Relaxation of Fermionic Excitations in a Strongly Attractive Fermi Gas in an Optical Lattice

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We theoretically study the relaxation of high energy single particle excitations into molecules in a system of attractive fermions in an optical lattice, both in the superfluid and the normal phase. In a system characterized by an interaction scale U and a tunneling rate t, we show that the relaxation rate scales as $\sim Ct\exp[-\alpha U^2/t^2\ln(U/t)]$ in the large U/t limit. We obtain explicit expressions for the temperature and density dependent exponent α, both in the low temperature superfluid phase and the high temperature phase with pairing but no coherence between the molecules. We find that the relaxation rate decreases both with temperature and deviation of the fermion density from half filling. We show that quasiparticle and phase degrees of freedom are effectively decoupled within experimental time scales allowing for observation of ordered states even at high total energy of the system.

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Ultracold atoms on optical lattices [1] can be used for simulating strongly interacting quantum many-body systems [2–4] with tunable Hamiltonian parameters. Although the main focus of cold atom experiments has been to obtain the equilibrium phase diagram of various models, ultracold atomic systems also provide a unique platform to study the intrinsic nonequilibrium dynamics of strongly interacting many-body systems. Their low energy scales and decoupling from external environment lead to long nonequilibrium time scales over which the system can be followed without ultrafast probes.

The issues of nonequilibrium relaxation dynamics are becoming an important consideration for the state-of-the-art cold atom experiments [5–11] as well as recent pump-probe experiments with electron systems [12]. The tunability of Hamiltonian parameters to access strongly interacting regimes is one of the central attractive features of cold atoms. However, an implied assumption in connecting the results obtained on optical lattices to the physics of condensed matter systems is that the atoms on the optical lattice have achieved thermal equilibrium at low temperatures after tuning the parameters. Hence, it is important to understand the relaxation dynamics and associated equilibration time scales [13–20] of these systems.

The attractive Hubbard model on optical lattices is a lattice implementation [21] of BCS–Bose-Einstein condensation crossover [1,22], which is a paradigm for understanding strongly interacting superfluids. The strong coupling physics is governed by formation of tightly bound molecules which undergo Bose-Einstein condensation at low temperatures. In this Letter, we study the relaxation dynamics of the attractive Hubbard model in the strong coupling limit, where most fermions are paired to form molecules. We focus on the decay of excess unpaired fermions present in the system (either due to an external drive like lattice modulation or due to sweeping of the Hamiltonian parameters) to form molecules. For these high energy excitations, energy conservation requirements lead to a very slow decay rate that scales superexponentially with the ratio of the interaction strength to the bandwidth of the system. Thus, at strong coupling, the fermionic quasiparticles and the motion of the bosonic molecules effectively decouple in the nonequilibrium dynamics of the system. This leads to the possibility of observing ordered states in these systems even at a high total energy of the system. Using a particle-hole transform to map this problem to that of spin mediated decay of double occupancies in the repulsive Hubbard model, we compute the decay rate both in the low temperature superfluid phase and in the high temperature paired phase for arbitrary filling fractions in the lattice. We find that the decay rate decreases both with temperature and with the deviation of the fermion density from half filling on either side. We discuss the implications of these results for maintaining adiabaticity during a sweep of Hamiltonian parameters.

We consider the one band attractive Hubbard model for fermions on a 3D cubic optical lattice

$$H = -t\sum_{\langle ij\rangle} c^{\dagger}_{i\sigma}c_{j\sigma} - U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \tag{1}$$

where t is the tunneling matrix and U is the local attraction between the fermions. For large U/t, the fermions are paired to form molecules with a large binding energy $\sim U$ which undergo Bose condensation at a temperature $\sim J = 4t^2/U$, controlled by the kinetic energy scale of the molecules. We consider two temperature regimes: (a) the low temperature ($T \ll J$) superfluid phase, where the molecules are Bose condensed, and (b) the high

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temperature ($T \sim t \gg J$) phase where the molecules do not have phase coherence, and calculate the decay rate of unpaired fermions in both phases.

The formation of a molecule from two unpaired fermions is forbidden unless the binding energy of the molecule ($\sim U$) is carried off by other excitations in the system. There are two different modes of excitations where this excess energy can be dumped: (a) kinetic energy of other unpaired fermions (with scale $\sim t$) and (b) kinetic energy of the molecules (with scale $\sim J$). In this Letter, we assume (b) is dominant, which limits the density of unpaired fermions $\rho_{\rm ex} < J/t \sim t/U$. To absorb the binding energy $n \sim U/J \sim U^2/t^2$ molecular excitations have to be created. The corresponding matrix element is

$$M \sim t\frac{t}{J}\frac{t}{2J}\cdots\frac{t}{nJ} = \frac{t}{n!}\left[\frac{t}{J}\right]^n \sim t\exp\left[-\alpha\frac{U^2}{t^2}\ln\frac{U}{t}\right],$$

where, to leading order, we have used $n! \sim n^n$ for large n and $nJ = U$ to write the final form. Here α is a temperature and density dependent constant which depends on the details of the process. Within Fermi's golden rule, the decay rate $\Gamma \sim M^2$ and thus decreases superexponentially with U/t.

To obtain a physical picture of the decay process, it is instructive to use a particle-hole transformation [23] which maps the attractive (negative U) Hubbard model to a repulsive (positive U) Hubbard model. The attractive model with zero magnetization at any density is equivalent to the repulsive model at half filling (one particle per site) with a finite magnetization proportional to the deviation of the fermion density in the attractive model from half filling, i.e., $m = (1/2)(1-\rho)$, where ρ is the fermion density in the attractive Hubbard model. Under this transformation, molecule formation is mapped to the formation of a Mott insulator, and the unpaired fermions are equivalent to the high energy double occupancy (doublon) hole excitation, with the binding energy of the molecules playing the role of the Mott gap. At half filling, the low energy physics of the repulsive Hubbard model reduces to an antiferromagnetic Heisenberg model which exhibits a canted antiferromagnetic (CAFM) order in its ground state in the presence of finite magnetization. This spin ordering is equivalent to the emergence of superfluidity in the attractive model with the kinetic energy of the molecules playing the role of spin wave fluctuations. The equivalence of the relevant quantities under the mapping is shown in Table. I. Here, we will use the language of the spin model to look at quantitative estimates of the decay time scales.

Decay in the superfluid phase.—The superfluid phase of the attractive fermions is represented by the CAFM phase for the spins in the repulsive model. As a hole (doublon) hops in the background of a Mott insulator with CAFM ordering [shown in Fig. 1(a)] from a site i to a site j, it disrupts the spin texture and creates purely ferromagnetic bonds between nearest neighbors, each of which gains an energy of $(Jx/2)$, where $x = 1 - 4m^2$ is proportional to the antiferromagnetic component of the spin order. Hopping of the hole along a path creates ferromagnetic bonds in the directions transverse to this path, thus creating a domain wall in the system, as shown in Figs. 1(b) and 1(c). In a cubic lattice each hop creates $z - 2 = 4$ broken bonds. In order to absorb the energy U, the hole needs to traverse a path of length $n = 2U/[(z-2)Jx]$. Within Fermi's golden rule, the decay rate is

TABLE I. Equivalence of different quantities under the mapping between the attractive and the repulsive Hubbard model.

Attractive model	Repulsive model
Unpaired fermions	Doublon hole pairs
Binding energy	Mott gap
Deviation from half filling	Magnetization
Superfluid order	Canted antiferromagnetic order
Kinetic energy of molecules	Superexchange energy

$$\Gamma = 2\pi\rho_{\rm ex}\nu(n)|M_{fi}(n)|^2, \tag{2}$$

where $\rho_{\rm ex}$ is the density of holes (or equivalently of unpaired fermion excitations), and $M_{fi}(n)$ is the matrix element connecting the initial state with a doublon and a hole to the final state with a domain wall of length n

$$M_{fi}(n) = \frac{t}{n!}\left[\frac{2t}{(z-2)Jx}\right]^n \sim t(t/U)^n. \tag{3}$$

Here, $\nu(n)$ is proportional to the number of self-avoiding paths of length n connecting the doublon and the hole

$$\nu(n) = \int d^3r \frac{2n}{(z-2)Jx} S(n, r)G(r), \tag{4}$$

where $S(n, r)$ is the number of self-avoiding paths of length n connecting two points at a distance r, and $G(r)$ is the dimensionless doublon-hole-pair correlation function.

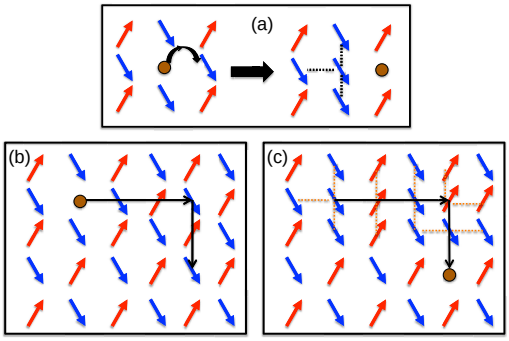

FIG. 1 (color online). Hopping of a hole in a canted antiferromagnetic background. (a) A single hop moves back one spin, creating broken bonds shown by dashed lines. (b), (c) Configurations before and after multiple hops of a hole. The solid line denotes the trajectory of the hole, while the dashed lines in (c) shows the broken bonds.

We assume that the doublons and holes are uncorrelated, i.e., $G(r) = 1$. This assumption is valid in the limit of low density of doublons, precisely the limit we are interested in. Then, $\nu(n) = \frac{2n}{(z-2)Jx} S(n)$, where $S(n)$, the total number of self-avoiding paths of size n. $S(n) \sim g^n n^k$ for large n, and the constants $g = 4.68$ [24] and $k = 1/6$ [25] for a cubic lattice have previously been computed in the context of polymer physics. Using these, we obtain the relaxation rate of doublons in the repulsive Hubbard model or equivalently the relaxation rate of the unpaired fermions in the attractive Hubbard model,

$$\Gamma \sim \frac{t\rho_{\rm ex}}{\sqrt{g}} \left(\frac{g}{8x}\right)^{2+k} \exp\left[-\left(\frac{U^2}{4xt^2} - 3 - 2k\right) \ln\left(\frac{U}{\sqrt{g}t}\right)\right].$$

Note that, for the attractive case, $x = 2\rho - \rho^2$ is a measure of the filling factor which vanishes both at $\rho = 0$ (empty band) and $\rho = 2$ (completely filled band) and attains its maximum value at half filling ($\rho = 1$). The low temperature decay rate, plotted for different densities in Fig. 2(a), shows the expected superexponential scaling with U/t. As we move away from half filling, the energy lost in a single hop decreases, and longer domain walls are required to absorb the excess energy, leading to a slower decay rate.

Decay in the high temperature normal state.—We now consider the decay of the single particle excitations in the high temperature phase ($T \sim t \gg J$), where the fermions are still paired into molecules but there is no superfluidity.

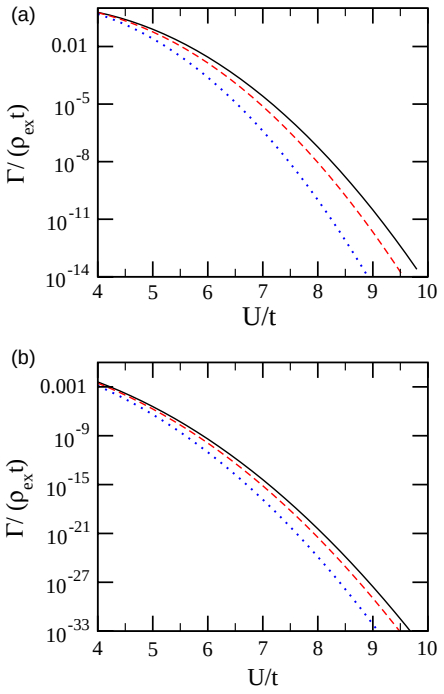

FIG. 2 (color online). The decay rate of unpaired fermions (a) in the superfluid phase and (b) in the high temperature normal state as a function of U/t for different fermion densities: (i) half filling (solid black line), (ii) $\rho_f = 0.7$ (red dashed line), and (iii) $\rho_f = 0.5$ (blue dotted line).

In terms of the spin model, this regime corresponds to a completely spin disordered phase with no spatial or dynamic correlations. The single site Hilbert space can be occupied by an $\uparrow$ spin with probability $1/2 + m$ or by a down spin with probability $1/2 - m$ (we are working at fixed magnetization).

As in the low temperature phase, the motion of holes (doublons) pushes the spins along the trajectory by one site. However, the energy lost in a given hop now depends on the configuration of the neighboring spins along the path. Since there is no spatial correlation between the spins, the energy lost in each hop can be treated as an independent random variable which takes the values $Jr/2$ ($r = -4, -3, \ldots, 4$), with the probability $P(r) = (a/b)^{r/2} \sum_{i=04}^{4-r} C_{i4} C_{i+r} a^i b^{4-i}$, where nC_k are the binomial coefficients, $a = (1/2 - m)^2$, and $b = (1/2 + m)^2$. The mean energy lost in each hop is 0, while the variance of the distribution is given by $J^2 x/2$. By central limit theorem, the total energy lost in l steps is a Gaussian random variable with zero mean and a variance $lJ^2x/2$,

$$P(E, l) = \frac{1}{\sqrt{\pi x l J}} \exp[-E^2/(J^2 l x)]. \quad (5)$$

Since the doublon needs to lose an energy U to decay, one must now average over decay processes from paths of length $l \geq n$ with the probability distribution $P(U, l)$. The square of the matrix element for a process involving l hops is given by $M^2 \sim t^2(t^2/\epsilon_1^2)(t^2/\epsilon_2^2) \cdots (t^2/\epsilon_l^2) \sim t^2(2t^2/lJ^2x)^l$, where ϵ_i is the energy lost after i steps and, to leading order, we have replaced ϵ_i^2 by its average value $iJ^2x/2$. To see the scaling in t/U, we note that the Gaussian probability distribution $P(U, l)$ has a width $l \sim 2U^2/(xJ^2)$, and hence the square of the matrix element scales as $t^2(t/U)^{2l}$. Then, summing over all paths with $l > n$,

$$\Gamma \sim 2\pi t^2 \rho_{\rm ex} \int_n^\infty dl g^l l^k P(U, l) \left(\frac{t}{U}\right)^{2l}. \quad (6)$$

The high temperature decay rate, plotted as a function of U/t in Fig. 2(b), is orders of magnitude smaller than the low temperature decay rate. To understand this, note that the motion of the high energy pair can both excite and deexcite low energy modes in the background system. At zero temperature, these low energy modes are unoccupied and the motion of the high energy pair then leads to excitation of these modes. As temperature increases, the occupation probability of the low energy modes increases and the motion of the high energy pair randomly leads to excitation and deexcitation of these modes. Thus the high energy pair loses its energy more efficiently at lower temperatures and decays faster.

Adiabaticity and sweep rates.—In cold atom experiments the strongly interacting regime of model systems is accessed by tuning the Hamiltonian parameters at a finite rate, which is limited by the lifetime of the atoms in the

trap. The tuning process should be adiabatic to remain in the interesting low temperature regime for the system. Since the microscopic relaxation processes determine the time scale for equilibration, the relaxation time scales, along with experimental sweep rates, would determine the limits of adiabaticity in these experiments. We now make these ideas more precise by looking at the constraints due to the slow decay of unpaired fermions.

In the large U/t limit of the attractive Hubbard model, the unpaired fermion density in equilibrium $\rho_{\mathrm{ex}} \sim \exp(-U/T)$, where T is the temperature of the system. We assume an adiabatic sweep of U/t at a constant rate $\gamma = (\dot{U}/t)$ and try to assess the limits where adiabaticity fails. At low temperatures, the entropy mainly comes from the kinetic motion of the molecules; so for a constant entropy process, $T/J = \lambda/4$ or $U/T = U^2/(\lambda t^2)$ along the sweep, where λ is a constant. Now, adiabaticity will be maintained in the regime where

$$\dot{\rho}_{\mathrm{ex}} = -(\dot{U}/T)\rho_{\mathrm{ex}} = -\frac{2}{\lambda}\frac{U}{t}\gamma\rho_{\mathrm{ex}} \leq -\Gamma(U/t)\rho_{\mathrm{ex}}. \quad (7)$$

As the microscopic rate Γ goes down superexponentially with U/t, this criterion would set an upper limit of $(U/t)_{\mathrm{max}}(\gamma)$, which is the maximum U/t up to which the system remains adiabatic with a sweep rate γ. Our analysis shows that it is extremely difficult to keep the system fully adiabatic in the strong coupling limit when either the tunneling or the interaction is being changed, as the relaxation time scale of unpaired atoms (or doublons for the repulsive case) can be anomalously long. Experimentally this long time scale should manifest itself as a saturation in the molecular fraction with the saturation occurring at smaller values of U/t for faster sweep rates.

At the same time, if relaxation of unpaired fermions is very slow (longer then the time scale of experimental measurements), then they can be considered as infinitely long lived and completely decoupled from other degrees of freedom in the system like the phase fluctuations of the superfluid order parameter. Similarly, in the repulsive Hubbard model, if the goal is to observe antiferromagnetism, one may worry that a small number of doublons can release enough energy to destroy magnetic order. If the doublons are very long lived, there will be a long time scale over which one can neglect relaxation of doublons and analyze the quasiequilibrium with "unbreakable" doublons. Thus, within experimental time scales, there is an effective spin-charge decoupling which makes it easier to observe spin ordering even in the presence of high energy charge excitations. The idea of realizing metastable states with long-lived doublons has also been discussed in the context of the η-paired state in the repulsive Hubbard model [26].

We have studied the decay of unpaired fermions in an attractive Hubbard model. We have shown that the decay rate scales as $\sim Ct\exp[-\alpha U^2/t^2\ln(U/t)]$ for large U/t and computed the exponent α both at low temperatures (superfluid phase) and high temperatures (normal state of molecules). We find the decay rate decreases with increase in both temperature and the deviation of the fermion density from half filling. We also discussed implications of our analysis for realizing many-body states in optical lattices. The downside of the long relaxation times is that it is difficult to change parameters of the system fully adiabatically. The upside of slow relaxation is that there is effective decoupling of different degrees of freedom. So, for example, one may be able to achieve equilibration of phase (magnetic) degrees of freedom, even when there is a finite density of unrelaxed single fermions (doublons).

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