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Structure of pairs in heavy weakly-bound nuclei

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Abstract

We study the structure of nucleon pairs within a simple model consisting of a square well in three dimensions and a delta-function residual interaction between two weakly-bound particles at the Fermi surface. We include the continuum by enclosing the entire system in a large spherical box. To a good approximation, the continuum can be replaced by a small set of optimally-determined resonance states, suggesting that in many nuclei far from stability it may be possible to incorporate continuum effects within traditional shell-model based approximations.

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In weakly-bound nuclei far from the valley of stability, the effects of continuum single-particle states can be significant. The size of these effects and the physical quantities in which they appear are largely unexplored subjects. Previous studies have focussed on specific issues. Dobaczewski et al. [1] formulated the Hartree-Fock-Bogoliubov equations in coordinate space to study pairing near the neutron drip line. Bertsch and Esbensen studied pairing in light halo nuclei, using a Green function framework in which the continuum was discretized [2]. Otsuka, also interested in light halo nuclei, introduced the Variational Shell Model, which implicitly includes effects of continuum states [3]. Our interest here is slightly different. Like Dobaczewski et al., we want to understand aspects of the structure of "heavy" nuclei far from stability. Our intent, however, is to study the adequacy of relatively simple shell-model approximations to a full treatment of the continuum, with the goal of eventually calculating beta decay in nuclei along the r-process path.

We perform all calculations in the following simple model, similar to that used in Ref. [2]: two particles move near the Fermi surface of an external one-body potential and interact via an attractive delta-function two-body potential. The one-body potential is a finite spherical square well plus a surface (derivative) spin orbit force. To include the continuum simply, we enclose the entire system in a large spherical box.

An attractive delta-function potential produces a two-particle bound state at infinitely negative energy when diagonalized in a complete space. To avoid the singularity we follow the procedure of Ref. [2], truncating the continuum so that the bound state appears at zero energy, a physically sensible value. The procedure imposes a relation between the interaction strength and the maximum two-particle kinetic energy; outside the well we take the interaction strength to be 831 MeV fm^3 [2], which implies a cutoff of 40 MeV. To

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simulate density-dependence, we reduce the strength of the interaction inside the well to 300 MeV fm^3, a value that has proved appropriate in shell-model studies that ignore the continuum [4]. We include all partial waves up to $\ell = 7$; neither increasing this number to $\ell = 17$ nor varying the box size between 30 and 50 fm changes the results significantly.

Although we treat only two particles as active, we would like in some measure to simulate the dynamics of heavy nuclei. To do so, we adjust the parameters of the one-body potential so that its single-particle spectrum resembles that in a nucleus with $A \approx 90$. The square well is therefore taken to have a radius R of roughly 5.2 fm and a depth in the range 40–50 MeV. A spin-orbit strength $V_{\text{s.o.}}$ of about 0.4–0.5 fm^2 then results in the standard ordering of single particle levels. We assume that all but the last bound level, or perhaps the last few bound levels, are fully occupied and inert. The two active particles are then distributed over the few remaining bound orbits and all the continuum orbits (i.e., those with positive energy) up to the cutoff. By changing slightly the radius and depth of the square well, we can alter the active single-particle levels and their energies. Here we focus on states with angular momentum zero and positive parity, which span a space of dimension $\approx$ 1000 (2500) two-particle states for a box size of 30 (50) fm.

In what follows, we compare the results of a complete diagonalization in the space of 0^+ states with those obtained at several levels of approximation. We first consider truncation of the continuum to states that are largely confined within the square well, i.e. resonances. We then further reduce the basis by constructing one single-particle state to represent each resonance (the resonances have widths and comprise several such states).

First we discuss the full calculations, some representative results of which appear in Table 1. Here the only bound state included is the $0g_{7/2}$ level. The energy (E_b) of this level ranges from about −300 keV to about −3 MeV; the table gives the largest components of the ground state wave function for three choices of E_b. In all three sets of calculations, the continuum single-particle states never make up more than 25% of the ground state eigenvector. Furthermore, this contribution does not depend strongly on the energy of the active bound orbit, at least within the range specified above. Neither of these two facts is surprising. The continuum states that couple most strongly to the bound orbit through a short-range interaction are those with large spatial overlap. Such states typically belong to resonances and are concentrated within the well. Even though they make up but a small fraction of the total continuum, the resonant states nevertheless provide nearly the full continuum contribution to the ground state; the plethora of non-resonant continuum states couple much more weakly, typically by factors of 1000 or more. But the resonant states are in general well separated in energy from the last bound state, limiting the amount of continuum mixing. Also, as the bound-state energies are lowered the resonances are as well, by roughly the same amount. The energy gap

Table 1
Ground state amplitudes (Amp.) for three sets of calculations involving a bound $0g_{7/2}$ state and its mixing with the continuum. The energy of the bound level is denoted E_b. The levels are labeled by j and l values, together with the unperturbed energies of the two particles. All energies are in MeV; the bound state has negative energy

	Amp.	ℓ_j	E_1	E_2
$E_b = -2.88$ MeV	0.891	$g_{7/2}$	−2.88	−2.88
	−0.307	$h_{11/2}$	1.58	1.58
	0.191	$d_{5/2}$	0.023	0.023
	−0.091	$h_{9/2}$	9.38	9.38
	0.071	$i_{13/2}$	11.2	11.9
	0.070	$i_{13/2}$	11.9	11.9
	−0.064	$h_{9/2}$	8.64	9.38
	−0.044	$h_{9/2}$	9.38	10.7
	0.043	$d_{3/2}$	2.49	3.29
$E_b = -1.24$ MeV	0.889	$g_{7/2}$	−1.24	−1.24
	−0.213	$h_{11/2}$	3.17	3.24
	−0.159	$h_{11/2}$	3.24	3.24
	−0.143	$h_{11/2}$	3.17	3.17
	0.117	$d_{5/2}$	1.07	1.43
	0.102	$d_{5/2}$	1.07	1.07
	−0.077	$h_{9/2}$	10.2	11.1
	0.070	$i_{13/2}$	12.9	13.9
	0.067	$d_{5/2}$	1.43	1.43
$E_b = -0.286$ MeV	0.878	$g_{7/2}$	−0.286	−0.286
	−0.294	$h_{11/2}$	4.07	4.07
	0.110	$d_{5/2}$	1.72	2.30
	−0.102	$h_{11/2}$	4.07	4.37
	0.096	$d_{5/2}$	1.72	1.72
	−0.075	$h_{9/2}$	11.7	11.7
	0.074	$i_{13/2}$	14.4	14.4
	0.068	$d_{5/2}$	1.72	3.20
	0.066	$d_{5/2}$	1.21	1.72

between the important states is therefore nearly independent of the Fermi energy, and consequently so is the continuum component of the ground state.

Several other important points are demonstrated in Table 1:

- For the case of a single bound $0g_{7/2}$ orbit, the dominant resonances that admix in the ground state are the $h_{11/2}$ and the $d_{5/2}$. These are remnants of what would be the "next major shell" in a deeper potential well.
- The dominant resonance contributions are of two types. Configurations in which the two continuum particles occupy the same level play an important role. There are also, however, significant contributions in which they occupy different levels *within the same resonance*. Such admixtures are difficult to incorporate into traditional treatments of pairing, which assume that pairs are composed of particles in time reversed orbits. We discuss a method for treating the "intra-resonance" pairing shortly.

The case reported in Table 1 has a relatively high-spin bound orbit, which couples primarily to continuum states that also have high spins. A somewhat different picture emerges when the bound level has quantum numbers $s_{1/2}$ and can strongly couple with s resonances. Even at low energies in the continuum, s resonances are typically very broad since there is no centrifugal barrier to help localize them. As a consequence, more continuum states admix into the ground state. Moreover, because the resonances are so broad the energy gap separating them from the bound states is smaller and components with one bound nucleon and one in the continuum appear. These facts are illustrated in Table 2, which present results for a case in which the only active bound orbit is the $2s_{1/2}$ with $E_b = -1.26$ MeV.

In more realistic scenarios, the valence nucleons may occupy more than one bound orbital. We find that very little of import is different when we include all the states of the bound 2s-1d-0g shell in our calculations. The bound orbits are much more likely to be occupied than the unbound ones, and only a few resonant states in the continuum play a significant role. These conclusions, which are nearly universal in this simple model, probably do *not* hold, however, in extremely weakly-bound nuclei very near the drip lines; some authors [5] have found that the nuclear mean field may be quite different there. In particular, shell structure may be smoothed out so that energy gaps between single-particle orbitals shrink. This would no doubt cause significantly more continuum mixing than in our calculations. Our focus, however, is not on nuclei at the drip lines. We are concerned instead with nuclei such as those along the r-process path, for which separation energies are typically 1–2 MeV [6]. There the results of our simple model should be relevant. They show, in short, that continuum contributions to the ground state wave function are fairly weak and are dominated by resonances.

Table 2
Ground state amplitudes involving a bound $3s_{1/2}$ state, with $E_b = -1.26$ MeV. All other notation is as in Table 1

Amp.	ℓ_j	E_1	E_2
0.944	$s_{1/2}$	−1.26	−1.26
0.110	$s_{1/2}$	0.994	−1.26
0.103	$s_{1/2}$	1.74	−1.26
0.101	$s_{1/2}$	0.449	−1.26
−0.092	$h_{9/2}$	4.16	4.16
0.089	$s_{1/2}$	2.69	−1.26
0.087	$i_{13/2}$	6.53	6.53
0.075	$s_{1/2}$	3.84	−1.26
0.064	$s_{1/2}$	0.114	−1.26
0.062	$s_{1/2}$	5.18	−1.26

These conclusions suggest that in treating nuclei away from stability, but not too near the drip lines, we may be able to simply eliminate non-resonant states without significantly changing the results. To test this idea, we need a working definition of a resonant state. To this end we define the quantity

$$I = \int_0^{\mathcal{R}} dr\, u^2(r), \tag{1}$$

where $u(r)$ is a normalized single-particle continuum radial wave function and $\mathcal{R} \sim R + 3$ fm. The resonant states are obviously those with large I. But any given resonance has a width, i.e. is spread over several of the continuum single-particle states. As a working definition, we will therefore count as resonant any single-particle continuum state within one standard deviation of the local maximum of I (corresponding to the peak of the resonance). If two resonances overlap, as sometimes occurs for s waves, we include all the states in both peaks.

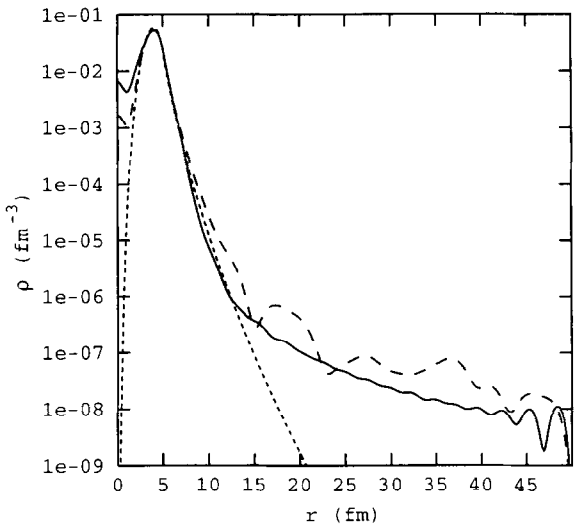

Fig. 1. One-body densities for calculations involving a bound $0g_{7/2}$ state with energy -1.24 MeV. The solid line is the full density, the long-dashed line is the density when nonresonant continuum states are omitted, and the dotted line is the density when the continuum is omitted entirely.

We may now truncate the continuum to include only these resonant states, diagonalize, and compare the results with those from the full space. Rather than compare spectra, we focus on the single-particle density, since it is likely to be particularly affected (mostly outside the nuclear radius) by continuum contributions in weakly-bound nuclei. In the two-particle model the density is given by

$$\rho(r) = \delta(r - r_1) + \delta(r - r_2). \tag{2}$$

Fig. 1 shows the one-body ground-state densities for a bound $0g_{7/2}$ level at energy $E_b = -1.24$ MeV, plus continuum admixtures. In addition to the full density distribution, we show the densities that arise when only the bound state is included and when only the bound state and resonances states are included. The ground state energies for the three calculations are -6.33 MeV, -2.48 MeV and -5.61 MeV, respectively.

The main effects of the continuum *in the full result* are to increase the density near the origin and outside the well (the latter effect has been carefully noted in Refs. [1,2]; the irregularities near 50 fm in Fig. 1 are caused by the box). The increased density at small radii is simply a consequence of mixing with states of low angular momentum and would occur whether the admixed states were bound or unbound. The truncation to resonances in most regions does not significantly change the density. The biggest deviations occur just outside the well, where the approximate result is too large, and in the long tail, where it oscillates around the full density. But for processes such as beta decay that are not extremely sensitive to details of the radial wave function, the truncation should serve admirably.

As noted earlier (see Table 1), the principal resonance admixtures involve either both particles in the same single-particle state or two particles in close-lying continuum states within a given resonance (and thus with the same l and j quantum numbers). As we also noted, the latter admixtures are difficult to incorporate in traditional shell-model treatments of pairing, based, e.g., on the broken-pair (generalized-seniority) approximation [7]. With this in mind, we have tried to identify an optimum single-particle state representing each resonance, which is usually a set of several continuum levels. There is no obviously best procedure for doing this, but a reasonable prescription is to define the single state that represents the set contained in a given resonance by

$$|R(l,j)\rangle = N \sum_i \sqrt{\frac{I_{ilj}}{E_{ilj} - E_0}} |ilj\rangle \,, \tag{3}$$

where N is a normalization constant, $|ilj\rangle$ are the states in a given (l,j) resonance, E_0 and E_{ilj} are the single-particle energies of the bound and resonance states, respectively, and I_{ilj} is the quantity defined in Eq. (1) as a measure of the probability of finding a particle near the potential well. Now, however, we include the specific quantum numbers i, l and j for the continuum single-particle state, to make evident the use of a separate state $|R(l,j)\rangle$ for each resonance with given l and j (the label i distinguishes the different single-particle states in a given resonance). If there is more than one bound state, we take E_0 to be the average bound-state single-particle energy. This definition of $|R(l,j)\rangle$ follows from a) the requirement that it roughly reproduce to lowest order in perturbation theory – justified since the admixtures of continuum states are small – the contribution of the set of states $|ilj\rangle$ to the ground-state eigenvector, and b) the assumption that the wave functions corresponding to the states $|ilj\rangle$ (with fixed l and j) are roughly proportional inside the well. Fig. 2 shows the results of this approximation when the active bound state has quantum numbers $0g_{7/2}$ and

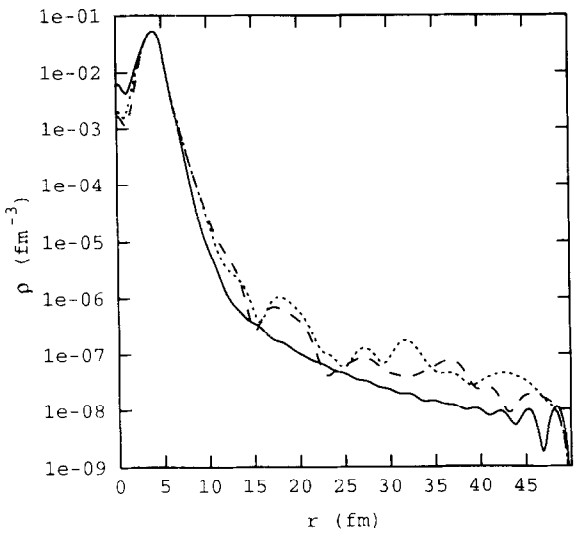

Fig. 2. One-body densities for calculations involving a bound $0g_{7/2}$ state with energy -1.24 MeV. The solid line is the full density, the long-dashed line is the density when nonresonant continuum states are omitted, and the dotted line is the density when each resonance is replaced by one optimal single-particle state (see text).

energy $E_b = -1.24$ MeV, alongside the corresponding results for the full calculation and the truncation to resonant states discussed earlier. [The ground state energies for the three calculations are -5.79 MeV, -6.33 MeV and -5.61 MeV, respectively.] The linear combination of states within the resonance prescribed by Eq. (3) naturally incorporates the effects of pairing between different states (within a given l, j resonance). Little, apparently, is lost in approximating each resonance by one well-chosen single-particle state.

This conclusion is even stronger for $J \neq 0$ pairs, since their components are coupled less by a short-range interaction. The approximation of each resonance by a single state should therefore also work in many nucleon systems (where $J \neq 0$ pairs can play an important role), allowing the use of techniques familiar from the long history of the shell model. We have not verified this explicitly since we treat only two particles here, and it is possible that the approximation will break down with the addition of more particles. We believe this to be unlikely, however. The two-body matrix elements connecting bound and resonant states with non-resonant continuum states are very small and it is hard to see how the latter could ever play an important role. We therefore intend to follow the procedure discussed here in calculating beta decay from nuclei along the r-process path, existing treatments of which [8–10] are schematic and not totally reliable. These nuclei, though far from stability, are nevertheless also sufficiently far from the drip lines that the approach we have described here should suffice.

One idea we have not explored in detail is the use of the canonical basis, which diagonalizes the ground-state one-body density matrix, as a way of truncating the single-particle spectrum and guiding the selection of optimal resonance states. Within HFB theory, states in this basis with lowest average energy are bound or quasibound, so that a truncation based on energy includes the most important states. Furthermore, each state in the canonical basis pairs only with its time-reversed partner; this feature of HFB is also present in our two-particle model. Finding the canonical basis, however, requires knowing the ground state one-body density matrix. In HFB this analysis is relatively simple, but in our case we would have to diagonalize the Hamiltonian within the full model space. The canonical states obtained from the HFB method and truncated at some energy, though, may provide a good basis for the number-conserving methods we envisage. In fact, HFB or other techniques more complicated than the one we have considered may be *necessary* for accurate treatment of observables, such as nuclear radii, that are sensitive to small features of the spatial wave function. The approximations discussed in this paper together with, e.g., the broken-pair approximation should be adequate for beta decay, however, provided one can reliably fix a single-particle potential and a two-body interaction.

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