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

Rajdeep Sensarma\(^1\), David Pekker\(^2\), Ana Maria Rey\(^3\), Mikhail D. Lukin\(^4\) and Eugene Demler\(^4\)
\(^1\) Condensed Matter Theory Center, University of Maryland, College Park, MD 20742, USA.
\(^2\) Department of Physics, California Institute of Technology, Pasadena, CA 91125, USA.
\(^3\) JILA, NIST and Department of Physics, University of Colorado, Boulder, CO 80309, USA.
\(^4\) Physics Department, Harvard University, Cambridge, MA 02138, USA.

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 \(\sim Ct\exp(-\alpha U^2/t^2)\) in the large \(U/t\) limit. We obtain explicit expressions for the exponent \(\alpha\), 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 timescales allowing for observation of ordered states even at high total energy of the system.

PACS numbers:

Ultracold atoms on optical lattices\(^1\) can be used for simulating strongly interacting quantum many body systems\(^2\)\(^-\)\(^4\) with tunable Hamiltonian parameters like interaction strength. Although the main focus of cold atom experiments has been to obtain the equilibrium phase diagram of various models, ultracold atomic systems also provide an unique platform to study the intrinsic non-equilibrium dynamics of strongly interacting many body systems. They are almost completely decoupled from external environment and their low energy-scales lead to long non-equilibrium time-scales over which it is possible to follow the system without ultra-fast probes.

The issues of non-equilibrium 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 timescales\(^13\)\(^-\)\(^20\) of these systems.

The attractive (or negative \(U\)) Hubbard model on optical lattices is a lattice implementation\(^21\) of BCS-BEC crossover\(^1\)\(^-\)\(^22\), which is a paradigm for understanding strongly interacting superfluids. At weak coupling, this model exhibits BCS superfluidity with an exponentially small critical temperature. At strong coupling, the physics is governed by formation of tightly bound molecules which undergo Bose-Einstein condensation at low temperatures. In this Letter, we consider the relaxation dynamics of the attractive Hubbard model in a cubic lattice 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 super-exponentially with the ratio of the interaction strength to the bandwidth 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

\[
H = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}
\]

where \(t\) is the tunneling matrix and \(U\) is the local attraction between the fermions. In the strong coupling limit (large \(U/t\)), the fermions are paired to form tightly bound bosonic 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. The separation of the energy scales \(U \gg t \gg J\) allows us to consider two different temperature regimes where most of the fermions are paired into molecules: (a) the low temperature \((T \ll J)\) superfluid phase, where the molecules are Bose condensed and (b) the high temperature \((T \sim J)\) phase where the molecules do not have phase coherence. We calculate the decay rate of unpaired fermions in these two regimes.

The simplest process, where two unpaired fermions hop on top of each other to form a molecule, 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 a scale \(\sim t\)) and (b) kinetic energy of the molecules, with a scale \(\sim J\). In this paper, we assume the later process is dominant, which limits
TABLE I: Equivalence of different quantities under the mapping between the attractive and the repulsive Hubbard model

<table>
<thead>
<tr>
<th>Attractive Model</th>
<th>Repulsive Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unpaired Fermions</td>
<td>Doublon hole pairs</td>
</tr>
<tr>
<td>Binding Energy</td>
<td>Mott gap</td>
</tr>
<tr>
<td>Deviation from half-filling</td>
<td>Magnetization</td>
</tr>
<tr>
<td>Superfluid order</td>
<td>Canted antiferromagnetic order</td>
</tr>
<tr>
<td>K. E. of Molecules</td>
<td>Superexchange energy</td>
</tr>
</tbody>
</table>

the density of unpaired fermions to be less than $J/t \sim t/U$. Since the kinetic energy has an energy scale of $J = 4t^2/U$, $n \sim U/J \sim U^2/t^2$ molecular excitations have to be created to release the binding energy. The matrix element for this process, within $n^{th}$ order perturbation theory, is given by

$$M \sim t^n \left( \frac{t}{J} \right)^n \sim C t \exp \left[ -\alpha \frac{U^2}{t^2} \ln(U/t) \right]$$

(2)

where we have used $n! = n^n$ for large $n$ and $nJ = U$ to write the final form. The decay rate $\Gamma \sim M^2$ thus decreases super-exponentially 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 (equal up and down spin densities) 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 $\rho$ 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 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 timescales.

Decay in the superfluid phase: The superfluid phase of the attractive fermions is represented by the canted antiferromagnetic phase for the spins in the repulsive model. As a hole hops in the background of a Mott insulator with canted spin ordering (shown in Fig. 1(a)) from a site $i$ to a neighboring site $j$, it pushes back the spin on the site $j$ to the site $i$. This 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 Fig. 1(b) and (c). It is to be noted that hopping of doublons in this background also leads to a similar process. In a cubic lattice each hop creates $z-2 = 4$ broken bonds. So, in order to accommodate an energy $U$ and decay, the hole (doublon) need to traverse a path of length $n = 2U/[(z-2)Jx]$. Within Fermi’s golden rule, the decay rate is given by

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

(3)

where $\rho_{ex}$ 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 $n$ given by

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

(4)

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

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

(5)

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. We assume that the doublons and holes are uncorrelated, i.e.
The attractive Hubbard model is studied, finally obtaining the relaxation rate of unpaired fermions in the superfluid phase. This has previously been computed in the context of polymer physics. Using an approximate expression for the pair distribution function, it is independent of \( r \), or \( G(r) = 1 \). This assumption is valid in the limit of low density of doublons, precisely the limit we are interested in. Then \( \nu(n) = \left( \frac{2n}{(2-\rho^2)} \right) S(n) \), where \( S(n) \) is the total number of self-avoiding paths of size \( n \), scales as \( \sim g^n n^k \) for large \( n \). The constants \( g = 4.68 \) [24] and \( k = 1/6 \) [25] for a cubic lattice has previously been computed in the context of polymer physics. Using these, finally obtain the relaxation rate of unpaired fermions in the attractive Hubbard model

\[
\Gamma \sim \frac{t \rho_{ex}}{\sqrt{\rho}} \left( \frac{g}{8x} \right)^{2+k} \exp \left[ -\left( \frac{U^2}{4x^2t^2} - 3 - 2k \right) \ln \left( \frac{U}{\sqrt{8t}} \right) \right]. \tag{6}
\]

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 as a function of \( U/t \) for different densities in Fig. 2, show the expected super-exponential scaling. As we move away from half-filling (with increasing magnetization), 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. 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 \( P(r) = (a/b)^{r/2} \sum_{i=0}^{4-r} 4C_i 4C_{i+r} a^{i-b^{r-i}} \), where \( nC_k \) is the Binomial co-efficient, \( a = (1/2 - m)^2 \) and \( b = (1/2 + m)^2 \). The mean energy lost in each hop is 0, while the variance of the distribution is given by \( J^2 x/2 \). The total energy lost in \( l \) steps is thus a Gaussian random variable with zero mean and a variance \( l J^2 x/2 \).

\[
P(E, l) = \frac{1}{\sqrt{\pi xlJ}} \exp[-E^2/(J^2 xl)] \tag{7}
\]

Since the doubloon 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 \( M^2 \sim l^2 (t^2/c_2^2)(t^2/c_2^2) \cdots (t^2/c_2^2) \sim l^2 (2t^2/J^2 l^2)^3 \), where \( c_i \) is the energy lost after \( i \) steps and, to leading order, we have replaced \( c_i^3 \) by its average value \( i J^2 x/2 \). To see the scaling in \( t/U \), we note that the Gaussian probability distribution \( P(U, l) \) would be cut-off at a typical lengthscale \( l \sim 2U^2/(xJ^2) \), and hence the square of the matrix element scales as \( t^2 (t/U)^2l \). Then, summing over all paths with \( l > n \)

\[
\Gamma \sim 2\pi t^2 \rho_{ex} \int_0^\infty dl \frac{1}{2} t^k P(U, l) \left( \frac{t}{U} \right)^{2l} \tag{8}
\]

The high temperature decay rate, plotted as a function of \( U/t \) in Fig. 3 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 de-excite 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 de-excitation 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 needs to be adiabatic in order to remain in the interesting low temperature regime for the system. Since the microscopic relaxation processes determine the timescale for equilibration, it is expected that the relaxation timescales, 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 (or equivalently doublon-hole pairs).

We consider a system of attractive fermions at low enough temperatures so that most of the fermions are paired to form molecules. In the large $U/t$ limit, the density of unpaired fermions in equilibrium $\rho_{ex} \sim \exp(-U/T)$, where $T$ is the temperature of the system. We assume an adiabatic sweep of $U/t$ at a constant rate $\gamma = (U/t)$ and try to assess the limits where adiabaticity fails. At these low temperatures, almost all the entropy comes from the kinetic motion of the molecules; so for a constant entropy process, we can assume $T/J = \lambda/4$ or $U/T = U^2/(\lambda t^2)$ along the sweep, where $\lambda$ is a constant. Now, adiabaticity will be maintained in the regime where

$$\rho_{ex} = -(U/T)\rho_{ex} = -\frac{2}{\lambda t} \gamma \rho_{ex} < -\Gamma(U/t)\rho_{ex}$$

where $\gamma$ is the experimental sweep rate. As the microscopic rate $\Gamma$ goes down super-exponentially with $U/t$, this criterion would set an upper limit of $(U/t)_{max}(\gamma)$, which is the maximum $U/t$ upto which the system remains adiabatic when the parameters are swept with a rate $\gamma$. 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 are being changed, as the relaxation timescale of unpaired atoms (or doublons for the repulsive case) can be anomalously long. Experimentally this long timescale 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 timescale 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 timescale over which one can neglect relaxation of doublons and analyze the quasi-equilibrium with "unbreakable" doublons. Thus, within experimental timescales, 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 $\eta$-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 $\sim C t \exp(-\alpha U^2/t^2)$ for large $U/t$ and computed the exponent $\alpha$ 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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