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SINGLE-PARTICLE EXCITATIONS AND THE ORDER PARAMETER FOR A TRAPPED SUPERFLUID FERMI GAS

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We reveal a strong influence of a superfluid phase transition on the character of single-particle excitations of a trapped neutral-atom Fermi gas. Below the transition temperature the presence of a spatially inhomogeneous order parameter (gap) shifts up the excitation eigenenergies and leads to the appearance of in-gap excitations localized in the outer part of the gas sample. The eigenenergies become sensitive to the gas temperature and are no longer multiples of the trap frequencies. These features should manifest themselves in a strong change of the density oscillations induced by modulations of the trap frequencies and can be used for identifying the superfluid phase transition.

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Physics of ultracold trapped atomic gases has attracted a lot of attention after the discovery of Bose–Einstein condensation [1–3]. Trapped neutral-atom Fermi gases, being cooled to a sufficiently low temperature, should also exhibit prominent macroscopic quantum phenomena which are mostly related to a superfluid pairing phase transition. Possible versions of this phase transition in atomic samples have recently been discussed in Refs. [4–7]. However, as only a small fraction of particles is influenced by the pairing, it is not entirely clear how the transition will manifest itself in dynamic and kinetic properties of the gas.

In this Letter we indicate a clear way of identifying the pairing transition in a trapped Fermi gas. We study single-particle excitations and show that they are strongly influenced by the pairing. Above the transition temperature T_c the excitation eigenfrequencies are multiples of the trap frequencies. It turns out that below T_c the presence of the order parameter shifts up the eigenenergies and ensures the existence of in-gap excitations localized in the outer part of the gas sample in the well formed by the gap and the trapping potential. The eigenenergies become sensitive to the gas temperature and are no longer multiplies of the trap frequencies. This should strongly change the response of the gas to modulations of the trap frequencies (see below).

The influence of pairing on single-particle excitations is essentially the same for all types of pairing discussed in Refs. [4–7], and for simplicity we confine ourselves to the case of the s-wave pairing. We consider a two-component neutral gas of fermionic atoms trapped in a spherically symmetrical harmonic potential. The two (hyperfine) components labeled as α and β are assumed to have equal concentrations. The Hamiltonian of the system has the form ($\hbar = 1$)

$$H = \sum_{i=\alpha,\beta} \int d\mathbf{r} \psi_i^+ H_0 \psi_i + V \int d\mathbf{r} \psi_\alpha^+ \psi_\alpha \psi_\beta^+ \psi_\beta, \qquad (1)$$

where $\psi_i(\mathbf{r})$ with $i = \alpha, \beta$ are the field operators of the α and β atoms, $H_0 = -\nabla^2/2m + m\Omega^2 r^2/2 - \mu$, Ω is the trap frequency, and μ is the chemical potential which greatly

exceeds Ω in the Thomas–Fermi limit (see e.g. Ref. [8]) discussed below. The second term in Eq. ([8]) assumes an attractive elastic interaction between atoms in the states α and β (s-wave scattering length $a < 0$), $V = 4\pi a/m$ being the coupling constant, and m the atom mass.

The presence of a negative s-wave scattering length for the inter-component interaction leads to a superfluid phase transition via Cooper pairing in the s-wave channel [6], with the critical temperature $T_c \ll \mu$. Being interested in the effect of this transition, we consider temperatures $T \ll \mu$, where the chemical potential coincides with the Fermi energy in the center of the trap: $\mu \approx \varepsilon_F = p_F^2/2m$, and the Thomas–Fermi radius of the gas sample $R_{TF} = v_F/\Omega$ serves as a unit of length ($v_F = p_F/m$). In this temperature range a small parameter of the theory is $\lambda = 2\,|a|\,p_F/\pi \ll 1$. The density profile of the gas is $n(R) = n_0(1 - R^2)^{3/2}$, where $n_0 = p_F^3/3\pi^2$ is the maximum gas density, and R the distance from the origin in units of R_{TF}. This density profile corresponds to the local Fermi momentum $p_F(R) = p_F(1 - R^2)^{1/2}$, and the density of states on the local Fermi surface $N(R) = mp_F(R)/(2\pi^2)$. To be precise, the above formulae should be modified in the presence of the interaction. The leading mean-field corrections are smooth and small ($\propto \lambda$). They also result in a uniform shift of particle eigenenergies in the vicinity of the chemical potential level. This shift can be absorbed by redefining μ.

We assume that the critical temperature T_c of the pairing transition is much larger than Ω and, hence, T_c is very close [7] to the critical temperature $T_c^{(0)} = 0.28\varepsilon_F \exp(-1/\lambda)$ in a spatially homogeneous gas with density n_0 [9]. Below T_c the gas is characterized by the presence of the order parameter $\Delta(\mathbf{R}) = |V|\,\langle\psi_\alpha(\mathbf{R})\psi_\beta(\mathbf{R})\rangle$. Following a standard mean-field procedure (see, e.g. [10]), the term describing the interparticle interaction in Eq. (1) can be written as $\Delta(\mathbf{R})\psi_\alpha(\mathbf{R})\psi_\beta(\mathbf{R}) + \Delta^*(\mathbf{R})\psi_\beta^\dagger(\mathbf{R})\psi_\alpha^\dagger(\mathbf{R})$. Then the Hamiltonian (1) becomes bilinear and can be reduced to a diagonal form by using the Bogolyubov transformation generalized for the spatially inhomogeneous case [10]:

$$\begin{pmatrix} \psi_\alpha(\mathbf{R}) \\ \psi_\beta(\mathbf{R}) \end{pmatrix} = \sum_\nu \left[U_\nu(\mathbf{R}) \begin{pmatrix} \alpha_\nu \\ \beta_\nu \end{pmatrix} + V_\nu^*(\mathbf{R}) \begin{pmatrix} \beta_\nu^\dagger \\ -\alpha_\nu^\dagger \end{pmatrix} \right],$$

where α_ν and β_ν are the operators of single-particle excitations. Their wave functions $U_\nu(\mathbf{R})$, $V_\nu(\mathbf{R})$ satisfy the Bogolyubov – de Gennes equations

$$H_0 \begin{pmatrix} U_\nu \\ V_\nu \end{pmatrix} + \begin{pmatrix} \Delta(\mathbf{R})V_\nu \\ -\Delta^*(\mathbf{R})U_\nu \end{pmatrix} = \varepsilon_\nu \begin{pmatrix} U_\nu \\ -V_\nu \end{pmatrix}, \tag{2}$$

with $\varepsilon_\nu \geq 0$ being the excitation energies.

In the vicinity of T_c the order parameter can be found from the Ginzburg–Landau equation [7]:

$$\Delta(R) = 5.15 \cdot T_c \sqrt{(T_c - T)/T_c} \exp\left(-R^2/2l_\Delta^2\right), \tag{3}$$

where $l_\Delta^2 = \kappa\sqrt{2\lambda/(1+2\lambda)} \ll 1$, and $\kappa = 0.13(\Omega/T_c)$. At lower temperatures, where the Ginzburg–Landau approach is not valid, $\Delta(R)$ can be obtained from the Eilenberger equations [11] which in the presence of a harmonic trapping potential read

$$\begin{aligned} ig'_\omega + (\Delta \cdot f_\omega - \Delta^* \cdot \tilde{f}_\omega)/\Omega &= 0 \\ if'_\omega - (2i\omega f_\omega + 2\Delta^* \cdot g_\omega)/\Omega &= 0 \end{aligned} \tag{4}$$

$$i\tilde{f}'_\omega + (2i\omega\tilde{f}_\omega + 2\Delta \cdot g_\omega)/\Omega \;=\; 0,$$

with the symbol prime standing for the operator $(p_F(R)/p_F)(\mathbf{n}\nabla_\mathbf{R})$. Eqs. (4) follow from the well-known Gor'kov equations [12] under the assumption $\varepsilon_F(R) \gg T$. The functions f_ω, $\tilde{f}_\omega$ and g_ω depend on the position $\mathbf{R}$ and a unit vector $\mathbf{n}$, $f_\omega = f_\omega(\mathbf{R},\mathbf{n})$ etc., and obey the constraint $f_\omega(\mathbf{R},\mathbf{n})\tilde{f}_\omega(\mathbf{R},\mathbf{n}) - g_\omega^2(\mathbf{R},\mathbf{n}) = 1/4$ (see [11] for more details).

Eqs. (4) should be completed by the self-consistency condition

$$\Delta(R) = |V| \cdot 2\pi N(R) T \sum_\omega \int \frac{d\mathbf{n}}{4\pi} f_\omega(\mathbf{R},\mathbf{n}), \tag{5}$$

where the summation is performed over the Matsubara frequencies $\omega = \pi T(2n+1)$.

For real Δ the function $\tilde{f}_\omega(\mathbf{R},\mathbf{n}) = f_\omega(\mathbf{R},-\mathbf{n})$, and the solution of Eqs. (4) for f_ω, omitting the terms of order $\left(\Omega/\sqrt{T^2+\Delta^2}\right)^3$, can be written as

$$f_\omega = \frac{\Delta}{2\sqrt{\omega^2+\Delta^2}} + \frac{\omega}{4}\frac{\Omega\Delta'}{(\omega^2+\Delta^2)^{3/2}} + \Omega^2\left[\frac{\omega^2}{16}\frac{2(\omega^2+\Delta^2)\Delta'' - 5\Delta(\Delta')^2}{(\omega^2+\Delta^2)^{7/2}}\right], \tag{6}$$

where the symbol prime has the same meaning as before. Eqs. (6) and (5) provide us with an equation for the order parameter $\Delta(R)$. Actually, the first term of Eq. (6) gives a formally divergent quantity $\sum_\omega \pi T/\sqrt{\omega^2+\Delta^2}$. To eliminate this divergency we renormalize the coupling constant V in the same way as it has been done in the Bogolyubov method (see, e.g., [13]). Then we obtain

$$\frac{\Delta}{\lambda N(R)} = \Delta \cdot \widetilde{S}_{1/2} + S_{5/2}\frac{1-R^2}{12}\left[\frac{d^2\Delta}{dR^2} + \frac{1}{R}\frac{d\Delta}{dR}\frac{2-3R^2}{1-R^2}\right] - S_{7/2}\frac{5(1-R^2)}{24\Omega^2}\left(\frac{d\Delta}{dR}\right)^2\Delta, \tag{7}$$

where $S_\alpha \equiv \pi T\sum_\omega \omega^2/(\omega^2+\Delta^2)^\alpha$ for $\alpha = 5/2, 7/2$, and

$$\widetilde{S}_{1/2} = \frac{1}{\lambda} - \gamma - \ln\frac{\Delta}{\pi T_c^{(0)}(1-R^2)} - \int_0^\infty \frac{2dx}{\exp(\frac{\Delta}{T}\cosh(x)) + 1},$$

with $\gamma = 0.577$ being the Euler constant.

At T close to T_c equation (7) reduces to the Ginzburg-Landau equation from Ref. [7]. For lower temperatures we solved Eq. (7) numerically, with the boundary conditions $\Delta'(0) = 0$ and $\Delta(1) = 0$. In Fig. 1 we present $\Delta(R)$ at various temperatures for $\lambda = 0.3$ and $T_c^{(0)} = 5\Omega$ ($T_c = 0.86T_c^{(0)}$). The comparison with results of the local-density approximation shows that the latter is adequate only at very low temperatures: with decreasing T, the spatial region where Δ is essentially nonzero increases and, hence, spatial derivatives of Δ, neglected in the local-density approximation, become less important.

In a spherically symmetrical trapping potential elementary excitations are characterized by the radial quantum number n, orbital angular momentum l, and its projection m. The excitation wave functions can be written as $(U_\nu, V_\nu) = R^{-1}Y_{lm}(\widehat{\mathbf{R}})(u_{nl}(R), v_{nl}(R))$, where the functions (u,v) are normalized by the condition $\int_0^\infty (u_{nl}u^*_{n'l} + v_{nl}v^*_{n'l})\,dR = \delta_{nn'}$. At temperatures $T \ll \varepsilon_F \approx \mu$ elementary excitations formed by particles with energies in a narrow vicinity of the Fermi surface are most important. In the classically accessible region of space the excitation wave functions exhibit strong spatial oscillations, with a period of order $p_F^{-1}(R) \ll R_{TF}$ and a slowly varying amplitude $\widetilde{u}_{nl}(R)$, $\widetilde{v}_{nl}(R)$:

$$\begin{pmatrix} u_{nl} \\ v_{nl} \end{pmatrix} = \frac{\exp\left(i\widetilde{\mu}\int_{R_1}^{R} p_{Fl}dR\right)}{\sqrt{p_{Fl}(R)}} \begin{pmatrix} \widetilde{u}_{nl} \\ \widetilde{v}_{nl} \end{pmatrix} + \text{h.c.}. \tag{8}$$

The partial Fermi momentum is defined as $p_{Fl}(R) = (1 - R^2 - (l+1/2)^2/\widetilde{\mu}^2 R^2)^{1/2}$, where $\widetilde{\mu} = 2\mu/\Omega \gg 1$, and the classically accessible region is specified by the condition $R_1 < R < R_2$, with the turning points $R_{1,2}$ from the equation $p_{Fl}(R_{1,2}) = 0$. Omitting the terms of order $\widetilde{\mu}^{-1}$ in Eq. (2), for the amplitudes $f_\pm = \widetilde{u} \pm i\widetilde{v}$ we obtain a pair of decoupled equations ($\widehat{\varepsilon}_{nl} = \varepsilon_{nl}/\Omega \geq 0$, $\widehat{\Delta} = \Delta/\Omega$):

$$\left[-\left(p_{Fl}\frac{d}{dR}\right)^2 + \widehat{\Delta}^2 \pm p_{Fl}\frac{d\widehat{\Delta}}{dR} - \widehat{\varepsilon}_{nl}^2\right] f_{nl\pm} = 0. \tag{9}$$

In classically inaccessible regions $0 < R < R_1$(due to the centrifugal barrier) and $R > R_2$(due to the trapping potential), Eqs. (9) should be modified by replacing $p_{Fl}(R)$ with $\mp i\,|p_{Fl}(R)|$, respectively, to obtain decaying solutions. Above T_c the order parameter is zero, and using a standard semiclassical procedure one can obtain the well-known result $E_{nl}^{(0)} = (2n + l + 3/2)\Omega$ for the eigenenergies counted off the bottom of the potential well. In a spherical harmonic trap the chemical potential $\mu = (j + 3/2)\Omega$, where j is a positive integer. Accordingly, we obtain $\varepsilon_{nl}^{(0)} = |2n + l - j|\,\Omega$ for the eigenenergies of particle-like ($2n + l \geq j$, $\widetilde{v}_{nl} = 0$) and hole-like ($2n + l \leq j$, $\widetilde{u}_{nl} = 0$) single-particle excitations.

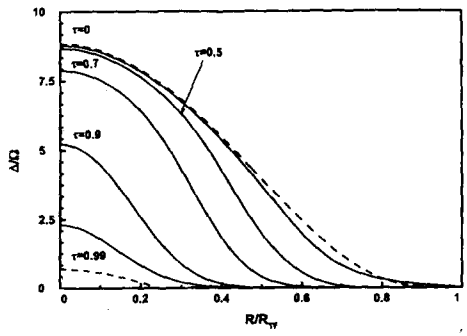

Fig.1. Order parameter $\Delta(R)$ at various temperatures $\tau = T/T_c$ (solid lines). The dashed lines correspond to $\Delta(R)$ in the local density approximation at $\tau = 0$ (upper curve) and $\tau = 0.99$ (lower curve)

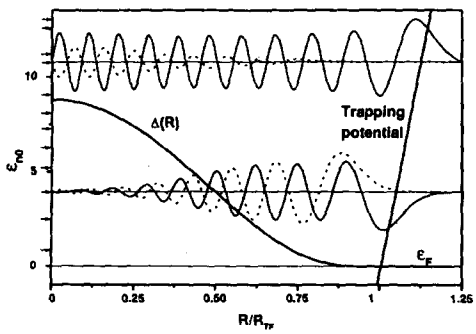

Fig.2. Wave functions u_{n0} (solid lines) and v_{n0} (dashed lines) for above-gap and in-gap excitations, obtained by numerical solution of Eqs. (8) for $l = 0$ at $T = 0$. For illustrative purpose only (to reduce the number of rapid oscillations) we take $\widetilde{\mu} = 63$ instead of the actual value $\widetilde{\mu} \approx 970$. Arrows indicate eigenenergies of the excitations

Below the transition point the appearance of the order parameter $\Delta(R)$ modifies the excitation spectrum. Just below T_c the order parameter is small and exists only in a small spatial region of radius $l_\Delta \ll 1$ (see Eq. (3)). Therefore, the presence of $\Delta(R)$ only influences the excitations with small l and slightly shifts up their eigenenergies: The shifts will be of order $\delta = \Delta(R_1)l_\Delta$, i.e. much smaller than the maximum value $\Delta(0)$ of the spatially inhomogeneous gap $\Delta(R)$. Hence, the lowest excitations, namely the ones with $\varepsilon_{nl}^{(0)} = 0$ at $T > T_c$, become in-gap, i.e., have energies below the top of the gap: $\varepsilon_{nl} \sim \delta \ll \Delta(0)$. With decreasing temperature, $\Delta(R)$ rapidly grows, which increases the number of in-gap excited states.

At temperatures well below T_c the characteristic radius of $\Delta(R)$ becomes of order the size of the gas sample R_{TF}, and all relevant excitations ($l \lesssim \tilde{\mu}/2$) are influenced by the presence of $\Delta(R)$. The wave functions of above-gap excitations ($\varepsilon_{nl} > \Delta(R_1)$) extend over the entire classically accessible region $R_1 < R < R_2$. On the contrary, the in-gap excitations with energies ε_{nl} well below $\Delta(R_1)$ are essentially "expelled" from the center of the trap: their wave functions are mostly localized in the well formed in the outer part of the sample by $\Delta(R)$ and the trapping potential (see Fig.2).

For T well below T_c we have $\widehat{\Delta}(0) \sim T_c/\Omega \gg 1$, and Eqs. (9) for the amplitudes $\widetilde{u}_{nl}$, $\widetilde{v}_{nl}$ can be solved in the semiclassical approach, omitting the terms with spatial derivatives of $\widehat{\Delta}(R)$ as they are small compared to $\widehat{\Delta}^2$. Then, in the spatial region where $\varepsilon > \Delta(R)$ we obtain

$$\begin{pmatrix} \widetilde{u}_{nl} \\ \widetilde{v}_{nl} \end{pmatrix} = \frac{\widehat{\Delta}(R)}{\sqrt{\omega(R)}} \sum_{\pm} C_{\pm} \begin{pmatrix} \pm(\widehat{\varepsilon} \mp \omega(R))^{-1/2} \\ \mp(\widehat{\varepsilon} \pm \omega(R))^{-1/2} \end{pmatrix} \exp\left\{ \pm i \int \frac{\omega(R)}{p_{Fl}(R)} dR \right\}. \qquad (10)$$

Here $\omega(R) = \sqrt{\widehat{\varepsilon}^2 - \widehat{\Delta}^2(R)}$, and $C_{\pm}$ are numerical coefficients. In the case of above-gap excitations ($\varepsilon_{nl} > \Delta(R_1)$) these coefficients can be found by making an analytical continuation of the solution (10) to the classically inaccessible regions $R < R_1$ and $R > R_2$. Since for $\varepsilon_{nl} > \Delta(R_1)$ there are only two (classical) turning points R_1 and R_2, the semiclassical quantization condition reads

$$\frac{2}{\pi} \int_{R_1}^{R_2} \frac{\sqrt{\varepsilon_{nl}^2 - \Delta^2(R)}}{p_{Fl}(R)} dR = \varepsilon_{nl}^{(0)}. \qquad (11)$$

This condition provides us with the energy spectrum of the above-gap excitations (see Fig. 2). The amplitudes $\widetilde{u}_{nl}$, $\widetilde{v}_{nl}$ of their wave functions oscillate in the entire region $R_1 < R < R_2$, and decay in classically inaccessible regions $R < R_1$ and $R > R_2$. As well as excitations above T_c, these excited states are doubly degenerate, but their energies are shifted up by the presence of $\Delta(R)$.

For the in-gap excitations the situation is more subtle due to the appearance of a peculiar turning point R_c determined by the condition $\varepsilon_{nl} = \Delta(R_c)$. At this point a particle undergoes the Andreev reflection [14] from the spatially inhomogeneous gap $\Delta(R)$ and transforms into a hole (and vice versa). As a result, these excitations acquire a superpositional particle-hole character and become non-degenerate, with a splitting increasing with $\Delta(0)$.

In the spatial region $R_c < R < R_2$ the amplitudes $\widetilde{u}_{nl}$, $\widetilde{v}_{nl}$ are determined by Eq. (10), with the coefficients $C_{\pm}$ following from an analytical continuation of Eq. (10) to the region $R_1 < R < R_c$. In the latter region the amplitudes are given by the same Eq. (10) where $\omega(R)$ is replaced by $-i\,|\omega(R)|$, and the coefficients $C_{\pm}$ are obtained by making an analytical continuation to the classically inaccessible region $R < R_1$. As a result, the quantization condition for the in-gap excitations reads

$$(-1)^{j-l} \cos(2\phi) = 2Z^2/(Z^4+1), \qquad (12)$$

$$Z = \sqrt{2} \exp\left\{ \int_{R_1}^{R_c} \sqrt{\Delta^2(R) - \varepsilon_{nl}^2}/p_{Fl}(R) dR \right\}, \quad \phi = \int_{R_c}^{R_2} \sqrt{\varepsilon_{nl}^2 - \Delta^2(R)}/p_{Fl}(R) dR.$$

The wave functions of these excitations are mainly localized in the region $R_c < R < R_2$, where the amplitudes $\widetilde{u}_{nl}$ and $\widetilde{v}_{nl}$ oscillate. For $R_1 < R < R_c$ they decay exponentially. In fact, these amplitudes behave themselves as wave functions of bound states in the potential well formed by the trapping potential from one side and by the order parameter $\Delta(R)$ from the other side (see Fig. 2). To a certain extent these excitations are analogous to localized states in the vortex core in ordinary superconductors [15].

For the lowest in-gap excitations the semiclassical approach for finding the eigenenergies ε_{nl} and amplitudes $\widetilde{u}_{nl}$, $\widetilde{v}_{nl}$ is not adequate, and one has to solve Eq. (9) numerically. The energies of these excitations are very sensitive to $\Delta(R)$, and, hence, to the gas temperature. For $\Delta(R)$ in Fig. 1 at $T = 0$ we find $\varepsilon_0 = 0.85\Omega$ for the lowest excitation with $l = 0$ (Eq. (12) gives $\varepsilon_0 = 1.06\Omega$). With increasing T the value of ε_0 decreases ($\varepsilon_0 = 0.23\Omega$ for $T = 0.99T_c$) and tends to zero for $T \to T_c$.

In conclusion, below the transition temperature, the excitation eigenfrequencies become temperature dependent and are no longer multiples of the trap frequencies. These features should lead to a strong change of the density oscillations induced by modulations of the trap frequency, which can be used for identifying the pairing transition. For example, spherically symmetrical modulations ($\delta\Omega \sim \cos(\nu t)$) cause single-particle transitions between the states with the same orbital angular momentum l, and above T_c the amplitude of the density oscillations will exhibit resonances at frequencies ν which are multiples of 2Ω. Below T_c the presence of $\Delta(R)$ changes the eigenfrequencies of some of the excitations, and those will not contribute to the density oscillations at the resonance frequencies. Hence, the resonance peaks broaden and become smaller. For $\Delta(R)$ in Fig. 1 already at $T = 0.5T_c$ the eigenfrequencies of all excitations with $l \lesssim \widetilde{\mu}/2$ are altered by the pairing. Thus, the resonances in the ν-dependence of the density oscillations, characteristic for the gas above T_c, will be smeared out. At low enough temperatures one should also expect the appearence of resonances related to collective modes of the order parameter. This issue will be addressed in a future publication.

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