Pairing Gap and In-Gap Excitations in Trapped Fermionic Superfluids

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We consider trapped atomic Fermi gases with Feshbach-resonance enhanced interactions in pseudogap and superfluid temperatures. We calculate the spectrum of RF(or laser)-excitations for transitions that transfer atoms out of the superfluid state. The spectrum displays the pairing gap and also the contribution of unpaired atoms, i.e. in-gap excitations. The results support the conclusion that a superfluid, where pairing is a many-body effect, was observed in recent experiments on RF spectroscopy of the pairing gap.
Fermionic superfluidity and superconductivity appear in several systems in nature such as metals, cuprates and helium. In the limit of weak interparticle interaction, the Bardeen-Schrieffer-Cooper (BCS) theory of superconductivity has been successful in explaining the observed phenomena as a Bose-Einstein Condensation (BEC) of weakly bound momentum-space pairs. In the limit of strong interactions, spatially small, strongly bound pairs are formed and undergo BEC. The intriguing question about the nature of the crossover from BCS pairing to BEC of dimers was theoretically addressed in 1980 (1, 2) and is closely related to uncovering the nature of high-temperature superconductivity. Trapped fermionic atoms offer a system where the crossover can be scanned by tuning the inter-particle scattering length using Feshbach resonances (3-7). At the crossover region, the scattering length diverges and a universal behaviour, independent of any length scale, is expected. The system is also genuinely mesoscopic due to the trapping potential for the atoms. Here we consider spectroscopic signatures of pairing in these systems at the onset of the superfluid transition and show that the mesoscopic nature of the system leads to pronounced signatures from unpaired atoms which can also be understood as in-gap excitations. The results are in agreement with the experimental results in (8).

The single-particle excitation spectrum of a fermionic superfluid is expected to show an energy gap. A spectroscopic method for observing the excitation gap in atomic Fermi gases has been proposed (9-11). RF-spectroscopy has been used for observing mean fields (12, 13) and, very recently, the excitation gap (8). Laser- or RF-fields are used for transferring atoms out of the superfluid state to a normal one. The superfluid state originates from the pairing of atoms in two different internal states, say \( |1\rangle \) and \( |2\rangle \). The field drives a transition from \( |2\rangle \) to a third state \( |3\rangle \); atoms in state \( |3\rangle \) are not paired i.e. they are in the normal state. The idea is closely related to observing the superconductor - normal metal current in metals and, similarly, it reflects the density of states and displays the excitation gap. Only, in this case, the superfluid-normal interface is realized by internal states of the atom, not by a spatial boundary.
The response, in the case of atoms, is qualitatively different from that of metals due to the exact momentum conservation in atomic transitions driven by homogeneous fields. Here, we calculate the response of this process, that is, the spectrum as a function of the detuning of the RF-field, taking into account the mesoscopic nature of the sample i.e. the trapping potential. This leads to pronounced signatures which can be utilized in confirming the onset of the excitation gap and the superfluid transition.

In the high-$T_c$ region of the BEC-BCS crossover, the BCS theory, in its simplest form, is expected to be incapable of describing the effects of strong interactions, such as the formation of a pseudogap. In atomic Fermi gases, the vicinity of the Feshbach resonance is associated with strong interactions, and preformed pairs causing a pseudogap may exist even above the critical temperature. The excitation gap, therefore, has contributions both from the superfluid gap ($\Delta_{sf}$) and the pseudogap ($\Delta_{pg}$). The many-body state is affected also by the existence of the molecular bound state which actually causes the Feshbach resonance phenomenon. These issues are considered in recent theory work on resonance superfluidity (14-17). We use such an approach for calculating the equilibrium state of the system (18).

The interaction with the (RF/laser) field is introduced as a perturbation and the response is calculated to the second order in the perturbation Hamiltonian. This corresponds to a Fermi Golden rule -type of derivation of the spectrum and allows a treatment of the complex many-body state with reasonable accuracy. The Hamiltonian $H_T$, describing the effect of the field, couples the states $|2\rangle$ and $|3\rangle$ (18). The offset from the resonance of the transition between $|2\rangle$ and $|3\rangle$ is given by the RF-field detuning $\delta = E_{RF} - (E_3 - E_2)$, where $E_{RF}$ and $E_3$, $E_2$ are the energies of the RF-photon and of the states $|3\rangle$ and $|2\rangle$, respectively. The spectrum is obtained from the response $I(\delta) = \langle N_3 \rangle$, where $N_3$ is the number of atoms in state $|3\rangle$, by neglecting terms of higher than second order in $H_T$ in the derivation (18). In the case of metals, such quantity would give the current $I(V)$, where $V$ is voltage, over the superconductor - normal
metal tunneling junction.

Trapped atomic gases have an inhomogeneous density distribution \( n(r) \) and therefore a spatially varying superfluid order parameter is expected. We treat the problem in the local density approximation, that is, we solve the equilibrium state by including \( n(r) \) given by the Thomas-Fermi distribution as a position dependent parameter (18, 19). Fig. 1 presents the position dependence of the atom density and the superfluid gap. This shows that only the atoms in the middle of the trap are condensed. Fig. 2 shows the fraction of condensed atoms and the mean (averaged over \( r \)) superfluid gap and pseudogap as functions of temperature. The parameters used in calculating the results in Figs. 1–3 correspond to the experiments in Fig. 3 of (8) and are given in (18).

The spectra \( I(\delta) \) at different temperatures are plotted in Fig. 3. The peak at the zero detuning, \( \delta = 0 \), originates from free (unpaired) atoms. Another peak, shifted right from the zero, appears with decreasing temperature. The shift reflects the excitation gap, i.e. the energy needed for breaking a pair. The free-atom peak gradually vanishes when the temperature is lowered and also the atoms at the borders of the trap become paired. The disappearance of the free atom peak shows that the border atoms have reached the pseudogap regime (18) and that the atoms in the middle of the trap are well below the superfluid transition temperature (20). We have neglected the effect of the mean (Hartree-Fock) field energy shifts (18), as they appear absent in the experiments (8, 13).

In a corresponding spatially homogeneous system, instead of the free-atom peak at zero detuning, a quasiparticle peak, shifted left from the zero, appears at high temperatures (11). The shift is to the left, to the opposite direction than that of the pair-peak, because thermal quasiparticles of the superfluid already possess the excess gap energy, that is, energy is gained in the RF-transfer process (21). As Fig. 3 shows, such quasiparticle peaks appearing in a homogeneous system are now shadowed by trapping effects and the free-atom peak. The unpaired atoms
in Fig. 3 can, however, be understood as in-gap excitations or quasiparticles. Instead of the
local density approximation, inhomogenous superfluids can be described by the Bogoliubov-deGennes equations. Solving the equations in a trap geometry (10, 22) results in in-gap excitations whose energies lie below the maximum (at the point of highest density) gap energy. The wave-functions of these excitations are located at the edges of the trap; they correspond to the free atoms at the borders of the trap in the local density treatment. The free atoms in Fig. 3 and observed in (8) can thus be understood as in-gap excitations of an inhomogeneous superfluid.

The spectra in Fig. 3 are in excellent qualitative agreement with the experimental results in (8). Also quantitatively they agree well with (8) (c.f. Fig. 3 in that article). The shift of the pair-peak, which gives the excitation gap, is at temperatures $T' \leq 0.2T_F$ about $0.2E_F$ in (8) and $0.3E_F$ for $T \leq 0.1T_F$ according our calculation. The widths of the peaks, which are determined by the gap, are about $0.3E_F$ and $0.4E_F$, respectively. The critical temperature at the center of the trap is in our case $T_c \sim 0.3T_F$ which may be used to estimate that in (8) it is $\sim 0.2-0.25 T_F$. The temperatures $T'$ in the experiment are determined in the BEC limit due to lack of precise thermometry in the unitarity limit. The adiabatic passage to the unitarity limit, where the spectra are actually measured, is expected to reduce the temperature due to entropy conservation so that $T < T'$ (23). This is consistent with the observation that the pair-peak in Fig. 3 starts to appear at $T \sim 0.35T_F$ and is clearly visible at $T \sim 0.2T_F$, but in (8) it appears and is clearly visible already at higher (BEC limit) temperatures of $T' \sim 0.75T_F$ and $T' \sim 0.45T_F$, respectively. The sensitivity of the free-atom (quasiparticle) peak to temperature and the possibility of direct comparison between theory and experiment may offer a route for developing a precise thermometry for the crossover region.

We emphasize that those spectra in (8) where the free-atom peak has disappeared correspond to the cases h) through j) in Fig. 3 where more than 80% of the atoms are condensed. This indicates that the pairing observed at the lowest temperatures in (8) corresponds to a su-
perfluid. At higher temperatures, either a pseudogap or a combined effect of a superfluid gap and a pseudogap occurs. In summary, the results presented here support the conclusion that a superfluid, where pairing is a many-body effect, was observed in (8). The mesoscopic nature of these novel Fermi superfluids shows up in an intriguing way.

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20. The pronounced free-atom peak at the zero detuning clearly reflects the strong dependence of the order parameter on density and the trapping potential. In the case of a very smooth density dependence of the energy gap, one would expect simply a broadening of the pair-peak. Such type of behaviour was actually observed in the experiments probing mean fields (12,13): there only one peak was observed and the effect of the trapping potential was a considerable broadening of the peak.

21. Note that since not only energy but also momentum is exactly conserved in the transfer process, these particles cannot be transferred at zero detuning. This is in contrast to superconductor - normal metal junctions where thermal quasiparticle currents flow freely for below-gap voltages.

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Materials and Methods
Figure 1: The superfluid gap and the atom density as functions of position at temperature $T = 0.2T_F$. Resonance superfluidity theory incorporating a pseudogap, together with Thomas-Fermi distribution in the local density approximation, is used. Only the atoms in the middle of the trap are condensed while the atoms closer to the borders are either free or in the pseudogap regime. The critical temperature in the middle of the trap is $T_c \approx 0.3T_F$.

Figure 2: The mean superfluid gap ($\Delta_{sf}$) and pseudogap ($\Delta_{pg}$) as functions of temperature. The fraction of condensed atoms $n_{\text{cond}}$ is defined as the fraction of atoms for which the temperature is below the local critical temperature. The temperature $T \approx 0.7T_c$ corresponds to $T = 0.2T_F$, showing that the superfluid gap distribution in Fig. 1 corresponds to a condensate fraction of $n_{\text{cond}} \approx 0.3$. 

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Figure 3: The spectra of the considered RF-transition as a function of the RF-field detuning $\delta$ for several temperatures. The peak at $\delta = 0$ is caused by free atoms. A peak shifted to the right from the zero gradually appears for lower temperatures, corresponding to paired atoms; the shift of the peak from the zero detuning gives the energy gap in the single particle excitation spectrum. The shift, that is, the gap grows with decreasing temperature. The plots show the disappearance of the free-atom peak when also the atoms at the borders of the trap enter the pseudogap regime and become paired. The critical temperature in the middle of the trap is $T_c \approx 0.3 T_F$. At the temperature $T = 0.1 T_F$, more than 80% of the atoms are condensed. The parameters used in the calculation correspond to the experiments in Fig.3 of (8). The gas is in the unitarity limit, i.e. close vicinity of the Feshbach resonance, which is the expected high-$T_c$ regime for the system.
Feshbach resonances are a powerful tool to tune interactions in degenerate Fermi gases of atoms. They have been used for creation of molecules and molecular Bose-Einstein condensates (BEC) out of fermionic atoms (1-5) and for exploring the crossover region between BEC of molecules and Bardeen-Schrieffer-Cooper (BCS) pairing of atoms (6-11). At the crossover region, the scattering length diverges and universal behaviour independent of any length scale is expected (12-16). This unitarity limit is predicted to be the high-$T_c$ region of the system (17-23).

We consider a gas of atoms in two different internal states $|1\rangle$ and $|2\rangle$, corresponding to Fermion annihilation operators $c^{(1)}$ and $c^{(2)}$, respectively. The interaction between these states is enhanced by a Feshbach resonance. We denote the magnetic field detuning from the Feshbach resonance position by $\nu_0$. For $\nu_0 < 0$, the scattering length between the atoms is positive and two-body physics supports a molecular bound state, for which we introduce a bosonic annihilation operator $b$. At positive detunings $\nu_0$, the scattering length is negative and pairing which is a many-body effect is expected at low temperatures. Near the resonance, $\nu_0 \sim 0$, the scattering length diverges and the system is in the unitarity regime. We use the resonance superfluidity theory (17-21) for calculating the equilibrium state of the system. The system is described by the Hamiltonian

$$H = \sum_{k,\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c^{\dagger}_{k\sigma} + \sum_q (E^0_q + \nu) b^{\dagger}_q b_q$$

$$+ \sum_{q,k,k'} U(q, k') c^{(1)}_{q/2+k} c^{(1)}_{q/2-k} c^{(2)}_{q/2-k'} c^{(2)}_{q/2+k'}$$

$$+ \sum_{q,k} (g(k) b^{\dagger}_q c^{(1)}_{q/2-k} c^{(2)}_{q/2+k} + h.c.).$$

(1)

The interaction parameters $U$, $g$ and the Feshbach detuning $\nu$ are obtained from the bare parameters $U_0$, $g_0$ and $\nu_0$ by a renormalisation procedure (18). The momentum cutoff required by the summations and used in the renormalisation is chosen as $K_c = 25 k_F$, where $k_F$ is the Fermi momentum. The energies $\varepsilon_k = k^2 / 2m$ and $E_q = q^2 / 2M$ are the kinetic energies of
a free fermion (with mass $m$) and a composite boson (mass $M = 2m$), here we have chosen $h/(2\pi) = 1$ where $h$ is Planck’s constant. Equilibrium parameters such as the chemical potential $\mu$, pseudogap $\Delta_{pg}$ and the order parameter $\Delta_{sf}$ are solved self-consistently, following (24). The total excitation gap is given by $\Delta^2 = \Delta_{sf}^2 + \Delta_{pg}^2$. For further details see (25).

The interaction with the (RF/laser) field is introduced as a perturbation and the response is calculated to second order in the perturbation Hamiltonian. The Hamiltonian describing the effect of the field is

$$H_T = \sum_k \frac{\delta}{2} \left( c_k^{(3)} c_k^{(3)*} - c_k^{(2)} c_k^{(2)*} - b_k^* b_k \right) + \sum_{kl} \left( M_{kl} c_k^{(2)} c_l^{(3)*} + h.c. \right) + \sum_{klq} \left( D_{qkl} b_q c_k^{(1)} c_l^{(3)} + h.c. \right), \tag{2}$$

where $M_{kl}$ and $D_{qkl}$ are proportional to the Rabi frequency of the field and $\delta = E_{RF} - (E_3 - E_2)$ is the RF-field detuning, where $E_{RF}$ and $E_3$, $E_2$ are the energies of the RF-photon and of the states $|3\rangle$, $|2\rangle$, respectively. We neglect the bosonic contribution in the perturbation Hamiltonian, assuming that the number of composite bosons is small. The assumption is well-founded at least on the attractive side of the Feshbach resonance, where the Feshbach detuning is positive.

Inclusion of the bosonic current is straightforward, but on the repulsive side and at the resonance one should consider many-particle correlation functions to get the correct asymptotic behaviour (26-28). The spectrum is obtained from the response $I(\delta) = \langle \dot{N}_3 \rangle = i \langle [(H + H_T), N_3] \rangle$, where $N_3$ is the number of atoms in state $|3\rangle$, by neglecting terms of higher than second order in $H_T$.

Applying Matsubara Green’s functions techniques, $I(\delta)$ can be written as

$$I(\delta) = 2 \sum_{kl} |M_{kl}|^2 \text{Im} \left\{ \sum_{x_n^{(2)}} n_F(x_n^{(2)}) G_{(3)^*}^{\text{ret}} (m, x_n^{(2)}) - \delta) \text{Res}_{z=x_n^{(2)}} G_{(2)} (n, z) + n_F(\epsilon_m^{(3)}) G_{(2)^{\text{adv}}}^{\text{adv}} (n, \epsilon_m^{(3)} + \delta) \right\}, \tag{3}$$

where $x_n^{(2)}$ are the (imaginary) poles of the Green’s functions $G_{(2)}$ and $n_F$ are the Fermi distribution functions.
We assume the three-dimensional Thomas-Fermi density distribution for the gas, where the density of atoms at distance \( r \) from the middle of the trap is

\[
n(r) = n(0) \left(1 - \left(\frac{r}{R_{TF}}\right)^2\right)^{3/2}.
\]

(4)

Here \( n(0) \) is the density in the middle of the trap and \( R_{TF} \) is the Thomas-Fermi radius, i.e. the size of the atom cloud. We treat the problem in the local density approximation, that is, we solve the equilibrium state including \( n(r) \) as a position dependent parameter. Note that our analysis is independent of the symmetry of the cloud, i.e. ball as well as cigar or pancake shapes are described by the same analysis with scaled coordinates. The use of the local density approximation is well grounded when the correlation length \( \xi \) over which the atoms affect each other is much smaller than the trap size \( l = \sqrt{\hbar/m\omega} \), where \( \omega \) is the trapping frequency (29-30). For typical traps (31), the radial frequency is of the order of 10 kHz yielding the radial trap size of \( l \approx 20000 a_0 \) while the axial frequencies are smaller by at least one order of magnitude. Using the correlation length of the order of \( \xi \approx O(1/k_F) \) (29) gives, for Fermi energies of the order of 2 \( \mu \)K, \( \xi \approx 3000 a_0 \) and the condition is well satisfied.

The trap parameters are calculated for the maximum atom density of \( 10^{13} \, 1/cm^3 \) in the center of the trap corresponding to the Fermi energy of 2 \( \mu \)K. We use a background scattering length of the order \( a_{bg} = -2000 a_0 \) (32), where \( a_0 \) is the Bohr’s radius, corresponding to the two lowest substates of the electronic 1\( s^22s \) ground state of \(^6\text{Li} \). With this \( a_{bg} \) one obtains as the background interaction energy \( U_0 = -0.5 E_F \). The boson-fermion coupling parameter is \( g_0 \sim 10 E_F \) in our calculations. The coupling \( g_0 \) cannot be directly obtained from experiments. It is defined in (17) as \( g_0 = \sqrt{\Delta\mu_L \Delta B U_0} \), where \( \Delta\mu_L \) is the magnetic moment difference for between the Feshbach state and the continuum state and \( \Delta B \) is the width of the Feshbach resonance. The RF-spectra are not sensitive to the exact value of \( g_0 \) but it affects the fraction of molecules in the system. In order to describe the system close to the resonance, we choose
the magnetic field detuning in the unitarity limit, $\nu_0 = 1 E_F$ (33). The state $|3\rangle$ is not populated initially.

In the results reported here, mean (Hartree-Fock) field effects are not included. In principle, shifts in the spectra occur if the atoms in the initial and final states of the RF-transfer, $|2\rangle$ and $|3\rangle$, feel a different mean field caused by atoms in state $|1\rangle$. We have analyzed the problem also assuming differing, density dependent mean fields for the states $|2\rangle$ and $|3\rangle$. In that case, a notable feature is that the free-atom peak position deviates from the bare-atom resonance position, also at temperatures well above $T_c$. In contrast, in the experiments (31), the free-atom peak is located at the bare-atom resonance position, displaying no mean field shift. Note that this is the case also at temperatures $\lesssim T_F$ where the free-atom peak is dominant and thus originates from atoms in the high density regions of the trap. The absence of such a mean field shift is related to the fact that, for $^6$Li, also the states $|1\rangle$ and $|3\rangle$ have a Feshbach resonance and unitarity limited interactions in close vicinity of the $|1\rangle - |2\rangle$ Feshbach resonance. Finally, the additional mean field shift that could be caused by the interaction between atoms in states $|2\rangle$ and $|3\rangle$ is absent due to the nature of the RF-field driven transition as was observed in (34).

Our method does not allow exact treatment of the onset of the pseudogap regime and precise study of the pseudogap transition temperature. However, the pseudogap pairing occurs at temperature $T^* \approx 0.7 T_F$. The Fermi temperature scales with the atom density as $T_F \propto n^{2/3}$, and the superfluid transition temperature follows approximately the same form at the unitarity limit. The free atom peak disappears at the temperature $T \sim 0.1 T_F$, which means that the temperature in terms of the local Fermi temperature of the border atoms is $T \sim 0.5 T_F^{0.1}$. Here $T_F^{0.1}$ is the local Fermi temperature scaled for density $n(r) = 0.1 n(0)$. Therefore, the free-atom peak disappears when the border atoms are clearly below their (local) pseudogap temperature (however not yet below their critical temperature). In such temperatures, the atoms at the center of the trap, actually the
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