reflection symmetry along the easy axis. The easy-axis direction is important, in particular, for the experimental detection of AFM correlations based on the Bragg spectroscopy analysis [4,6] and on the quantum-gas-microscope technique (QGMT). Despite the fact that temperatures and entropies[1] achieved with recent successful developments of the QGMT for fermionic mixtures [7–12] are high to observe long-range magnetic correlations, thus further optimizations and improvements in cooling protocols are required, it is important to study characteristic dependencies of these thermodynamic quantities on other system parameters (including different symmetries of magnetic ground states), thus determine the most optimal regime for *in situ* imaging of the long-range AFM correlations.

2. Theoretical description

Ultracold two-component fermionic mixtures in optical lattices with a sufficiently strong lattice potential, $V_{\mathrm{lat}} \gtrsim 5E_{\mathrm{r}}$, where E_{r} is

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[1] The entropy per particle is more crucial quantity in the context of ultracold-atom experiments, since the system does not exchange heat with environment and its parameters can be changed adiabatically.

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the recoil energy of atoms, are well described by the single-band Hubbard model with the Hamiltonian

$$\hat{\mathcal{H}} = -\sum_{\langle ij\rangle}\sum_{\sigma} t_\sigma (\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}) + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + V\sum_i (r_i/a)^2\hat{n}_i - \sum_i\sum_\sigma \mu_\sigma \hat{n}_{i\sigma}, \quad (1)$$

where t_σ is the hopping amplitude of fermionic species in a particular atomic hyperfine state that we denote by the spin-1/2 index $\sigma = \{\uparrow, \downarrow\}$, thus we consider here and below two atomic components as pseudospins, $\hat{c}^\dagger_{i\sigma}$ ($\hat{c}_{i\sigma}$) is the corresponding creation (annihilation) operator of atoms at the lattice site i, the notation $\langle ij\rangle$ indicates a summation over nearest-neighbor sites, and U is the magnitude of the on-site repulsive ($U > 0$) interaction of the two different species with corresponding densities $\hat{n}_{i\uparrow}$ and $\hat{n}_{i\downarrow}$ ($\hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$). In the third term, V is the amplitude of the external harmonic potential, r_i is the distance from the lattice site i to the trap center, and a is the lattice spacing. In the last term, μ_σ is the chemical potential that determines the total number of atoms of each spin component in the system.

Note that the asymmetric Hubbard model (1) (it can also be recognized as the extended Falicov–Kimball model for spinless fermions in the context of solid-state materials [13]) can be transformed to an anisotropic Heisenberg (or a spin-1/2 XXZ) model in the limit of $U/t_\sigma \gg 1$ and $n_i \approx 1$. The latter is described by the Hamiltonian

$$\hat{\mathcal{H}}_{XXZ} = J_\parallel \sum_{\langle ij\rangle} \hat{S}^Z_i \hat{S}^Z_j + J_\perp \sum_{\langle ij\rangle} (\hat{S}^X_i \hat{S}^X_j + \hat{S}^Y_i \hat{S}^Y_j) - \Delta\mu \sum_i \hat{S}^Z_i, \quad (2)$$

with the constants $J_\parallel = 2(t^2_\uparrow + t^2_\downarrow)/U$, $J_\perp = 4t_\uparrow t_\downarrow/U$, $\Delta\mu = (\mu_\uparrow - \mu_\downarrow)$, and the spin-1/2 operators $\hat{S}^R_i = \frac{1}{2}\hat{c}^\dagger_{i\alpha}\sigma^R_{\alpha\beta}\hat{c}_{i\beta}$ (here and below we use units $\hbar = 1$), where σ^R are the Pauli matrices ($R = \{X, Y, Z\}$). Hence, we see that the presence of hopping imbalance ($t_\uparrow \neq t_\downarrow$) results in $J_\parallel > J_\perp$, thus breaks the SU(2) rotational spin symmetry towards $\mathrm{U}(1)\times\mathbb{Z}_2$, where the discrete symmetry $\mathbb{Z}_2$ can be broken either spontaneously by long-range AFM ordering along the Z axis or by the chemical potential difference $\Delta\mu \neq 0$ that plays a role of the external magnetic field favoring the ferromagnetic configuration along the same axis. Naturally, with an increase of $\Delta\mu$ at the fixed asymmetry in hopping amplitudes the easy-axis (Ising-type) AFM configuration becomes less and less energetically favorable, thus a transition to another AFM-ordered easy-plane (canted) many-body state becomes possible (see Refs. [14–16] for more details).

Therefore, to avoid a potential competition between different types of AFM ordering that can also result in a significant suppression of critical temperatures, in the original model (1) we consider chemical potentials the same for both spin components (i.e., $\mu_\uparrow = \mu_\downarrow \equiv \mu$). Note that asymmetric hopping amplitudes $t_\uparrow \neq t_\downarrow$ together with $\mu_\uparrow = \mu_\downarrow$ result in a nonzero polarization, i.e. not equal total numbers of particles in two spin states ($N_\uparrow \neq N_\downarrow$), of the trapped system [2,16], but this condition is the most optimal for the easy-axis AFM ground state of the model (1) at half filling (e.g., at $\mu = U/2$ and $r_i = 0$), as discussed above.

Below, we consider a three-dimensional optical lattice setup with the Hubbard parameters entering Eq. (1) that are set close to the experimental values [1]. In particular, we focus on two opposite limits: (i) zero (or very small) hopping imbalance $t_\uparrow = t_\downarrow = t$ and (ii) large hopping imbalance (e.g., $t_\uparrow = 0.54t$ and $t_\downarrow = 0.06t$). According to Ref. [1], both cases can be effectively realized by the magnetic-field-gradient technique with a high level of control.

Our theoretical analysis is based on the dynamical mean-field theory (DMFT) [17] with the exact diagonalization solver [18] and the number of orbitals $n_s = 5$ per each spin component in the corresponding Anderson impurity model. Since we are interested mostly in the easy-axis observables, in DMFT it is enough to account for the standard hybridization terms between the impurity and the bath [18]. The corresponding Anderson parameters of the impurity model are found iteratively till the convergence based on DMFT self-consistency conditions [17] is reached. For the given values of the Hubbard parameters our approach allows to calculate the local observables, such as expectation values of the density of particles of any spin component, the double and the hole occupancy, as well as the fluctuations of the particle number on a particular lattice site.

To account for the inhomogeneity effects produced by the external trap, we use DMFT with the local density approximation (LDA + DMFT). Note that LDA does not account for the proximity effects close to the phase boundaries, however in the cases under study these effects do not play a crucial role leading only to minor corrections. Within LDA we obtain the local observables at the specific point r of the trap from the condition $\mu(r) = \mu_0 - V(r/a)^2$, where μ_0 is the chemical potential in the trap center that for the fixed values of the Hubbard parameters defines also the total number of particles in the system.

From the converged solutions of LDA + DMFT on different lattice sites (i.e., with different r) one can analyze the dependence of the local observables on the distance r (see also Ref. [19] for more details). In particular, by combining the results with the Maxwell relation $\partial s/\partial\mu = \partial n/\partial T$ we obtain the entropy per lattice site at the particular point r_0 of the trap (for simplicity, we use the units of $k_B = 1$ and $a = 1$ below)

$$s(r_0) = 2V \int_{r_0}^{R_{\max}} \frac{\partial n(r, U, T)}{\partial T} r dr, \quad (3)$$

where the cut-off distance $R_{\max}$ is determined from the condition $n(R_{\max}, U, T) = 0$.

A subsequent integration of the entropy and density distributions in the trap determine the total entropy S and the total number of particles N in the system (here and below we assume the axial-symmetric three-dimensional setup)

$$S = \int_0^{R_{\max}} s(r) 4\pi r^2 dr, \quad N = \int_0^{R_{\max}} n(r) 4\pi r^2 dr. \quad (4)$$

Both quantities, S and N, can be considered as the preserved numbers in the experiment (and, in particular, during the lattice ramp) that allows to access the initial values for the entropy and temperature. Note that, alternatively, one can also introduce an additional term corresponding to the amount of entropy per particle Δs that is added to the system due to uncontrolled heating processes during the lattice ramp, as it was done in Ref. [3]. Below, for simplicity and consistency reasons, we consider that the change in system parameters can be performed adiabatically ($\Delta s = 0$).

In order to determine the initial temperature $\widetilde{T}$ in the system that is necessary for observations of the many-body quantum phases under study we use the expression for the entropy of the Fermi gas under assumption of a moderate scattering length a_s ($k_\mathrm{F}|a_s| < 1/2$) [20]

$$S \approx N\pi^2 \widetilde{T}/T_\mathrm{F}. \quad (5)$$

Eqs. (3)–(5) allow to set a direct correspondence between thermodynamic quantities before and after the lattice ramp. Therefore, the problem can be effectively solved under assumption of adiabaticity of the ramp process.