Few-to-many particle crossover of pair excitations in a superfluid

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(Dated: August 9, 2022)

Motivated by recent advances in the creation of few-body atomic Fermi gases with attractive interactions, we study theoretically the few-to-many particle crossover of pair excitations, which for large particle numbers evolve into modes describing amplitude fluctuations of the superfluid order parameter (the “Higgs” modes). Our analysis is based on a Richardson-type pairing model that captures interactions between time-reversed fermion pairs. The model is integrable, which allows a systematic quantitative study of the few-to-many particle crossover with only minor numerical effort. We first establish a parity effect in the ground state energy, which is quantified by a so-called Matveev-Larkin parameter that generalizes the pairing gap to mesoscopic ensembles and which behaves quantitatively differently in a few-body and a many-body regime. The crossover point for this quantity is widely tunable as a function of interaction strength. We then compute the excitation spectrum and demonstrate that the pair excitation energy shows a minimum that deepens with increasing particle number and shifts to smaller interaction strengths, consistent with the finite-size precursor of a quantum phase transition to a superfluid state. We extract a critical finite-size scaling exponent that characterizes the decrease of the gap with increasing particle number.

A fundamental question in physics is how the constituents of interacting systems behave collectively to yield the emergent properties of matter [1]: How many particles are required to transition from a few-body ensemble to a collective many-body state? Experiments that explore this crossover are scarce: Examples include the emergence of metallic behavior in colloidal clusters [2], semiconductor quantum dots [3, 4], or superconductivity in nanograins [5–7]. Recent experiments on few-body ensembles of ultracold fermions provide a new platform in which the few-to-many body crossover can be studied [8–9]. These cold atom setups offer several advantages over solid-state systems: For example, they are free of disorder or impurities, and parameters such as the trap geometry and the interaction strength are controlled very accurately. Moreover, precise measurement techniques exist, such as modulation spectroscopy [10] or even direct fluorescence imaging of the few-body wave function [11, 12].

In this Letter, we show how the excitation spectrum of a paired superfluid emerges at large particle numbers, with a Higgs mode that describes amplitude fluctuations of the superfluid order parameter. Corresponding experiments in the few-body limit were recently carried out in two-dimensional harmonically-trapped atomic Fermi gases [10], which create pair excitations on top of a few-body ground state by modulating the interaction strength. For particular closed-shell configurations, these excitations transfer an atom pair to a higher oscillator shell and are hence gapped. With increasing attractive interaction, however, the excitation energy decreases below the noninteracting value and assumes a minimum before it increases again at strong interactions. The expectation is that in the limit of large particle numbers, the minimum shifts to weaker interactions and decreases to zero energy, signaling a quantum phase transition to a superfluid state [13]. Hence, the observations [10] are interpreted as the few-body precursor of a quantum phase transition. Here, we corroborate this picture with exact results beyond the few-body limit, allowing in particular the extraction of a finite-size exponent for the gap closing at large particle number.

In order to highlight the crucial role of pair interactions, we consider a model with an effective interaction between time-reversed fermion pairs and show that it quantitatively describes current experiments. The model belongs to a class of so-called Richardson models [14–17], which are solved by an algebraic Bethe ansatz (see Refs. [18, 19] for reviews), allowing for an efficient calculation of many-body states at only minor numerical effort compared to other methods such as a full configuration-interaction approach [20–27], coupled-cluster methods [24], or Monte-Carlo calculations [28–30]. We study the following Hamiltonian:

\begin{equation}
H = \sum_{j} \varepsilon_j n_j - g \sum_{ij} A_i^\dagger A_j.
\end{equation}

Here, \(\varepsilon_j\) is a single-particle energy labelled by a primary quantum number \(j\), and the level is \(d_j\)-fold degenerate with degenerate states distinguished by a second quantum number \(m\). For a 2D harmonic oscillator, for example, we have \(\varepsilon_j = j + 1\) (\(j = 0, 1, \ldots\)) [all energies are expressed in units of the harmonic oscillator energy] with \(d_j = j + 1\) per spin and \(m = -j, -j + 2, \ldots\). \(j\) is the angular momentum projection within a shell \(j\). Furthermore, we define the particle number operator in a given shell

\begin{equation}
n_j = \sum_m (c_j^m c_j^\dagger m + c_j^\dagger m c_j^m),
\end{equation}

where \(c_j^m\) creates a fermion in a state \((j, m)\) and \(c_j^\dagger m\) creates a fermion in a corresponding time-reversed state.
The interaction term couples pairs of fermions annihilated by

$$A_j = \sum_m c_{jm}^c c_{jm}^\dagger,$$  

(3)

Note that for a box potential, the pairing interaction retains precisely the matrix elements giving rise to superfluidity. For an oscillator potential, Eq. (1) neglects some matrix elements with pair-breaking transitions compared to a contact interaction (and will thus not reproduce certain features of the contact interaction such as a nonrelativistic conformal symmetry at weak interactions), but as we will demonstrate it accurately describes the pair excitation spectrum.

Fermionic systems with pairing interactions as in Eq. (1) are integrable. A key observation for the solution is that the interaction only couples empty and pair-occupied levels while singly-occupied levels decouple from the Fock space. Restricted to a set $\mathcal{U}$ of pair levels, Eq. (1) describes a quadratic Bose Hamiltonian with a hard-core constraint on $A_j$, characterized by $[A_j, A_j^\dagger] = \delta_{ij}(d_j - n_j)$. Intriguingly, this constraint only leads to a small modification of the free Bose gas solution: Interacting eigenstates evolve continuously from non-interacting states and are thus described by a set of $M$ occupied pair levels $\{(j_0, m_0), \ldots, (j_{M-1}, m_{M-1})\} \subset \mathcal{U}$. The corresponding state

$$\{|j_0, m_0), \ldots, (j_{M-1}, m_{M-1})\rangle = B_0^\dagger \ldots B_{M-1}^\dagger |0\rangle$$  

(4)

is created by acting on the empty state $|0\rangle$ with the same creation operators as for the Bose problem

$$B_\ell^\dagger = \sum_{\ell=0}^L \frac{A_{\ell}^\dagger}{2\varepsilon_\ell - E_\nu}.$$  

(5)

Here, the $E_\nu$ are generalized pair level energies (called roots), which are the central objects in the Richardson solution, and $L$ is a cutoff on the single-particle spectrum. In particular, the energy of the state (4) is

$$E = \sum_{\nu=0}^{M-1} E_\nu$$  

(6)

with additional single-particle contributions of blocked levels. The state (4) is an eigenstate of Eq. (1) provided that the roots $E_\nu$ solve the Richardson equations

$$\frac{1}{\tilde{\gamma}} - \sum_{\ell,\mu} \frac{d_\ell}{2\varepsilon_\ell - E_\nu} + \sum_{\mu=0,\mu\neq\nu}^{M-1} \frac{2}{E_\mu - E_\nu} = 0.$$  

(7)

Here, the first two terms are the same as for bosons and the last term, which couples different occupied levels, is a hard-core contribution.

We solve the Richardson equations (7) iteratively starting from a noninteracting configuration with a set of blocked and pair-occupied levels, the latter setting the initial conditions for the roots $E_\nu$. Throughout the Letter, to make contact with the experiment [10], we consider a 2D harmonic oscillator with a cutoff at twice the Fermi level of an $N$-particle ground state configuration. We subtract a linear divergence in the second term of the Richardson equations by defining a renormalized coupling

$$\tilde{\gamma}^{-1} = \frac{1}{\tilde{\gamma}^{-1}} + \sum_{\ell=0}^L d_\ell/2\varepsilon_\ell.$$  

Roots derived from degenerate levels are split in the complex plane, and with increasing interaction strength there can be singular points at which two or more roots merge and bifurcate. These singularities are not reflected in the energy or other observables, but they need to be resolved by any solution algorithm, see Ref. [35] for a detailed discussion of the numerical implementation.

We first examine the ground state configurations: To illustrate the Richardson solution, Fig. 4(a) shows the roots $E_\nu$ as a function of the interaction strength for $N = 12$ particles, which has a singular point at $\tilde{\gamma} = 0.5$ (here involving the merging of three roots). The inset depicts the corresponding noninteracting parent state from which the state evolves. [Note that the pairing Hamiltonian couples states within a shell equally, hence the ordering of pair- or singly-occupied states within a shell is not important.] The parent configuration here is nondegenerate with completely filled orbitals (for the 2D harmonic oscillator, this happens for so-called “magic” numbers $N = 2, 6, 12, 20, \ldots$). For comparison, Fig. 4(b) shows an $N = 10$ configuration with an open shell at the Fermi level, where degenerate roots are split in the complex plane without further merging.

Figure 2(a) shows the ground state energy as a function of particle number for three different interaction strengths $\tilde{\gamma} = 0.1, 0.3$, and 1. Here, we consider configurations with nondegenerate ground states, corresponding to the closed-shell configurations discussed above as well as open-shell configurations in which all states at the Fermi level are filled with one spin species [see the inset for an illustration]. As is apparent from the figure, closed-shell states have an enhanced pairing energy compared to their open-shell neighbors, which is a gen-
eral feature of attractive pairing interactions [36] that we here generalize to degenerate systems. The excess energy of open-shell configurations is [31]

$$\Delta_{ML} = \tilde{E}_{gs}(n_F) - \frac{1}{2}(E_{gs}(n_F-1) + E_{gs}(n_F)) \quad (8)$$

as indicated in Fig. 2(a). Here, $\tilde{E}(n_F)$ and $E_{gs}(n_F)$ are open-shell and closed-shell ground-state energies with Fermi level $n_F$, respectively. The quantity (8) is called the Matveev-Larkin parameter [31] and it generalizes the bulk gap $\Delta$ to mesoscopic ensembles: Indeed, for large particle number, it is (up to finite-size corrections) [31, 37]

$$\Delta_{ML} = d_{n_F} \Delta, \quad (9)$$

where $\Delta$ solves the gap equation

$$\frac{1}{g} = \sum_{\ell=0}^{L} \frac{d_{\ell}}{2E_{\ell}} \quad (10)$$

with $E_{\ell} = \sqrt{(\varepsilon_{\ell} - \mu)^2 + \Delta^2}$ and $\mu$ is a chemical potential that constrains $N = \sum_{\ell}(1 - (\varepsilon_{\ell} - \mu)/E_{\ell})$. For the harmonic oscillator, $\Delta \sim \sqrt{N}$ for large $N$ such that the Matveev-Larkin parameter is extensive. By contrast, for small particle numbers and interaction strength, its value is set by the perturbative result

$$\Delta_{ML} = d_{n_F} \frac{\tilde{g}}{2}, \quad (11)$$

which scales as $O(\sqrt{N})$ with much smaller magnitude. Indeed, a full solution of the pairing model agrees with this picture as shown in Fig. 2(b) which shows the intensive quantity $\Delta_{ML}/N$ for the same interaction strengths as in Fig. 2(a). The crossover between the perturbative and the bulk regime is most apparent for $\tilde{g} = 0.1$, and the crossover region shifts to smaller particle number with increasing interaction [dotted line]. Note that even a small increase in the interaction strength has a strong effect on the crossover region compared to 1D systems [38], which we attribute to the increased density of states in 2D traps. While existing experiments on one-dimensional quantum wires [39] or trapped atoms [9] appear firmly in the perturbative limit [32, 38], our calculations indicate that experiments on 2D Fermi gases may allow to explore this crossover problem in full even for moderate particle numbers.

We proceed to discuss excited states, which are the main results of the Letter. Figure 3(a) shows the excitation spectrum for $N = 12$ particles, which has a closed-shell ground state, where we include with each excitation branch the occupation of the noninteracting parent state. Excitations are obtained either by creating pair excitations or by breaking pairs and promoting single fermions to higher levels, where we show pair-breaking excitations only up to the second level. We include the parent state configuration for several excitations. The dashed line is the mean field prediction $2\Delta$ for the Higgs excitation.
few-to-many body crossover, which we describe in the following.

Figure 4 shows the evolution of the pair excitation for 15 closed-shell configurations with \( N = 6, 12, 20, 30, 42, 56, 72, 90, 110, 132, 156, 182, 210, 240, \) and 272 [gray lines]. For larger particle numbers, the gap decreases, and the position of the minimum shifts to smaller coupling. Indeed, it extrapolates to infinite particle number in a power-law form \( E_{\text{min}} \sim g_{\text{min}}^{-\alpha} \) with \( \alpha = 0.29(1) \) [bold blue line]. This behavior is consistent with the expectation that in the thermodynamic limit, the pairing instability occurs at arbitrarily weak interaction strength \( \tilde{g} \). An important benchmark of our results are configuration-interaction calculations in the few-body limit \([25]\) shown as orange and green crosses, where the latter calculations restrict the Hilbert space to three shells near the Fermi level. In both cases, we identify an effective interaction strength \( \tilde{g} \) by relating the coupling in the respective calculations to the Fermi energy as \( \tilde{g} = A \varepsilon_F/\langle n_F \rangle \) or \( \tilde{g} = A g/\langle n_F \rangle \) with a joint fit parameter \( A \) for different \( N \), where \( \varepsilon_F \) is a critical bound-state energy (in units of the trap frequency) and \( g \) a bare contact interaction parameter. In all cases, the location of the minimum is quite well reproduced, indicating that the pairing model accurately captures pairing interactions at the Fermi level. Moreover, while there is a deviation of 10% for the minimum excitation energy between our calculations and the results of \([25]\) for \( N = 6 \) (indicating the relevance of pair-breaking matrix elements neglected in the pairing model), the agreement improves to 2% with the three-shell calculation at \( N = 30 \). This improved agreement with increasing \( N \) suggests that the pairing model complements exact few-body calculations and provides a reliable extrapolation to large particle numbers. In addition, data points in the figure [green diamonds] show experimental measurements for \( N = 6 \) and \( N = 12 \) by Bayha et al. \([10]\). We are able to fit the experimental data by including a small trap anisotropy of 1% for \( N = 6 \) and of 0.4% for \( N = 12 \) in our calculations [thin green lines], in line with the experimental anisotropy \([10]\).

To describe the few-to-many crossover quantitatively, we show in Fig. 5(a) the position of the minimum of the pair excitation in Fig. 4 as a function of particle number, and Fig. 5(b) shows the excitation minimum. Both quantities vanish as a power law with increasing particle number: First, for the position of the minimum, we obtain \( \tilde{g}_{\text{min}} \sim N^{-\nu} \) with \( \nu = 1.50(5) \) [blue line]. The location of the minimum compares well with the mean-field prediction for the critical coupling [gray points], which further corroborates the interpretation of the pairing excitation as the few-body precursor of a quantum phase transition. Second, the excitation minimum decreases as \( E_{\text{min}} \sim N^{-\beta} \) with an exponent \( \beta = 0.20(1) \) [blue line] that is characteristic of the finite-size scaling of the superfluid transition.

In summary, we provide a description of trapped Fermi
gases with attractive pairing interactions that captures the full crossover between the few-body and the many-body regime. Our results indicate that the finite-size scaling of the quantum phase transition sets in early and is observable in experiments with few-body Fermi gases. Moreover, the pairing model used here is very versatile, in particular, it can be used to compute correlation functions [43, 44] as recently measured in [12].

We thank Johannes Bjerlin for discussions and Stephanie Reimann for discussions and comments on the manuscript. This work is supported by Vetenskapsrådet (grant number 2020-04239).

FIG. 5. (a) Position and (b) Size of the minimum of the pair excitation energy as a function of particle number.

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