Pairing correlations and transitions in nuclear systems

A. Belić\textsuperscript{a}, D. J. Dean\textsuperscript{b}, and M. Hjorth-Jensen\textsuperscript{c}

\textsuperscript{a}Institute of Physics, P.O.B. 57, Belgrade 11001, Serbia and Montenegro
\textsuperscript{b}Physics Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6373, USA
\textsuperscript{c}Department of Physics and Center of Mathematics for Applications, University of Oslo, N-0316 Oslo, Norway

Abstract

We discuss several pairing-related phenomena in nuclear systems, ranging from superfluidity in neutron stars to the gradual breaking of pairs in finite nuclei. We describe recent experimental evidence that points to a relation between pairing and phase transitions (or transformations) in finite nuclear systems. A simple pairing interaction model is used in order to study and classify an eventual pairing phase transition in finite fermionic systems such as nuclei. We show that systems with as few as $\sim 10^{16}$ fermions can exhibit clear features reminiscent of a phase transition.

1 Introduction

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. [1,2] for recent reviews. 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 [3]; however, recent experiments on superconducting ultrasmall aluminum grains by Tinkham et al. [4] 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 [5,6,7,8] 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 $T_c \approx 0.5 - 1$ MeV or the nuclear shape transitions of deformed nuclei associated with the melting of shell effects at $T_c \approx 1 - 12$ MeV. Pairing correlations are expected to play an essential role in nuclear systems, ranging from the binding energy, excitation spectrum and odd-even effects in finite nuclei to superfluidity in the interior of neutron stars. In recent theoretical and experimental studies [9,10] 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 eventual transitions in e.g., nuclear 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. [11]. 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. [10,11,12,13,14,15]. 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.

In this work we give first a brief review in Sec. 2 of pairing features in infinite neutron matter. In Sec. 3 we discuss experimental results indicating the gradual breaking of pairs in nuclei. A simple pairing model is in turn used in Sec. 4 to show the similarities between the experimental results and the gradual breaking of pairs. Concluding remarks are presented in Sec. 5.
2 Pairing in infinite neutron matter

The presence of neutron superfluidity in the crust and the inner part of neutron stars are considered well established in the physics of these compact stellar objects. In the low density outer part of a neutron star, the neutron superfluidity is expected mainly in the attractive $^1S_0$ channel. At higher density, the nuclei in the crust dissolve, and one expects a region consisting of a quantum liquid of neutrons and protons in beta equilibrium. The proton contaminant should be superfluid in the $^1S_0$ channel, while neutron superfluidity is expected to occur mainly in the coupled $^3P_2-^3F_2$ two-neutron channel. In the core of the star any superfluid phase should finally disappear.

The presence of two different superfluid regimes is suggested by the known trend of the nucleon-nucleon (NN) phase shifts in each scattering channel. In both the $^1S_0$ and $^3P_2-^3F_2$ channels the phase shifts indicate that the NN interaction is attractive. In particular for the $^1S_0$ channel, the occurrence of the well known virtual state in the neutron-neutron channel strongly suggests the possibility of a pairing condensate at low density, while for the $^3P_2-^3F_2$ channel the interaction becomes strongly attractive only at higher energy, which therefore suggests a possible pairing condensate in this channel at higher densities. In recent years the BCS gap equation has been solved with realistic interactions, and the results confirm these expectations.

The $^1S_0$ neutron superfluid is relevant for phenomena that can occur in the inner crust of neutron stars, like the formation of glitches, which may to be related to vortex pinning of the superfluid phase in the solid crust [16]. The results of different groups are in close agreement on the $^1S_0$ pairing gap values and on its density dependence, which shows a peak value of about 3 MeV at a Fermi momentum close to $k_F \approx 0.8$ fm$^{-1}$ [17,18,19,20]. All these calculations adopt the bare NN interaction or effective interactions without screening corrections as the pairing force. It has been pointed out that the screening by the medium of the interaction could strongly reduce the pairing strength in this channel [20,21,22]. However, the issue of the many-body calculation of the pairing effective interaction is a complex one and still far from a satisfactory solution.

The precise knowledge of the $^3P_2-^3F_2$ pairing gap is of paramount relevance for, e.g., the cooling of neutron stars, and different values correspond to drastically different scenarios for the cooling process. Generally, the gap suppresses the cooling by a factor $\sim \exp(-\Delta/T)$ (where $\Delta$ is the energy gap) which is severe for temperatures well below the gap energy.

For $\beta$-stable matter in equilibrium, the neutron $^1S_0$ pairing gap appears at densities corresponding to the crust of the star. It is generally believed that
it is the proton contaminant and its $^1S_0$ pairing gap which dominates in the region from the inner crust to the densities 2-3 times nuclear matter saturation density, together with the $^3P_2$ gap. The general picture can be summarized as follows:

- The $^1S_0$ proton gap in $\beta$-stable matter is $\leq 1$ MeV, and if polarization effects were taken into account [20], it could be further reduced by a factor 2-3.
- The $^3P_2$ gap is also small, of the order of $\sim 0.1$ MeV in $\beta$-stable matter. If relativistic effects are taken into account, it is almost vanishing. However, there is quite some uncertainty with the value for this pairing gap for densities above $\sim 0.3$ fm$^{-3}$ due to the fact that the NN interactions are not fitted for the corresponding lab energies.
- Higher partial waves give essentially vanishing pairing gaps in $\beta$-stable matter.

Thus, the $^1S_0$ and $^3P_2$ partial waves are crucial for our understanding of superfluidity in neutron star matter. However, hyperons such as $\Sigma^{-1}$ and $\Lambda$ may be present at twice or more nuclear matter saturation energy. There are indications that the $\Lambda\Lambda$ interaction is too weak to support a $\Lambda$ gap, while $\Delta_{\Sigma^{-1}} \sim 10$ MeV. Recent cooling simulations seem to indicate that available observations of thermal emissions from pulsars can aid in constraining hyperon gaps. However, all these calculations suffer from the fact that the microscopic inputs, pairing gaps, composition of matter, emissivity rates, etc. are not computed at the same many-body theoretical level. This leaves a considerable uncertainty.

We have not mentioned recent developments beyond the BCS approach, nor have we discussed results for proton-neutron pairing in symmetric or asymmetric matter. Such topics are addressed in the recent works of Lombardo, Schulze and collaborators, see e.g., Refs. [2,23,24] and references therein.

3 Thermodynamic properties of nuclei and pairing

The thermodynamical properties of nuclei deviate from infinite systems, although the spectroscopy of finite nuclei and especially many isotopes, are dominated by the same partial waves which are important in neutron star matter, see ref. [2].

While the quenching of pairing in superconductors is well described as a function of temperature, the nucleus represents a finite many body system characterized by large fluctuations in the thermodynamic observables. A long-standing problem in experimental nuclear physics has been to observe the transition from strongly paired states, at around $T = 0$, to unpaired states at
higher temperatures.

In nuclear theory, the pairing gap parameter $\Delta$ can be studied as function of temperature using the BCS gap equations [25,26]. From this simple model the gap decreases monotonically to zero at a critical temperature of $T_c \sim 0.5 \Delta$. However, if particle number is projected out [27,28], the decrease is significantly delayed. The predicted decrease of pair correlations takes place over several MeV of excitation energy [28]. Recently [10], structures in the level densities in the 1–7 MeV region were reported, structures which probably are due to the breaking of nucleon pairs and a gradual decrease of pair correlations.

Experimental data on the quenching of pair correlations are important as a test for nuclear theories. Within finite temperature BCS and RPA models, level density and specific heat are calculated for e.g., $^{58}$Ni [29]; within the shell model Monte Carlo method (SMMC) [30,31] one is now able to estimate level densities [32] in heavy nuclei [33] up to high excitation energies. Here we report on the observation of the gradual transition from strongly paired states to unpaired states in rare earth nuclei at low spin. The canonical heat capacity is used as a thermometer. Since only particles at the Fermi surface contribute to this quantity, it is very sensitive to phase transitions. It has been demonstrated from SMMC calculations in the Fe region [34,35], that breaking of only one nucleon pair increases the heat capacity significantly.

The experiments were carried out with 45 MeV $^3$He projectiles from the MC-35 cyclotron at the University of Oslo. In that experiment, one could extract level densities and $\gamma$ strength functions for the $^{161,162}$Dy and $^{171,172}$Yb nuclei. The data for the even nuclei are published recently [10].

The partition function in the canonical ensemble $Z(T) = \sum_{n=0}^{\infty} \rho(E_n) e^{-E_n/T}$ is determined by the measured level density of accessible states $\rho(E_n)$ in the present nuclear reaction. Strictly, the sum should run from zero to infinity. Here we calculate $Z$ for temperatures up to $T = 1$ MeV. However, the experimental level densities only cover the excitation region up close to the neutron binding energy of about 6 and 8 MeV for odd and even mass nuclei, respectively. For higher energies it is reasonable to assume Fermi gas properties, since single particles are excited into the continuum region with high level density. Therefore, due to lack of experimental data, the level density is extrapolated to higher energies by the shifted Fermi gas model expression [37]. The extraction of the microcanonical heat capacity $C_V(E)$ gives large fluctuations which are difficult to interpret [10]. Therefore, the heat capacity $C_V(T)$ is calculated within the canonical ensemble, where $T$ is a fixed input value in the theory, and a more appropriate parameter, see e.g., Schiller et al. [10] for further details.

The deduced heat capacities for the $^{161,162}$Dy nuclei are shown in Fig. 1 to-
together with the SMMC results of Liu and Alhassid [36] for various iron isotopes. The results labelled 'model' are discussed further in Refs. [2,10]. We note that both the theoretical and experimental results exhibit S-shaped $C_V(T)$-curves. The S-shaped curve is interpreted as a fingerprint of a phase transition in a finite system from a phase with strong pairing correlations to a phase without such correlations. Due to the strong smoothing introduced by the transformation to the canonical ensemble, we do not expect to see discrete transitions between the various quasiparticle regimes, but only the transition where all pairing correlations are quenched as a whole. It is worth noticing that the S-shape is much less pronounced for the odd system, again a possible indication of the importance of pairing correlations. This can also be seen from Fig. 2, taken from Ref. [10].

Here we notice that the entropy of the even and odd systems merge at a temperature $T \approx 0.5$ MeV, in close agreement with the point where the S-shape of the heat capacity of the $^{161,162}$Dy nuclei appears in Fig. 1. The temperature where the experimental entropies merge, could in turn be interpreted as the point where other degrees of freedom than pairing take over. A theoretical interpretation in terms of the vanishing of pairing correlations is given in Refs. [10]. The extraction of the microcanonical heat capacity $C_V(E)$ gives large fluctuations which are difficult to interpret [10]. Therefore, the heat capacity $C_V(T)$ is calculated within the canonical ensemble, where $T$ is a fixed input value in the theory, and a more appropriate parameter, see e.g., Schiller et al. [10] for further details.
Fig. 2. Experimental entropy in the canonical ensemble for $^{161,162}$Dy and for $^{171,172}$Yb.

The deduced heat capacities for the $^{161,162}$Dy nuclei are shown in Fig. 1 together with the SMMC results of Liu and Alhassid [36] for various iron isotopes. The results labelled ‘model’ are discussed further in Ref. [10]. We note that both the theoretical and experimental results exhibit S-shaped $C_V(T)$-curves. The S-shaped curve is interpreted as a fingerprint of a phase transition in a finite system from a phase with strong pairing correlations to a phase without such correlations. Due to the strong smoothing introduced by the transformation to the canonical ensemble, we do not expect to see discrete transitions between the various quasiparticle regimes, but only the transition where all pairing correlations are quenched as a whole. It is worth noticing that the S-shape is much less pronounced for the odd system, again a possible indication of the importance of pairing correlations. This can also be seen from Fig. 2, taken from Ref. [10]. Here we notice that the entropy of the even and odd systems merge at a temperature $T \approx 0.5$ MeV, in close agreement with the point where the S-shape of the heat capacity of the $^{161,162}$Dy nuclei appears in Fig. 1. The temperature where the experimental entropies merge, could in turn be interpreted as the point where other degrees of freedom than pairing take over. A theoretical interpretation in terms of the vanishing of
pairing correlations is given in Ref. [10] and in the next section.

4 Simple pairing model and nature of the pairing transition

We aim here to identify the nature of the pairing transition and give a theoretical interpretation of the results from the previous section. Since we are dealing with pairing correlations, our Hamiltonian is

\[ H = \sum_i \varepsilon_i a_i^\dagger a_i - G \sum_{ij>0} a_i^\dagger a_j^\dagger a_j, \]  

(1)

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. 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 \( \sim 16 - 18 \) 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 [38], 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

\[ S_N(E) = k_B \ln \Omega_N(E), \]  

(2)
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

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

(3)

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),

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

(4)

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

The above free energy was used by e.g., Lee and Kosterlitz [39], based on the histogram approach for studying phase transitions developed by Ferrenberg and Swendsen [40], 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. Since we are dealing with finite systems, we can study the development of the two minima as function of the dimension of the system and thereby extract information about the nature of the phase transition. If we are dealing with a second order phase transition, the behavior of $F(E)$ does not change dramatically as the size of the system increases. However, if the transition is first order, the difference in free energy, i.e., the distance between the maximum and minimum values, will increase with increasing dimension.

To elucidate the nature of the transition 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. 3 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 $S = 0, 2, 4, 6$. 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 4 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. 3, 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 [39]. We find a similar result for the minima developed at $T = 0.95$ MeV, where both $S = 6$ and $S = 8$ coexist. However, due to population inversion, these minima are only seen clearly for $N = 12, 14$ and 16 particles.

Table 4 reveals that $\Delta F/N$ is nearly constant, with $\Delta F/N \approx 0.5$ MeV, indicating a transition of second order. This result is in agreement with what is expected for an infinite system. It is also easy to see from Fig. 3, that the entropy in the microcanonical ensemble can be convex for certain excitation energy ranges, resulting in eventual negative heat capacities, as inferred from

\begin{table}[h]
\centering
\begin{tabular}{cccc}
\hline
$N$ & 10 & 12 & 14 & 16 \\
\hline
$\Delta F/N$ [MeV] & 0.531 & 0.505 & 0.501 & 0.495 \\
\hline
\end{tabular}
\caption{\Delta F/N for $T = 0.85$ MeV. See text for further details.}
\end{table}
Fig. 3. Free energy from Eq. (4) 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.

the authors of Refs. [11,12]. The analysis above however, does not lend support to interpreting this as a sign of a first order phase transition.

We note the important result that for $d/G > 1.5$, our free energy, for $N \leq 16$, develops only one minimum for all temperatures. That is, for larger single-particle spacings, there is no sign of a phase transition. This means that there is a critical relation between $d$ and $G$ for the appearance of a phase transition-like behavior, being a reminiscence of the thermodynamical limit. This agrees also with e.g., the results for ultrasmall metallic grains [8].

We have thus indications 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 [31] together with the histogram method of Refs. [39,40], 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.

5 Conclusions

In summary, the $^{1}S_{0}$ and $^{3}P_{2}$ partial waves are crucial for our understanding of superfluidity in neutron star matter. The role of polarization terms and hyperon pairing are still open and unsettled topics, see ref. [2] for further discussions. Furthermore, we have also discussed recent experimental and theoretical studies of thermodynamical properties of finite nuclei and their interpretation in terms of eventual pairing transitions in finite nuclei. For a more detailed theoretical analysis we would however need extensive shell-model Monte Carlo simulations in order to test the role played by e.g., pairing terms in the interaction. It is an open question whether such calculations lend support to the experimentally observed level densities.

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