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Spectroscopic Bogoliubov features near the unitary limit

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We analyze the single-particle excitation spectrum of the ultracold fermion atom system close to the unitary limit where there has been found experimental evidence for the Bogoliubov quasiparticles below as well as above the transition temperature \( T_c \). We consider the short-range correlations originating from the preformed pairs and try to discuss the experimental data adapting phenomenological self-energy previously used for description of the antinodal spectra of the underdoped cuprate superconductors. We show that this ansatz qualitatively accounts for the momentum-resolved rf spectroscopic data obtained for \(^{40}\)K atoms.

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I. INTRODUCTION

Spectroscopic tools such as the Bragg scattering technique \([1]\), the rf-pulse spectrometry \([2]\), and its \( k\)-resolved improvement \([3]\) were able to provide a clear-cut evidence for the superfluid nature of the ultracold fermion atom systems. Especially intriguing among the obtained data is the quasiparticle back-bending dispersion near the Fermi momentum observed below and above the superfluid transition temperature \( T_c \) \([4]\). This fact indicates that the Bogoliubov-type quasiparticles survive even in a normal state where the long-range coherence between fermion pairs no longer exists.

Similar fingerprints of the dispersive Bogoliubov quasiparticles have been previously detected above \( T_c \) in the underdoped cuprate superconductors by the angle-resolved photoemission spectroscopy (ARPES) \([5]\) and Fourier-transformed scanning tunnelling microscopy (STM) \([6]\) measurements. They confirmed expectations motivated by the local solution of the Feshbach resonant interactions can be described by the following local Hamiltonian \([18]\):

\[
\hat{H}_{\text{loc}}(\mathbf{r}) = \sum_{\sigma=\uparrow, \downarrow} \varepsilon(\mathbf{r}) \hat{c}_\sigma^\dagger(\mathbf{r}) \hat{c}_\sigma(\mathbf{r}) + E(\mathbf{r}) \hat{b}_0^\dagger(\mathbf{r}) \hat{b}(\mathbf{r}) + g [\hat{b}_\uparrow(\mathbf{r}) \hat{c}_\uparrow^\dagger(\mathbf{r}) + \hat{c}_\downarrow^\dagger(\mathbf{r}) \hat{b}(\mathbf{r})],
\]

where \( g \) denotes the \( s\)-wave channel scattering strength, \( \hat{c}_\sigma^\dagger(\mathbf{r}) \) are fermion operators of the single atoms in two hyperfine states \( \sigma = \uparrow, \downarrow \), and operators \( \hat{b}_\sigma^\dagger(\mathbf{r}) \) correspond to the molecular state. Spatial variations of the energies \( \varepsilon(\mathbf{r}) \), \( E(\mathbf{r}) \) come from the trapping potential and usually take the parabolic dependence with some characteristic radial and axial frequencies.

II. LOCAL SCATTERING ON PAIRS

The momentum-resolved spectroscopic measurements of the Boulder group \([4]\) have been done using \(^{40}\)K atoms equally populated in the hyperfine states \(|9/2, -9/2\rangle \) and \(|9/2, -7/2\rangle \) (we shall denote them symbolically as \( \sigma = \uparrow \) and \( \sigma = \downarrow \)). By applying the magnetic field, the atoms were adiabatically brought to the vicinity of the unitary limit, slightly on the BEC side \((k_F a)^{-1} = 0.15\). Under such conditions, energies of the atoms are nearly degenerate with the weakly bound molecular configurations; thereby, single atoms and molecules are strongly scattered from each other through the conversion processes.

At a given position \( \mathbf{r} \) in the magneto-optical trap, such Feshbach resonant interactions can be described by the following local Hamiltonian \([18]\):

\[
\hat{H}_{\text{loc}}(\mathbf{r}) = \sum_{\sigma=\uparrow, \downarrow} \varepsilon(\mathbf{r}) \hat{c}_\sigma^\dagger(\mathbf{r}) \hat{c}_\sigma(\mathbf{r}) + E(\mathbf{r}) \hat{b}_0^\dagger(\mathbf{r}) \hat{b}(\mathbf{r}) + g [\hat{b}_\uparrow(\mathbf{r}) \hat{c}_\uparrow^\dagger(\mathbf{r}) + \hat{c}_\downarrow^\dagger(\mathbf{r}) \hat{b}(\mathbf{r})],
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Hilbert space of the local Hamiltonian \((1)\) is spanned by four fermion configurations \(|F\rangle = |0\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\) and two molecular ones \(|B\rangle = |0\rangle, |\uparrow\downarrow\rangle\) altogether eight states. Six of these states \(|F\rangle \otimes |B\rangle\) are eigenfunctions of Eq. \((1)\) and two vectors \(|\uparrow\downarrow\rangle \otimes |0\rangle\) and \(|0\rangle \otimes |\uparrow\downarrow\rangle\) get mixed by the Feshbach interaction. With the suitable unitary transformation, we can determine the true eigenfunctions,

\[
|\psi_A\rangle = u|0\rangle \otimes |1\rangle + v|\uparrow\downarrow\rangle \otimes |0\rangle,
\]

\[
|\psi_B\rangle = -v|0\rangle \otimes |1\rangle + u|\uparrow\downarrow\rangle \otimes |0\rangle,
\]

where \( u^2, v^2 = \frac{1}{2}[1 \pm (\varepsilon - E/2)/\sqrt{(\varepsilon - E/2)^2 + g^2}] \) and the eigenvalues are given by \( \varepsilon + E/2 \pm \sqrt{(\varepsilon - E/2)^2 + g^2} \). Equations \((2)\) and \((3)\) are reminiscent of the Bogoliubov-Valatin transformation of the standard BCS problem, where true quasiparticles are represented by linear combinations of the
long-range order $\langle \hat{F}(r,t) \hat{F}(0,0) \rangle = 0$. To account for superconducting fluctuations, the authors [17] assumed certain temporal $\tau_\phi$ and spatial $\xi_\phi$ scales, over which the pairs remain short-range correlated,

$$\langle \hat{F}^\dagger(r,t)\hat{F}(0,0) \rangle \propto |\chi|^2 \exp \left(-\frac{|r|}{\tau_\phi} - \frac{|r|}{\xi_\phi} \right). \quad (6)$$

Taking into account the pairing field (6) by means of the lowest order perturbative scheme, they have determined the single-particle Green’s function $\hat{G}(\mathbf{k},i\omega_n) = [i\omega_n - \epsilon_\mathbf{k} - \Sigma(\mathbf{k},i\omega_n)]^{-1}$, interpolating it by [17]

$$\Sigma(\mathbf{k},i\omega_n) = -\Delta^2 \frac{i\omega_n - \epsilon_\mathbf{k}}{\omega_n^2 + \epsilon_\mathbf{k}^2 + \pi\Gamma^2}. \quad (7)$$

where $\Delta \propto |\chi|$ is a magnitude of the energy gap due to pairing and parameter $\Gamma$ is related to the in-gap states. At low energies (i.e., for $|\omega| \ll \Delta$) a dominant contribution of the spectrum comes from the in-gap quasiparticle residue $Z = (1 + \frac{\Delta^2}{\omega^2})^{-1}$, whereas at higher energies the BCS-type quasiparticles are formed. All these features are present in our exact solution (4) of the local Feshbach scattering problem (1), for which we obtain

$$\Sigma_{\text{loc}}(i\omega_n) = -[1 - Z(T)]g^2 \frac{i\omega_n - \epsilon}{\omega_n^2 + \epsilon^2 + Z(T)g^2}. \quad (8)$$

IV. PHENOMENOLOGICAL PAIRING ANSÄTZ

Combining the local physics (1) with the itinerancy $\hat{T}_\text{kin}(r)$ of fermions and molecules is a nontrivial task. Certain aspects of the complete Hamiltonian

$$\hat{H} = \int d\mathbf{r} [\hat{T}_\text{kin}(\mathbf{r}) + \hat{H}_{\text{loc}}(\mathbf{r})] \quad (9)$$

have been addressed so far by the self-consistent perturbative treatment [20], dynamical mean-field theory [21], self-consistent $T$-matrix approach [22], conserving diagrammatic approximations [15], renormalization group (RG) approach [23], path integral formulation for the bond operators [24], and several other techniques. Some of these studies directly [23,24] or indirectly [15] pointed at the Bogoliubov quasiparticles surviving above $T_c$.

Here we would like to focus on the qualitative outcomes, which could be relevant to the experimental situation of the Boulder group [4]. For this purpose, we apply the phenomenological self-energy,

$$\Sigma(\mathbf{k},\omega) = \frac{\Delta^2}{\omega + \epsilon_\mathbf{k} + i\gamma(T)} - i\Sigma_0, \quad (10)$$

which, according to the argumentation outlined in Sec. III in Ref. [17], originates from Eq. (7) and, similarly, Eq. (8). The particular structure (10) has been suggested also by previous studies for the precursor pairing in the cuprates [16,25] and ultracold gases [15]. The essential effects are here provided by temperature-dependent parameter $\gamma(T)$ related to scattering caused by the preformed pairs and responsible for filling in the low-energy states (instead of closing the energy gap as in classical superconductors). Its role is hence similar to $Z(T)$ of
dependence: be modified, if necessary. We obtained some resemblance a temperature scale, we have imposed the ratio 2 of preformed pairs stays constant [26,27] (this constraint can

uous studies [16,17]. To establish some correspondence with the line broadening, so we simply take it as a structureless constant.

For specific numerical computations, we used $\Sigma_0 = \Delta$, assuming $\Delta = \text{const}$. Such an assumption seems reasonable for a temperature region exceeding $T_c$ as long as the binding energy of preformed pairs stays constant [26,27] (this constraint can be modified, if necessary). We obtained some resemblance to the experimental data [4] using the following temperature dependence:

$$\gamma(T) = 4k_B T Z(T).$$  \hfill (11)

At low temperatures, $\gamma(T)$ is predominantly governed by an exponential decay due to $Z(T)$, while at higher temperatures it acquires a linear relation $\lim_{T \to \infty} \gamma(T) \propto T$ suggested by various studies [16,17]. To establish some correspondence with a temperature scale, we have imposed the ratio $2\Delta/k_B T_c = 6$ which, according to the recent quantum Monte Carlo (QMC) studies [28], seems to be realistic for the ultracold superfluids when approaching the unitarity limit. Since $\gamma(T)$ has indirect relation to the critical temperature (see the solid line in Fig. 1), we can treat Eq. (11) as a starting guess, which can be verified a posteriori. We use $\Delta$ as a convenient unit for energies.

Energy dependence of the single-particle excitation spectrum $A(k,\omega) = -\frac{1}{2}\text{Im}[(\omega - (\epsilon_k - \mu) - \Sigma(k,\omega))^{-1}$ at the Fermi momentum $k_F$ is shown in Fig. 2. Up to this point, we have neglected the trapping potential; therefore, strictly speaking, such function $A(k,\omega)$ describes the spectrum at a center of the trapping potential $r = 0$. Using the constant pairing energy $\Delta$, we obtain at low temperatures the characteristic BCS-type gapped structure. With increasing temperature, it gradually evolves into the singly peaked spectrum for $T \gtrsim 1.5T_c$.

In Fig. 3, we show the momentum dependence of the spectral function $A(k,\omega)$ at temperatures $T/T_c = 0.76, 1.24, 1.47,$ and 2.06. The two-peak shape of $A(k_F,\omega)$ versus $\omega$ is always accompanied by the presence of the Bogoliubov quasiparticle branches with their characteristic bending-down (for $\omega < 0$) and bending-up features (for $\omega > 0$), the latter unfortunately hardly accessible by ARPES and $k$-resolved rf measurements. This effect comes from preexisting pairs, which above $T_c$ remain correlated over some short-range scales. The Bogoliubov quasiparticles have been, in fact, detected in the underdoped cuprates by the diamagnetic response [9], the large Nernst effect, and the single-particle spectroscopy [5,6].

Let us emphasize that evolution of the Bogoliubov branches above $T_c$ is not followed by similar behavior of the local density of states $\rho(\omega, r = 0) = \sum_k A(k,\omega)$. This effect is illustrated in Fig. 4. For temperatures above $1.5T_c$, when the spectral function acquires the singly peaked structure (Figs. 2 and 3), the local density of states is still clearly depleted around $\omega \sim 0$, even for temperatures up to $3T_c$. Such a property

FIG. 3. (Color online) Momentum and energy dependence of the spectral function $A(k,\omega)$ for the set of temperatures reported experimentally by the Boulder group [4]. We can notice that the Bogoliubov quasiparticle features (bending-down dispersion) are preserved to nearly $1.5T_c$.  

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The chemical potential is then effectively replaced by trapping potential applying the local density approximation. Aspects become meaningful. We can treat the effects of the \( \mu \) parts of the harmonic trap is in practice contributed by atoms originating from all parts of the harmonic trap \( V(r) \), thereby the inhomogeneity aspects become meaningful. We can treat the effects of the trapping potential applying the local density approximation. The chemical potential is then effectively replaced by \( \mu(r) = \mu - V(r) \) and in \( k \) space the relative energies \( \xi_k(r) = \xi_k - \mu(r) \) become spatially dependent. Since our objective here is to investigate the qualitative features caused by the short-range superconducting correlations, we focus simply on the isotropic superconducting case \( \beta \), with respect to temperature, reducing the spectral weights of \( Z \) outside the center of the trapping potential, \( V(r) \). The rf spectroscopy provides information on the occupied part \( |E(r)| < \Omega_1 \) of the spatially averaged single-particle excitation spectrum. Neglecting the final-state effects [29] and using the linear response theory, the current can be expressed as a convolution of the spatially dependent spectral function \( A(k, \omega, r) \) and the Fermi distribution [13,30]

\[
I(|k|, \Omega) = \frac{1}{\pi m^2 R_F^2} \int dr |k|^2 A(k, \xi_k - \Omega, r) \frac{2}{\beta} \frac{1}{\pi m^2 R_F^2} 1, \tag{13}
\]

with \( \beta = 1/k_B T \) and the partition function given by \( Q(T,r) = 1 + 2 e^{-\beta E(r)} + 2 e^{-\beta E(r) + E(r)} + e^{-\beta E(r) + E(r)} + 2 \cosh[\beta (|E(r)| - E(r)/2)^2 + g^2] e^{-\beta (|E(r)| - E(r)/2)} \).

Influence of the trapping potential \( V(r) \) on the spectral weight (12) and the related damping rate (11) is shown for \( |r| = 0.5 R_F \) by the dashed lines in Fig. 1. We notice that, outside the center of the trapping potential, \( Z(T,r) \) increases with respect to temperature, reducing the spectral weights of the bonding and antibonding states. Since the corresponding damping parameter \( \gamma \) [which acquires \( r \) dependence via \( Z(T,r) \)] is also enhanced (see the main panel of Fig. 1), we expect a partial suppression of the energy gap upon increasing \( |r| \).

FIG. 4. (Color online) Evolution of the local density of states \( \rho(\omega, r = 0) \) in the center of the harmonic trap.

FIG. 5. (Color online) Spatial dependence of the spectral function \( A(k, \omega, r) \) at temperature \( T = 1.2 T_c \) for \( k = k_F \).

To analyze spectroscopic consequences of the inhomogeneity, we determine the spectral function \( A(k, \omega, r) = -\frac{1}{2} \Im \left[ \omega - \xi_k(r) - \Sigma(k, \omega, r) \right] \) using the phenomenological self-energy [10] with \( r \)-dependent damping rate (11). In Sec. IV, we have shown that \( A(k, \omega, r = 0) \) develops, at low temperatures, the gapped structure with the characteristic Bogoliubov peaks. Away from the trap center, these Bogoliubov peaks move closer to each other as marked by the filled points in Fig. 5. At some temperature-dependent critical radius \( r_c(T) \), the Bogoliubov features finally merge into the single peak. Figure 6 illustrates such an \( r \)-dependent energy gap determined for a number of representative temperatures.

We notice that the effective pairing gap is quite flat with respect to \( r \) and has a rapid drop approaching \( r_c(T) \). This is related to the fact that, for increasing temperature and/or radius, the spectral gap is “filled in” instead of closing, as would be characteristic for the BCS systems. Pair fluctuations (responsible for disordering the phase of the order parameter) cause the missing low-energy states to be bit by bit filled in until \( T^* \) (as illustrated in Fig. 4) or \( r_c(T) \) (Fig. 6), when the pairs dissociate and the related energy gap finally closes.

FIG. 6. (Color online) Spatial variation of the effective energy gap \( \Delta_{\text{eff}}(r) \) (in units of \( k_B T_F \)) for several temperatures as indicated.
where $\Omega$ is the detuning frequency, $R_F$ denotes the Thomas-Fermi radius, and $\Gamma$ corresponds to the tunneling matrix, which we assume as a constant.

Integrating Eq. (13) with respect to $r$, we have determined the energy distribution curves for several temperatures corresponding to the experimental situation [4]. In Fig. 7, we show two examples of the obtained results. Integration of the spectral function convoluted with the Fermi distribution practically yields the negative $\omega < 0$ region of the spatially averaged spectrum; therefore, only the lower part of the Bogoliubov excitation branch remains visible. Furthermore, we notice that the quasiparticle peaks become smeared and a magnitude of the effective gap is suppressed in comparison to $\Delta_{pg}(r = 0)$. Such a result is rather obvious if we recall that pairing effects weaken aside from the trap center (the energy gap of atoms contributing to the EDC curve decreases versus $|r|$ as shown in Fig. 6). Nevertheless, the $k$-resolved rf profiles exhibit the characteristic bending-down feature manifesting the BCS properties not only below $T_c$, but also clearly preserved over the temperature region up to $\sim 1.5T_c$.

VI. SUMMARY AND OUTLOOK

Transition to the superconducting-superfluid state is near the unitary limit [26] accompanied by a number of the *preparing* signatures [31] showing up above $T_c$. Among such hallmarks, there are the Bogoliubov-type quasiparticles representing the mixed particle and hole entities characteristic for the symmetry broken BCS state. Recent experimental data obtained for the underdoped cuprate oxides [5] and the ultracold fermion gasses [4] unambiguously show that such Bogoliubov quasiparticles survive even beyond the superconducting-superfluid domes. The origin of these features is related to the preformed pairs, which above $T_c$ remain correlated over some finite spatial and/or temporal distances (the long-range coherence establishes only below $T_c$).

Preformed pairs affect the single-particle spectra via the interconversion processes (1). In this paper, we have examined the influence of the preformed pairs on the single-particle excitation spectrum guided by the exact solution (4) of the local Feshbach scattering problem (1). We have shown that, upon increasing temperature, the free fermion states emerge gradually out of the Bogoliubov quasiparticles [strictly speaking from the bonding and antibonding states (2) and (3)]. We have next incorporated the local correlations and itinerancy of atoms or molecules through the pairing ansatz (10).

Our phenomenological analysis based on the self-energy (10) with the temperature-dependent pair-damping parameter $\gamma$ was motivated by the perturbative studies of the short-range superconducting correlations [17] and by the rigorous solution (4) of the local atom-molecule scattering (1). It turns out that, on a qualitative level, our results seem to agree with the predictions obtained by other sophisticated techniques, such as a diagrammatic $t$-matrix approximation, where the fermionic self-energy includes the pairing fluctuations [30], the crossover studies taking into account the condensed and noncondensed pairs (especially the scheme using one bare and one dressed Green’s functions) [10], the quantum cluster expansion [32], the ladder approximation for the hard-sphere Fermi gas [12], the conserving ($\Phi$-derivable) approach for the interacting fermion system following Luttinger and Ward [14], *ab initio* QMC simulations [26,28], the dynamical cluster QMC [27], etc.

We hope that the self-energy (10) originally proposed for reproducing the ARPES spectra of the underdoped cuprates [16] and considered in various self-consistent treatments [15] could be derived in a systematic way, using nonperturbative tools like, for instance, the contractor method [33] or the flow equation procedure [23]. Our study indicates that Eq. (10) can describe the spectroscopic data of the ultracold fermion atom superfluids. Similar BCS-type self-energy has been recently shown to be applicable also in the STM studies of the low-$T_c$ superconducting material Bi$_2$Sr$_2$CuO$_{6+\delta}$, where $d$-wave pairing features appear in a close neighborhood of the van Hove singularity and where the pseudogap region extends all over the superconducting dome, including the overdoped regime [34].

As a complementary technique to the momentum-resolved rf spectroscopy [4], we would like to suggest for future studies the Andreev tunneling [35]. If feasible in the ultracold fermion systems, such Andreev spectroscopy could very precisely establish the temperature region over which the short-scale superconducting-superfluid correlations survive above $T_c$.

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