Classification of the pairing transition in finite fermionic systems

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In this work we employ a simple pairing interaction model in order to study and classify an eventual pairing phase transition in finite fermionic systems. We show that systems with as few as \( \sim 10 - 16 \) fermions can exhibit clear features reminiscent of a phase transition. To classify the nature of the transition we apply two different numerical methods, one based on standard thermodynamics, and another based on a recently proposed scheme by Borrmann et al. [Phys. Rev. Lett. 84, 3511 (2000)]. The transition is shown to be of second order, in agreement with results for infinite fermionic systems.

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The standard BCS theory has been widely used to describe systems with pairing correlations and phase transitions to a superconducting phase for large systems, from the solid state to nuclear physics, with neutron stars as perhaps the largest object in the universe exhibiting superfluidity in its interior. An eventual superfluid phase in a neutron star will condition the neutrino emission and thereby the cooling history of such a star, in addition to inducing mechanisms such as sudden spin ups in the rotational period of the star; see, for example, Ref. [1] for a recent review. For an infinite system, such as a neutron star, the nature of the pairing phase transition is well established as second order.

When a system of correlated fermions such as electrons or nucleons is sufficiently small, the fermionic spectrum becomes discrete. If the spacing approaches the size of the pairing gap, superconductivity is expected to break down; however, recent experiments on superconducting ultrasmall aluminum grains by Tinkham et al. revealed the existence of a spectroscopic gap larger than the average electronic level density. This feature was interpreted as a reminiscence of superconductivity and renewed the interest in studies of what is the lower size limit for superconductivity.

Other finite fermionic systems such as nuclei are expected to exhibit a variety of interesting phase-transition like phenomena, like the disappearance of pairing at a critical temperature \( T_C \approx 0.5 - 1 \text{ MeV} \) or the nuclear shape transitions of deformed nuclei associated with the melting of shell effects at \( T_C \approx 1 - 12 \text{ MeV} \). In recent theoretical and experimental studies of thermodynamical properties of finite nuclei, the heat capacity has been found to exhibit a non-vanishing bump at temperatures proportional to half the pairing gap. These bumps were interpreted as signs of the quenching of pair correlations, representing in turn features of the pairing transition for an infinitely large system.

In the study of phase transitions in e.g., solid state, nuclear and high energy physics, it is important to know whether a given transition really is of first order, discontinuous, or if there is a continuous change in a physical quantity like the mean energy, as in phase transitions of second order. If one works in the canonical or grand canonical ensembles, for finite systems it is rather difficult to decide on the order of the phase transition. This is due to the fact that in ensembles like the canonical, any anomaly is smeared over a temperature range of \( 1/N \), \( N \) being the number of particles. In the analysis of finite systems, both a \( \delta \)-function peak and a power law singularity sharpen as the number of particles is increased, making it difficult to distinguish between the two cases, see, for example, Ref. [10].

In addition, first order phase transitions in finite systems have recently been inferred, theoretically and experimentally, from observed negative heat capacities that are associated with anomalous convex intruders in the entropy versus energy curves, resulting in backbendings in the caloric curves; see, for example, Refs. [11, 12]. Negative heat capacities are often claimed to appear only in calculations done in the microcanonical ensemble and are thought to vanish in the canonical or grand-canonical ensembles.

We aim in this Letter to identify the nature of the pairing transition, if any, in a finite fermionic system. Since we are dealing with pairing correlations, our Hamiltonian is

\[
H = \sum_i \varepsilon_i a_i^\dagger a_i - G \sum_{ij} a_i^\dagger a_j^\dagger a_j a_j,
\]

where \( a^\dagger \) and \( a \) are fermion creation and annihilation operators, respectively. The indices \( i \) and \( j \) run over the number of levels \( L \), and the label \( \bar{i} \) stands for a time-reversed state. The parameter \( G \) is the strength of the
pairing force while $\varepsilon_i$ is the single-particle energy of level $i$.

We assume that the single-particle levels are equidistant with a fixed spacing $d$. Moreover, in our simple model, the degeneracy of the single-particle levels is set to $2J+1 = 2$, with $J = 1/2$ being the spin of the particle. Introducing the pair-creation operator $S_i^+ = a_{i m}^{\dagger} a_{i -m}^{\dagger}$, one can rewrite the Hamiltonian in Eq. (1) as

$$H = d \sum_i i N_i - G \sum_{ij} S_i^+ S_j^-, \quad (2)$$

where $N_i = a_{i m}^{\dagger} a_i$ is the number operator. Seniority $S$ is a good quantum number and the eigenvalue problem can be block-diagonalized in terms of different seniority values. Loosely speaking, the seniority quantum number $S$ is equal to the number of unpaired particles.

For systems with less than $16 - 18$ particles, this model can be diagonalized exactly, and we can obtain all eigenstates. In our studies below, we will always consider the case of half-filling, i.e., equally many particles and single-particle levels. This case has the largest dimensionality: for 16 particles in 16 doubly degenerate single-particle shells, we have a total of $4 \times 10^8$ states. We choose units MeV for the energy and set $G = 0.2$ MeV in all calculations while we let $d$ vary.

Through diagonalization of the above Hamiltonian we can define exactly the density of states $\Omega_N(E)$ for an $N$-particle system with excitation energy $E$. An alternative to the exact diagonalization, would be to use Richardson’s well-known solution [13]; however, we are interested in all eigenstates, and the amount of numerical labor will most likely be similar. The density of states is an essential ingredient in the evaluation of thermal averages and for the discussion of phase transitions in finite systems. For nuclei, experimental information on the density of states is expected to reveal important information on nuclear shell structure, pair correlations and other correlation phenomena in the nucleonic motion.

The density of states $\Omega_N(E)$ is the statistical weight of the given state with excitation energy $E$, and its logarithm

$$S_N(E) = k_B \ln \Omega_N(E), \quad (3)$$

is the entropy (we set Boltzmann’s constant $k_B = 1$) of the $N$-particle system. The density of states defines also the partition function in the microcanonical ensemble and can be used to compute the partition function $Z$ of the canonical ensemble through

$$Z(\beta) = \sum_E \Omega_N(E) e^{-\beta E}, \quad (4)$$

with $\beta = 1/T$ the inverse temperature. With $Z$ it is straightforward to generate other thermodynamical properties such as the mean energy $\langle E \rangle$ or the specific heat $C_V$.

The density of states can also be used to define the free energy $F(E)$ in the microcanonical ensemble at a fixed temperature $T$ (actually an expectation value in this ensemble),

$$F(E) = -T \ln \left[ \Omega_N(E) e^{-\beta E} \right]. \quad (5)$$

Note that here we include only configurations at a particular $E$.

The above free energy was used by e.g., Lee and Kosterlitz [16], based on the histogram approach for studying phase transitions developed by Ferrenberg and Swendsen [17], in their studies of phase transitions of classical spin systems. If a phase transition is present, a plot of $F(E)$ versus $E$ will show two local minima which correspond to configurations that are characteristic of the high and low temperature phases. At the transition temperature $T_C$, the value of $F(E)$ at the two minima equal, while at temperatures below $T_C$, the low-energy minimum is the absolute minimum. At temperatures above $T_C$, the high-energy minimum is the largest. If there is no phase transition, the system develops only one minimum for all temperatures.

To elucidate the nature of the pairing transition we employ two different approaches, which both rely on our ability of computing the exact density of states $\Omega(E)$.

First, we calculate exactly the free energy $F(E)$ of Eq. (4) through diagonalization of the pairing Hamiltonian of Eq. (1) for systems with up to 16 particles in 16 doubly degenerate levels. For $d/G = 0.5$ and 16 single-particle levels, we develop two clear minima for the free energy. This is seen in Fig. 4 where we show the free energy as function of excitation energy using Eq. (4) at temperatures $T = 0.5$, $T = 0.85$ and $T = 1.0$ MeV. The first minimum corresponds to the case where we break one pair. The second and third minima correspond to cases where two and three pairs are broken, respectively. When two pairs are broken, corresponding to seniority $S = 4$, the free energy minimum is made up of contributions from states with $S = 0, 2, 4$. These contributions serve to lower the free energy. Similarly, with three pairs broken we see a new free energy minimum which receives contributions from states with $S = 0, 2, 4, 6$.

At higher excitation energies, population inversion takes place, and our model is no longer realistic.

We note that for $T = 0.5$ MeV, the minima at lower excitation energies are favored. At $T = 1.0$ MeV, the higher energy phase (more broken pairs) is favored. We see also, at $T = 0.85$ MeV, that the free-energy minima where we break two and three pairs equal. Where two
minima coexist, we may have an indication of a phase transition. Note however that this is not a phase transition in the ordinary thermodynamical sense. There is no abrupt transition from a purely paired phase to a nonpaired phase. Instead, our system develops several such intermediate steps where different numbers of broken pairs can coexist. At e.g., $T = 0.95$ MeV, we find again two equal minima. For this case, seniority $S = 6$ and $S = 8$ yield two equal minima. This picture repeats itself for higher seniority and higher temperatures.

If we then focus on the second and third minima, i.e., where we break two and three pairs, respectively, the difference $\Delta F$ between the minimum and the maximum of the free energy, can aid us in distinguishing between a first order and a second order phase transition. If $\Delta F/N$ remains constant as $N$ increases, we have a second order transition. An increasing $\Delta F/N$ indicates a first order phase transition. In Table 1 we display $\Delta F/N$ for $N = 10, 12, 14$ and $16$ at $T = 0.85$ MeV. It is important to note that the features seen in Fig. 1, apply to the cases with $N = 10, 12$ and $14$ as well, where $T = 0.85$ MeV is the temperature where the second and third minima equal. This means that the temperature where the transition is meant to take place remains stable as function of number of single-particle levels and particles. This is in agreement with the simulations of Lee and Kosterlitz [10]. We find a similar result for the minima developed in agreement with the simulations of Lee and Kosterlitz [19], Grossmann et al. [20] and Borrmann et al. [21]. The authors of Ref. [21] showed that the distributions of zeros are able to reveal the thermodynamic secrets of small systems in a distinct manner. Major contributions to the specific heat come from zeros close to the real axis, and a zero approaching the real axis infinitely closely causes a divergence in the specific heat. To characterize the DOZ close to the real axis, one assumes that the zeros lie approximately on a straight line. Defining the three parameters $\tau, \gamma$ and $\alpha$, see Ref. [21] for details, one can define entirely the nature of the phase transition. For a true phase transition in the Ehrenfest sense we have $\tau \rightarrow 0$. For this case it has been shown [21] that a phase transition is completely classified by $\alpha$ and $\gamma$. In the case $\alpha = 0$ and $\gamma = 0$ the specific heat $C_V(\beta)$ exhibits a $\delta$-peak corresponding to a phase transition of first order. For $0 < \alpha < 1$ and $\gamma = 0$ (or $\gamma \neq 0$) the transition is of second order. A higher order transition occurs for $1 < \alpha$ and arbitrary $\gamma$.

In Fig. 2 we show contour plots of the specific heat $C_\nu(B)$ in the complex temperature plane for $N = 11$ (a), 14 (b), and 16 (c) particles at normal pairing $d/G = 0.5$ and the $N = 14$ (d) in the weak pairing limit, $d/G = 2$. The poles are at the center of the dark contour regions. We see evidence of two phases in these systems. The first phase, labeled $I$ in Fig. 2, is a mixed seniority phase while the second phase, $II$, is a paired phase with zero seniority and exists only in even-$N$ systems. No paired phase exists in the $N = 11$ system and no clear boundaries are evident in the weak pairing case. We find that for (b) and (c) the DOZ are apparently distributed along two lines where the intersection occurs at $\tau_1$, which is the pole closest to the real axis. As the pairing branch (for $\beta > \beta_1$) only encompasses two points, we are unable to precisely determine $\alpha$ along this branch while $\gamma > 0$. Based on our free energy results discussed above, we believe $\alpha$ along this branch will be positive. In the mixed phase branch (for $\beta < \beta_1$) we find $\gamma < 0$, and $\alpha < 0$ in all normal-pairing cases. The parameter $\tau_1$, which is a measure of discreteness shows a $\tau_1 \sim N^{-1.4 \pm 0.12}$ dependence.

We note several significant results of this work. From two independent methods we find that the transition from the paired seniority zero ground state to a mixed phase state is second order. The free-energy analysis also demonstrates that each transition in seniority phases in the microcanonical ensemble is of second order. The strength of the pairing in these systems determines the nature of the phase transitions. In particular, for a weakly paired system, we found no evidence for two phases, while normal pairing strengths, such as those found in nuclei, may well exhibit the paired-phase and mixed seniority phases that we demonstrated in this model. We will include more realistic interactions to investigate this point in future work. We also found, using Auxiliary Field Monte Carlo computations for this system together with the histogram method of Refs. [14,17], that the energy fluctuations in the canonical ensemble make it rather difficult to extract useful
information on the nature of the phase transitions from these techniques.

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|   | 10  |   | 12  |   | 14  |   | 16  |   |
|---|-----|---|-----|---|-----|---|-----|---|
| $N$ | $\Delta F/N$ [MeV] | 0.531 | 0.505 | 0.501 | 0.495 |

TABLE I. $\Delta F/N$ for $T = 0.85$ MeV. See text for further details.
FIG. 1. Free energy from Eq. (5) at $T = 0.5$, 0.85 and $T = 1.0$ MeV with $d/G = 0.5$ with 16 particles in 16 doubly degenerate levels. All energies are in units of MeV and an energy bin of $10^{-3}$ MeV has been chosen.
FIG. 2. Contour plots of the specific heat in the complex temperature plane for a) $N = 11$, b) $N = 14$, and c) $N = 16$ particles. Panel d) shows the $N = 14$ case with weak pairing. The spots indicate the locations of the zeros of the canonical partition function.