Enhancing quantum order with fermions by increasing species degeneracy

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Enhancing quantum order with fermions by increasing species degeneracy

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One of the challenges for fermionic cold atom experiments in optical lattices is to cool the systems to low enough temperature that they can form quantum degenerate ordered phases. In particular, there has been significant work in trying to find the antiferromagnetic phase transition of the Hubbard model in three dimensions, without success. Here, we attack this problem from a different angle by enhancing the ordering temperature via an increase in the degeneracy of the atomic species trapped in the optical lattice. In addition to developing the general theory, we also discuss some potential systems where one might be able to achieve these results experimentally.

I. INTRODUCTION

While the off-diagonal long-range order in cold bosonic atomic gases has been observed many years ago, quantum magnetism in fermionic gases is still a challenge for experimentalists. Despite the possibility to control the interaction between spin states of atoms in an optical lattice [1], the temperatures required to obtain magnetic ordering remain lower than those achievable with current techniques. Therefore, it is easier to demonstrate the presence of magnetic correlations, before the true long-range magnetic order is established. Using the spin-sensitive Bragg scattering of light, antiferromagnetic correlations in a two-spin-component Fermi gas, magnetic correlations have been observed at a temperature 40% higher than the putative temperature for the transition to the antiferromagnetic state in three dimensions [2]. In this experiment, the two lowest hyperfine ground states of fermionic ^{6}Li atoms in a simple cubic optical lattice were labeled as spin-up and spin-down states. The repulsive interaction between atoms in these states was controlled by a magnetic Feshbach resonance. Since the magnetic superexchange interaction is given by $J = 4t^2/U$, the experiment controlled the value of J and in a particular regime, it measured antiferromagnetic correlations as extracted from the spin structure factor. Very recently it was demonstrated that spin (and charge) correlations can be detected also with the help of site-resolved imaging. In Refs. [3–5] quantum gas microscopy was used to determine spatial correlations for fermionic atoms in a two-dimensional optical lattice. While there is no phase transition in 2D, the measurements have shown an increase of the correlation length as the temperature was lowered. Similar antiferromagnetic correlations extending up to three lattice sites have also been observed in a 1D system [6].

In this work, we study the simplest many-body model that has a nonzero phase transition in two dimensions. This would be the Ising model [7] for a spin system. But we examine instead its fermionic analog, the Falicov-Kimball (FK) model [8], which also displays a nonzero transition temperature in two dimensions and behaves Ising-like when the interaction strength becomes large. This system can be easily simulated with mixtures of cold atoms on optical lattices, because it involves mobile fermions interacting with localized fermions [9]. One simply needs to have the hopping of the two atomic species to be drastically different. The simplest case of one trapped atomic state for each of the fermionic species maps onto the spinless version of the FK model. This model has been solved exactly in infinite dimensions via dynamical mean-field theory (DMFT) [10, 11] and numerically in two dimensions with Monte Carlo (MC) [12].

The atomic lithium-ytterbium mixture is an example of a system with an extreme mass imbalance and a controllable interspecies interaction [13]. When confined in an optical lattice, it can be well described by the FK model. Refs. [14–20] present other such atomic mixture systems. But mass imbalance is not the only way to realize the FK model. Recently a versatile method for creating widely tunable state-dependent lattices was demonstrated by the Esslinger group [21]. If the renormalized hopping amplitude of one of the spin states is tuned to be close to zero, such a system can also be described by the FK model. Independent control of lattice depths has also been demonstrated in a bosonic mixture of rubidium and potassium up to the localization transition for rubidum in Ref. [22].

The remainder of the paper is organized as follows. In Sec. II, we provide the formalism for our calculatons, followed by the results in Sec. III. Conclusions follow in Sec. IV.

II. FORMALISM

Our motivation for this work stems from the DMFT solution to the problem. There, one can derive a condition for the transition to an ordered phase with a checkerboard pattern [10, 11], which takes the form $1 = \sum_n \gamma(n)$, with the sum running over all integers [which label fermionic Matsubara frequencies $i\omega_n = \pi i(2n+1)T$, with T the temperature]. The function $\gamma(n)$ is a complicated function that is constructed from the mobile fermion Green's function, its self-energy, the on-site interation between the localized and mobile fermions U and the density of the localized fermions w_1. The important point to note, is that if we increase the degeneracy of the mobile fermions (while enforcing that they do not interact with themselves), then the T_c equation is modified by $\gamma(n) \to N\gamma(n)$, where N is the number of degenerate states for the mobile fermions [11]. Since one can immediately show that $\sum_n \gamma(n) \to C/T$ for $T \to 0$ and $\sum_n \gamma(n) \to C'/T^4$ for $T \to \infty$ [10], we expect that the transition temperature for the degenerate system will initially grow linearly in N and then turn over to a slower increase, proportional to $N^{1/4}$ for larger N. It is the rapid growth with degeneracy for small N, which makes these effects so spectacular. (These ideas are further supported by the observation that increasing species degeneracy *lowers* the final temperature after the optical lattice is ramped up in alkaline-earth systems [23])

The argument that T_c grows linearly with the degeneracy at low temperature can be made more general. We start with the Hamiltonian for the FK model on a lattice Λ that has $|\Lambda|$ lattice sites. The Hamiltonian for a given configuration of the heavy atoms $\{w\}$ is

$$\begin{aligned}\mathcal{H}(\{w\}) &= -t\sum_{\langle ij\rangle}\sum_{\sigma=1}^{N} c_{i\sigma}^\dagger c_{i\sigma} + U\sum_i\sum_{\sigma=1}^{N} n_{i\sigma}w_i \\ &= \sum_{\sigma=1}^{N}\mathcal{H}_\sigma(\{w\}),\end{aligned} \tag{1}$$

where σ denotes the N different "flavors" of the mobile fermions and $w_i = 1$ or 0, denotes whether site i has a localized fermion on it, or not, respectively (the localized fermions continue to be spinless). The hopping matrix is chosen to be nonzero only for nearest neighbors, and we set $t = 1$ as our energy unit (we also set $k_B = 1$). We define $E_i \equiv \varepsilon_i - \mu$, with μ the chemical potential and $\{\varepsilon_i\}$ the set of (degenerate) eigenvalues of $\mathcal{H}_\sigma(\{w\})$, which is independent of the specific value of σ because the mobile fermions are noninteracting amongst themselves, and they share the same interaction with the localized fermions. Here, the index i runs over $i = 1, \ldots, |\Lambda|$ (we will be working on a square lattice of edge L which then has $|\Lambda| = L \times L$).

The corresponding grand partition function is given by

$$\mathcal{Z} = \sum_{\{w\}}\prod_{i=1}^{|\Lambda|}\left[1 + e^{-\beta E_i(\{w\})}\right]^N, \tag{2}$$

with $\beta = 1/T$ the inverse temperature. Introducing the free energy $\mathcal{F}$, Eq. (2) can be rewritten as

$$\mathcal{Z} = \sum_{\{w\}} e^{-\beta\mathcal{F}(\{w\})}, \tag{3}$$

where

$$\begin{aligned}\mathcal{F}(\{w\}) &= -\frac{N}{\beta}\sum_i \ln\left[1 + e^{-\beta E_i(\{w\})}\right] \\ &= N\sum_i E_i\theta\left[-E_i(\{w\})\right] \\ &\quad - \frac{N}{\beta}\sum_i \ln\left[1 + e^{-\beta|E_i(\{w\})|}\right],\end{aligned} \tag{4}$$

and $\theta(\ldots)$ is the Heaviside unit step function. In the low-temperature limit the second term on the RHS vanishes. Inserting the limiting form of $\mathcal{F}$ into Eq. (3) yields

$$\mathcal{Z} = \sum_{\{w\}} e^{-\beta N\sum_i E_i\theta[-E_i(\{w\})]}. \tag{5}$$

Note, that this result can be recognized to be the condition for the filling of mobile fermions into the Fermi sea determined by the bandstructure corresponding to the particular configuration of the localized fermions, as given by the configuration $\{w\}$. Since, in the low-temperature limit $\mathcal{F}$ does not depend on temperature, the partition function depends on temperature only through the term βN. This means that the thermodynamics of the system depends only on the ratio T/N, with initial corrections expected to be small as T rises (because they will be proportional to T/T_F with some suitably large Fermi temperature T_F). As a result the critical temperature T_c in the low-temperature limit will necessarily increase linearly with increasing degeneracy N. This is an exact result, independent of the details of the lattice or the dimensionality—it only requires there to be a phase transition.

There are two assumptions that went into this anaylsis, which turn out not to hold when we actually calculate the maximal T_c as a function of N. First, the lowest T_c values are not so low, so the linear regime fairly rapidly crosses over to a slower increasing behavior and second, the interaction value $U_{\max}(N)$, where the maximal $T_{c,\max}(N)$ occurs, actually changes with N (see the inset in Fig. 2), so the arguments about the precise functional dependence of the $T_{c,\max}(N)$ on N turns out not to hold in the actual data; our arguments assumed we compared systems with the same U. The first effect is to reduce how T_c increases with N, while the second enhances how T_c increases with N.

Corrections to the linear dependence of T_c on N come mostly from states close to the Fermi level [$E_i \approx 0$, see the second term in the RHS of Eq. (4)]. Therefore, we can expect that the linear section of the $T_c(N)$ curve can be longer for bipartite lattices for which the density of states is reduced close to the Fermi energy, e.g., for

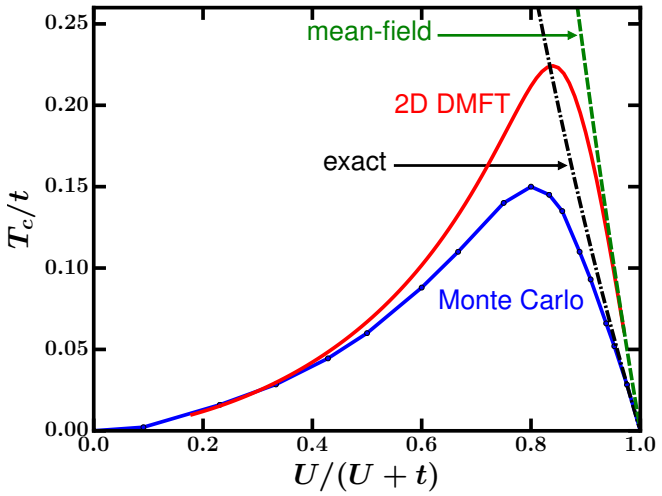

FIG. 1. (Color on-line) Comparison of the 2D DMFT (solid red line) and MC (blue dots, connected with a solid line as a guide to the eye) critical temperatures to the checkerboard density wave at half filling for both species on a square lattice with $N = 1$. The lines marked as "Ising mean-field" (green) and "Ising exact" (black) show the critical temperatures for the corresponding Ising model, which become exact for the respective theories when $U \to \infty$.

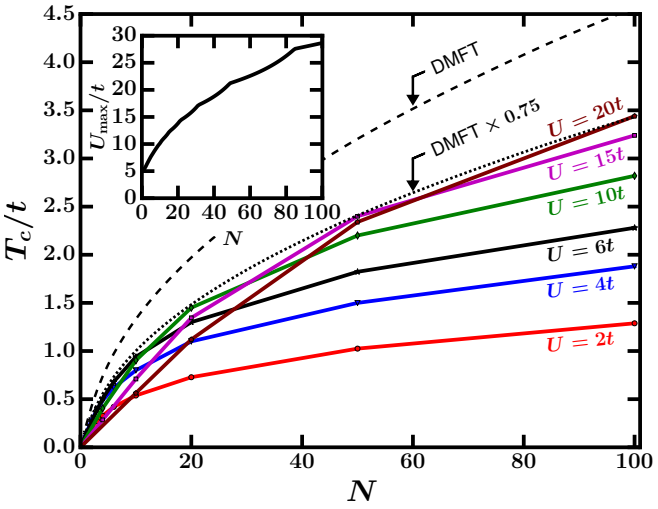

FIG. 2. (Color on-line.) The maximal critical temperature T_c plotted as a function of mobile fermion degeneracy N (as calculated with MC). The dashed line shows the corresponding DMFT T_c calculated at $U = U_{\max}$(DMFT). The solid lines show MC T_c's for different values of U. The black dotted line shows T_c(DMFT) $\times$ 0.75, which agrees well with nearly all the MC results. In the inset, $U_{\max}$(DMFT) is plotted as a function of degeneracy N, indicating it changes significantly with N.

a hexagonal lattice. Also in 3D, where there is no Van Hove singularity (the singularity for the square lattice is reduced by the interaction with the heavy atoms) the linear part can persist to even higher temperatures.

III. RESULTS

In Fig. 1, we plot the transition temperature to the checkerboard density wave on a square lattice with $N = 1$. The top curve is for the DMFT approximation, while the bottom curve is for the exact MC results. Note that the interaction strength for the peak of the curve lies in the range of $U \approx 4 - 5$ with the maximal U value slightly higher for DMFT versus MC. The DMFT results are semiquantitative, and clearly overestimate the T_c, but the overall error is not that large.

As N increases, we find that the maximum T_c increases as does the value of the interaction strength where the $T_c(U)$ curve is maximized. The full curve out to $N = 100$ is plotted in Fig. 2. The DMFT results are calculated for each N by first finding the interaction strength at the maximum of the T_c curve. For the MC results, we work with fixed U, varying N and then constructing the "maximal hull" of the data. It turns out that these MC results are nearly perfectly fit to the DMFT results when the latter are renormalized by a factor of 0.75. The DMFT curve initially grows linearly with N, but then settles into an increase that grows proportional to $\sqrt{N - 1.7}$, which is in between our linear and 0.25 power results, as we expected, due to the fact that $U_{\max}$ increases with N.

We find the enhancement of the maximal T_c for higher N versus $N = 1$, given by $T_{c,\max}(N)/T_{c,\max}(1)$ satisfies: 1.98 (MC, $N = 2$), 1.899 (DMFT, N=2); 2.84 (MC, $N = 3$), 2.651 (DMFT, $N = 3$); and 3.60 (MC, $N = 4$), 3.287 (DMFT, $N = 4$). Since the maximal T_c(DMFT) for the FK model is about one half the maximal T_c(DMFT) for the corresponding Hubbard model, we need to be able to have a degeneracy of $N \geq 3$ before this effect will have a high enough T_c that it can reach current experimentally accessible values for the 3D case.

In the above, we have demonstrated that by increasing degeneracy one can increase the critical temperature. The question remains as to whether this increased T_c also corresponds to an increased entropy per particle at the transition point. In MC, it is quite difficult to calculate the entropy in a reliable way because it requires integrating from infinite temperature down to the temperatue of interest. Since we have already shown good agreement between the MC and DMFT results (up to a numerical factor), we calculate the entropy S only within DMFT. This should be a good estimate of whether the entropy is increasing or decreasing with the number of mobile fermions N. The entropy for the FK model is given by [11]

$$\begin{aligned} S_{\rm tot}(T) &= -N \int d\varepsilon \, \{ f(\varepsilon) \ln f(\varepsilon) \\ &\quad + [1 - f(\varepsilon)] \ln [1 - f(\varepsilon)] \} \, \rho(\varepsilon) \\ &\quad - w_1 \ln w_1 - (1 - w_1) \ln (1 - w_1) \\ &= S_{\rm mob}(T) + S_{\rm loc}(T), \end{aligned} \tag{6}$$

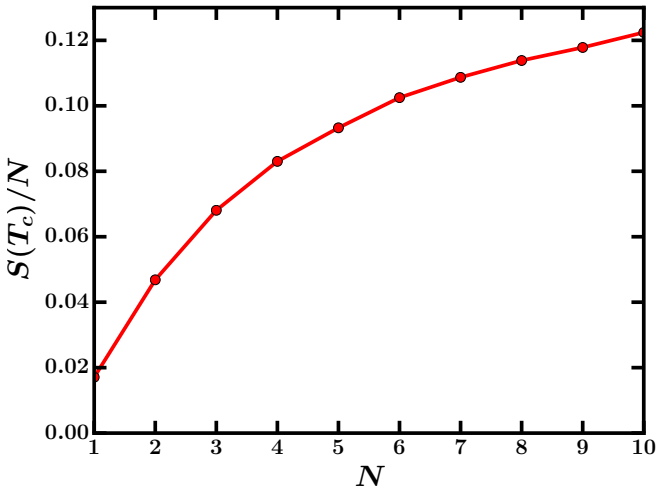

FIG. 3. (Color on-line) The entropy of the mobile fermions $S_{\rm mob}(T_c)/N$ *per mobile fermion* at the critical temperature T_c calculated in DMFT as a function of the mobile fermion degeneracy N.

where $f(\varepsilon) = 1/[1 + \exp(\varepsilon/T)]$ is the Fermi–Dirac distribution function and $\rho(\varepsilon)$ is the local density of states of the mobile fermions. The third line in Eq. (6) is the entropy of the localized particles $S_{\rm loc}(T)$ and since it depends only on their concentration w_1, and that concentration is fixed in the disordered state, it provides a constant shift to the overall entropy, which is independent of N (and given by $S_{\rm loc}(T) = \ln 2$). Hence, it is the integral, which is the entropy *per mobile fermion* at T_c which will determine whether the transition temperature is easier to reach for higher degeneracy. As shown in Fig. 3, this is clearly the case. We have $S_{\rm mob}(T_c)/N$ initially increasing linearly with N and then tailing off as N increases.

We focus the remainder of this article on discussing possible experimental realizations for such higher degeneracy mixtures. The FK model has zero interaction between the mobile fermions. One can argue, on rather general grounds, that the modification of T_c due to a nonzero intraspecies interaction u will have corrections to T_c of order u^2. Hence, if u is small, the effect we discuss here should continue to hold, with only slight reductions. This allows us to formulate our search criterion for physical systems that will show this degenerate species effect.

In searching for appropriate mixtures, we want to find systems that (i) can have a degeneracy of three or more for the light fermionic species, (ii) have a similar interspecies interaction U between the mobile and localized fermions, which will be tuned either via an interspecies Feshbach resonance, or via the depth of the trapping potential for the light species; and (iii) have a small intraspecies interaction u between the mobile fermions. We also note, that as long as the localized particle is nondegenerate, then it can actually be either Bose or Fermi, since its statistics does not enter the analysis because it does not move. (However, if the heavy particle is a boson, we do need its intraspecies interaction to be large and positive, so it generically forms a Mott insulator with at most one particle per site and it does not Bose condense on the lattice.)

We start with examining some prototypical systems which have already been demonstrated to be trapped on optical lattices. The first choice to examine is mixtures of ^{40}K (mobile fermion) and ^{87}Rb (localized boson) [24]. If we could trap the $m_F = -5/2, -7/2$, and $-9/2$ states of K, we would have an $N = 3$ mixture. This system is nice, in the sense that it has a tunable interspecies interaction via a Feshbach resonance, and the intraspecies interactions for K have a scattering length on the order of 100 a_0 (in some cases one of the pairs can be tuned to zero scattering length). The challenge is that the Rb-Rb interaction is too small (on the order of 100 a_0), and is not tunable, which would make it difficult to satisfy the required conditions for this effect. If we instead try ^{133}Cs (localized boson) [25], we find that the Cs-Cs interaction is large, with a scattering length near 2000 a_0 at $B \approx 260$ G, but the interspecies interaction is small (≈ -40 a_0) and not simultaneously tunable for all three K species.

Moving on to other possibilities, if we use mixtures of ^{171}Yb or ^{173}Yb (mobile fermion) [26, 27] and ^{133}Cs (localized boson) [28, 29], we only have a degeneracy of $N = 2$ for ^{171}Yb, even though its intraspecies scattering is small, while for ^{173}Yb the intraspecies scattering length is ≈ 200 a_0, which is still viable, given the potentially large Cs-Cs scattering length, but it would require a tunable Cs-Yb scattering length that is large, and although this has not yet been measured, we do not anticipate that there is any reason why it should be particularly large. If we tried Rb as the localized boson [30], it suffers from the same issues as with K-Rb—namely, the Rb-Rb scattering is too small.

Using ^{6}Li as the mobile fermion appears attractive [31, 32]. However, the interspecies scattering length is only small for low fields, and when a mixture is formed from the $N = 3$ trappable states, at least one intraspecies interaction will be large (although the other two can be close to zero). So, this case is suboptimal.

Next, we consider mixtures of ^{87}Sr (light fermion) which has up to $N = 10$ and a Sr-Sr scattering length on the order of 100 a_0 [33, 34]. If we use Cs as the (localized boson), then if the Cs-Cs scattering length can be set to the order of a few 1000 a_0, and the Sr-Cs scattering length is on the order of 500 a_0, then this system might work to illustrate this degenerate species effect, and it has the potential to be spectacularly large.

The remaining choices that might be workable seem to be longshots, but cannot yet be ruled out because we do not have enough information about their interspecies interactions. We discuss some of these possibilities next.

^{43}Ca is a fermion with a nuclear spin of 7/2 [35, 36], ^{25}Mg is a fermion with a nuclear spin of 5/2 [37], Ba has two spin 3/2 fermionic species [38], and ^{201}Hg is also spin

3/2 [39]. It is unknown what the intraspecies interactions are amongst these different spin states, how many can be trapped, and what their interspecies interactions are with potential heavy particles. So they all are possible, but at this stage quite difficult systems to work with. Finally, there are all of the magnetic-dipole systems, like Er [40, 41], Dy [42, 43], and Cr [44–46]. These systems often have chaotic intraspecies interactions due to a huge number of resonances, but they might show some small interactions at low fields, and hence may also be viable candidates for the light fermions.

IV. CONCLUSIONS

In summary, we have illustrated the idea that by enhancing species degeneracy, one can enhance T_c for fermionic neutral atoms trapped on optical lattices such that their T_c to an ordered state can be raised high enough that they would be accessible to explore with current experimental technology in cooling. This idea comes at this problem from a different angle than the many different cooling strategies that have been proposed, and could provide the ability to truly study spatially ordered quantum phases. The challenge is to find the right mixture of atoms where this effect can be fully exploited. We have examined a number of possible experimental systems, with Yb-Cs ($N = 2$) and Sr-Cs ($N = 10$) mixtures as the most promising, but it is clear the experiments will be challenging to carry out. Other experimental systems are more speculative, because the interspecies interactions are not yet known, but there are likely to be some additional experimental systems that can be tried for this enhancement effect on the ordering T_c.

We want to end by commenting that similar work has examined $SU(N)$ symmetric Hubbard models. The repulsive case actually sees a decrease in the antiferromagnetic T_c with increasing N [47], while the attractive case sees an enhancement similar to what we see for the density-wave instability [48], but we do not know of any large $N > 3$ systems with attractive interactions. Furthermore, there are challenges with finding atomic systems with a small enough U value (for large N), since a maximal hopping is required to have an accurate single-band description. So it will be more difficult to attain the Hubbard-like system than the Falicov-Kimball-like system that we propose.

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