

Exactly solvable pairing Hamiltonian for heavy nuclei

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We present a new exactly solvable Hamiltonian with a separable pairing interaction and nondegenerate single-particle energies. It is derived from the hyperbolic family of Richardson-Gaudin models and possesses two free parameters, one related to an interaction cutoff and the other to the pairing strength. These two parameters can be adjusted to give an excellent reproduction of Gogny self-consistent mean-field calculations in the Hartree-Fock basis.

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Pairing is one of the most important ingredients of the effective nuclear interaction in atomic nuclei, as was recognized early on by Bohr *et al.* [1] in an attempt to explain the large gaps observed in even-even nuclei. They suggested that the newly proposed Bardeen-Cooper-Schrieffer (BCS) [2] theory of superconductivity could be a useful tool in nuclear structure, although care should be taken with the violation of particle number in finite nuclei. Since then, BCS or the more general Hartree-Fock-Bogoliubov (HFB) theory, combined with effective or phenomenological nuclear forces, has been the standard tool to describe the low-energy properties of heavy nuclei. Improvements over BCS or HFB came through the restoration of broken symmetries, especially particle-number projection, which is still a problem not satisfactorily solved with density-dependent forces [3]. From a different perspective, Richardson found an exact solution of the constant-pairing problem with nondegenerate single-particle energies as early as 1963 [4]. Though highly schematic, the constant-pairing force has been used for decades in nuclear structure with several approximations [BCS, random-phase approximation (RPA), projected BCS (PBCS), etc.], but rarely resorting to the exact solution. Almost forgotten, the exact Richardson solution was recovered within the framework of ultrasmall superconducting grains [5], in which not only number projection but also pairing fluctuations were essential to describe the disappearance of superconductivity as a function of the grain size.

By combining the Richardson exact solution with the integrable model proposed by Gaudin [6] for quantum spin systems, it was possible to derive three families of integrable models called Richardson-Gaudin (RG) models [7]. The rational family, extensively used since then, contains the Richardson model as a particular exactly solvable Hamiltonian, as well as many other exactly solvable Hamiltonians of relevance in quantum optics, cold-atom physics, quantum dots, etc. [8]. However, the other families did not find a physical realization until very recently when it was shown that the hyperbolic family could model a p -wave pairing Hamiltonian in a two-dimensional lattice [9], such that it was possible to study, with the exact solution, an exotic phase diagram having

a nontrivial topological phase and a third-order quantum phase transition [10]. In this Rapid Communication, we will show that the hyperbolic family gives rise to a separable pairing Hamiltonian with two free parameters that can be adjusted to reproduce the properties of heavy nuclei as described by a Gogny HFB treatment.

Let us start our derivation with the integrals of motion of the hyperbolic RG model [7], which can be written in a compact form [11] as

$$R_i = S_i^z - 2\gamma \sum_{j \neq i} \left[\frac{\sqrt{\eta_i \eta_j}}{\eta_i - \eta_j} (S_i^+ S_j^- + S_i^- S_j^+) + \frac{\eta_i + \eta_j}{\eta_i - \eta_j} S_i^z S_j^z \right], \quad (1)$$

where S_i^z and S_i^\pm are the three generators of the $SU(2)_i$ algebra of copy i with spin representation s_i such that $(S_i^z)^2 = s_i(s_i + 1)$. We assume L $SU(2)$ -algebra copies, $i = 1, \dots, L$. The L operators R_i contain L free parameters η_i plus the strength of the quadratic term γ . The integrals of motion (1) commute among themselves and with the z component of the total spin, $S^z = \sum_{i=1}^L S_i^z$. Therefore, they have a common basis of eigenstates, which are parametrized by the ansatz

$$|\Psi_M\rangle = \prod_{\beta=1}^M S_\beta^+ |v\rangle, \quad S_\beta^+ = \sum_i \frac{\sqrt{\eta_i}}{\eta_i - E_\beta} S_i^+, \quad (2)$$

where $|v\rangle$ is the vacuum of the lowering operators, $S_i^- |v\rangle = 0$, and the E_β ($\beta = 1, \dots, M$) are the pair energies or pairons, which are determined by the condition that the ansatz (2) must satisfy the eigenvalue equations $R_i |\Psi_M\rangle = r_i |\Psi_M\rangle$ for every i .

In the pair representation of the $SU(2)$ algebra, the generators are expressed in terms of fermion creation and annihilation operators $S_i^+ = c_i^\dagger c_{\bar{i}}^\dagger = (S_i^-)^\dagger$ and $S_i^z = (c_i^\dagger c_i + c_{\bar{i}}^\dagger c_{\bar{i}} - 1)/2$. Each $SU(2)$ copy is associated with a single-particle level i , where \bar{i} is the time-reversed partner, and M is the number of active pairs. The vacuum $|v\rangle$ is defined by a set of seniorities, $|v\rangle = |v_1, v_2, \dots, v_l\rangle$, where the *seniority* $v_i = 0, 1$ is the

number of unpaired particles in level i , which determines the spin associated to the level as $s_i = (1 - \nu_i)/2$. The blocking effect of the unpaired particles reduces the number of active levels to $L_c = L - \sum_i \nu_i$.

Although any function of the integrals of motion generates an exactly solvable Hamiltonian, we will restrict ourselves in this presentation to the simple linear combination $H = \lambda \sum_i \eta_i R_i$. By defining $\lambda = [1 + 2\gamma(1 - M) + \gamma L_c]^{-1}$, and after some algebraic manipulations, the Hamiltonian reduces to

$$H = \sum_i \eta_i S_i^z - G \sum_{i,i'} \sqrt{\eta_i \eta_{i'}} S_i^+ S_{i'}^-, \quad (3)$$

where $G = 2\lambda\gamma$ is a free parameter.

This Hamiltonian, expressed in a two-dimensional momentum-space basis, gave rise to the celebrated $p_x + ip_y$ model of p -wave pairing [9,10]. However, if we interpret the parameters η_i as single-particle energies corresponding to a nuclear mean-field potential, the pairing interaction has the unphysical behavior of increasing in strength with energy. In order to reverse this unwanted effect, we define $\eta_i = 2(\varepsilon_i - \alpha)$, where the free parameter α plays the role of an energy cutoff and ε_i is the single-particle energy of the mean-field level i . Making use of the pair representation of the $SU(2)$, the exactly solvable pairing Hamiltonian (3) takes the form

$$H = \sum_i \varepsilon_i (c_i^\dagger c_i + c_{\bar{i}}^\dagger c_{\bar{i}}) - 2G \sum_{i,i'} \sqrt{(\alpha - \varepsilon_i)(\alpha - \varepsilon_{i'})} c_i^\dagger c_{\bar{i}}^\dagger c_{\bar{i}'} c_{i'}, \quad (4)$$

with eigenvectors given by (2), and eigenvalues

$$E = 2\alpha M + \sum_i \varepsilon_i \nu_i + \sum_\beta E_\beta. \quad (5)$$

Here, the pairons E_β correspond to a solution of the set of nonlinear Richardson equations,

$$\sum_i \frac{s_i}{\eta_i - E_\beta} - \sum_{\beta' (\neq \beta)} \frac{1}{E_{\beta'} - E_\beta} = \frac{Q}{E_\beta}, \quad (6)$$

where $Q = \frac{1}{2G} - \frac{L_c}{2} + M - 1$. Each particular solution of Eq. (6) defines a unique eigenstate (2).

In order to get an insight into the solutions of (6), we show in Fig. 1 the ground-state pairon dependence on the pairing strength G for a schematic system of $M = 10$ pairs moving in a set of $L = 24$ equally spaced single-particle levels ($\varepsilon_i = i$) and a cutoff $\alpha = 24$. For $G \rightarrow 0$, the pairons are all real and stay close to a set of M parameters η_i (the M lowest η 's for the ground-state configuration) in order to cancel the divergence in the right-hand side of (6). As G increases, the pairons move down in energy until they reach a critical value of $G \approx 0.012$ for which the two pairons closest to the Fermi level collapse to $\eta = -30$. Immediately thereafter, they acquire an imaginary part and expand in the complex plane as a complex-conjugate pair. The same phenomenon happens to the other pairons as G is further increased, forming an arc in the complex plane, as can be seen in the inset of Fig. 1. Even though the behavior of the pairons resembles that of the rational model [8], there are qualitative differences associated to the nonconstant form of

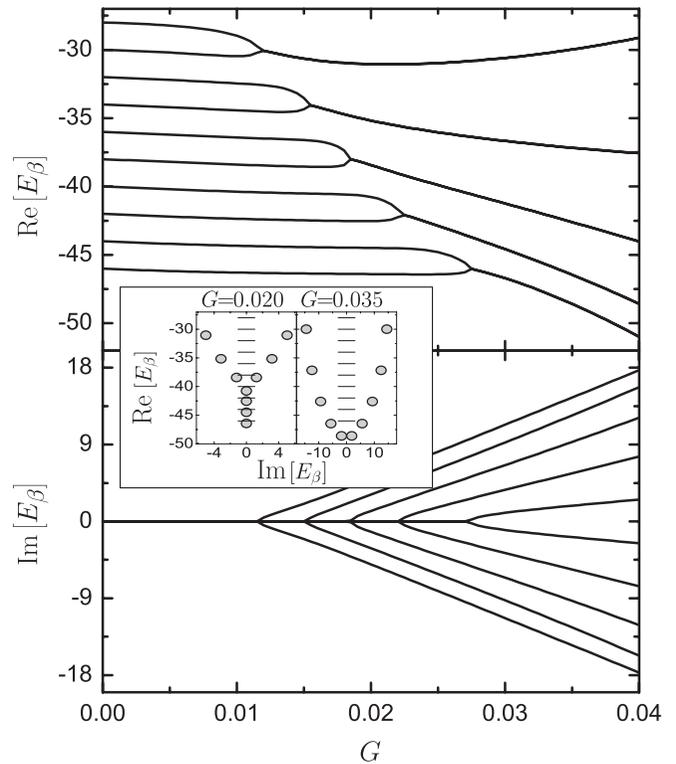


FIG. 1. Real and imaginary parts of the ground-state pairons as a function of pairing strength, for a set of 24 equally spaced single-particle levels ($\varepsilon_i = i$), a cutoff $\alpha = 24$, and $M = 10$ pairs. The inset shows the pairon distribution in the complex plane for two different pairing strengths.

the pairing interaction that will turn out to be essential for the description of heavy nuclei.

In what follows, we will derive the two free parameters G and α of the integrable Hamiltonian (4) by fitting its BCS wave function to a Gogny HFB calculation in the basis that diagonalizes the Hartree-Fock (HF) matrix. The HFB calculations with the Gogny force have been carried out with the standard DIS parametrization [12]. The pairing tensor is not exactly diagonal, but we have checked that the off-diagonal contributions are much smaller than the diagonal ones. In this approximation, HFB in the HF basis is equivalent to BCS.

Due to the separable character of the integrable pairing interaction, the state-dependent gaps and the pairing tensor in the BCS approximation are

$$\Delta_i = 2G\sqrt{\alpha - \varepsilon_i} \sum_{i'} \sqrt{\alpha - \varepsilon_{i'}} u_{i'} v_{i'} = \Delta\sqrt{\alpha - \varepsilon_i}, \quad (7)$$

$$u_i v_i = \frac{\Delta\sqrt{\alpha - \varepsilon_i}}{2\sqrt{(\varepsilon_i - \mu)^2 + (\alpha - \varepsilon_i)\Delta^2}}. \quad (8)$$

Note that the gaps Δ_i and the pairing tensor $u_i v_i$ depend on a single gap parameter Δ and have a square-root dependence on the single-particle energy. Hence, the model has a highly restricted form for both magnitudes that we will test against the Gogny gaps $\Delta_i^G = \sum_{i'} V_{i\bar{i},\bar{i}'i'}^G u_{i'}^G v_{i'}^G$ and pairing tensor $u_i^G v_i^G$, where $V_{i\bar{i},\bar{i}'i'}^G$ are the matrix elements of the Gogny force in the HF basis and $(u^G v^G)$ is the HFB eigenvector. We take the

single-particle energies ε_i of the integrable Hamiltonian from the HF energies of the Gogny HFB calculations and we set up an energy cutoff of 30 MeV on top of the Fermi energy. Occupation probabilities above this cutoff are lower than 10^{-3} and oscillate randomly. In order to fit the two parameters of the model α and G , and to fulfill the BCS equations for the chemical potential μ and the gap Δ , we solve the following three coupled equations for the chemical potential μ , the gap Δ , and the parameter α :

$$2M - L + \sum_i \frac{\xi_i}{E_i} = 0, \quad (9)$$

$$\sum_{i=i_F-n}^{i_F+n+1} \left[u_i^G v_i^G - \frac{\Delta}{2} \frac{t_i}{E_i} \right] \frac{t_i \xi_i^2}{E_i^3} = 0, \quad (10)$$

$$\sum_i \frac{(\Delta_i^G - \Delta \sqrt{\alpha - \varepsilon_i})}{\sqrt{\alpha - \varepsilon_i}} = 0, \quad (11)$$

where $t_i = \sqrt{\alpha - \varepsilon_i}$, $\xi_i = (\varepsilon_i - \mu)$, and the quasiparticle energy $E_i = \sqrt{\xi_i^2 + \Delta_i^2}$. Equation (9) is the BCS number equation that fixes the chemical potential μ . Equation (10) is a fitting of the Gogny pairing tensor $u_i^G v_i^G$ with respect to the gap parameters Δ , i.e., we minimize $\sum_{i=i_F-n}^{i_F+n+1} (u_i^G v_i^G - u_i v_i)^2$ with respect to Δ . Here, we select n levels above and below the Fermi energy in order to enhance the quality of the fit for the most correlated levels. We typically choose $n \sim 10$. Finally, Eq. (11) fixes the interaction cutoff α by minimizing the differences $\sum_i (\Delta_i^G - \Delta \sqrt{\alpha - \varepsilon_i})^2$ between the state-dependent Gogny gaps Δ_i^G and Δ_i , with respect to α . Once μ , α , and Δ are fixed, the pairing strength is determined from Eqs. (7) and (8),

$$\frac{1}{G} = \sum_i \frac{(\alpha - \varepsilon_i)}{\sqrt{\xi_i^2 + (\alpha - \varepsilon_i) \Delta^2}}.$$

As a first step to ascertain the quality of the hyperbolic Hamiltonian (4) to reproduce the superfluid features of heavy nuclei, we show in Fig. 2 the state-dependent gaps Δ_i and the pairing tensor $u_i v_i$ for protons corresponding to two heavy nuclei, ^{154}Sm and ^{238}U . Following the fitting procedure, we consider all levels below 30 MeV above the Fermi energy and solve self-consistently Eqs. (9)–(11) for the chemical potential μ , the gap parameter Δ , and the interaction cutoff α . Figure 2 shows a remarkable agreement between the Gogny force and the hyperbolic Hamiltonian for the pairing tensor. The Gogny state-dependent gaps exhibit large fluctuations due to the details of the two-body Gogny force. However, the general trend of the gaps is very well described by the square root $\sqrt{(\alpha - \varepsilon_i)}$ of the hyperbolic model. Although ^{238}U has 50% more proton pairs than ^{154}Sm , the quality of the mapping is excellent for both nuclei. It is interesting to note that the rational model, leading to the constant-pairing, exactly solvable, Richardson Hamiltonian, has a constant gap (a horizontal line) failing completely to describe the Gogny gaps. Table I shows the fitted values of pairing strength G and the interaction cutoff α . It also shows the gap parameter Δ and

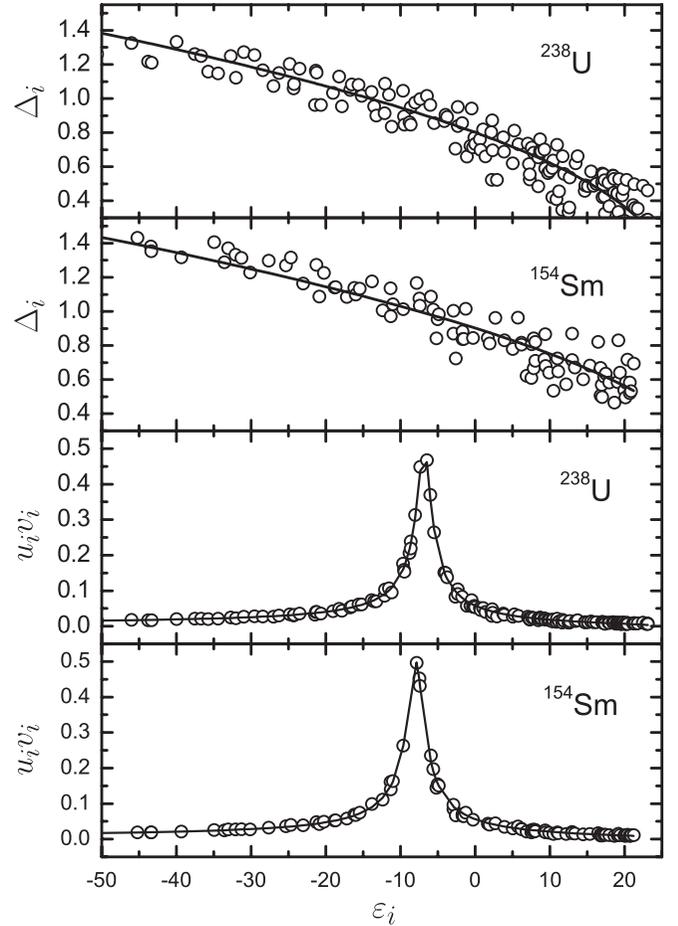


FIG. 2. State-dependent gaps Δ_i and pairing tensor $u_i v_i$ for protons in ^{238}U and ^{154}Sm . Open circles are Gogny HFB calculations in the HF basis, while the solid lines are the BCS results of the integrable Hamiltonian.

the correlations energies, defined as the total energy minus the HF energy, for both nuclei.

Once we have set up the procedure to define the parameters of the hyperbolic Hamiltonian in the BCS approximation, we are ready to explore the exact solution. For a general pairing Hamiltonian, the dimension of the Hilbert space is given by the binomial $B(L, M)$. Taking into account that (M, L) are (31, 91) for ^{154}Sm and (46, 148) for ^{238}U , the corresponding dimensions of the Hamiltonian matrices are 1.98×10^{24} and 4.83×10^{38} , respectively. These dimensions are well beyond the limits of a large-scale diagonalization. However, the integrability of the hyperbolic Hamiltonian allows us to

TABLE I. Parameter values, gaps, and correlation energies in MeV units for protons in ^{154}Sm and ^{238}U . E^G is the Gogny energy, and E^{BCS} and E^{Exact} are the BCS and the exact energies of the integrable Hamiltonian (4), respectively.

	G	α	Δ	E_{Corr}^G	$E_{\text{Corr}}^{\text{BCS}}$	$E_{\text{Corr}}^{\text{Exact}}$
^{154}Sm	2.24×10^{-3}	32.72	0.1577	1.3254	1.0164	2.9247
^{238}U	1.99×10^{-3}	25.25	0.1594	0.8613	0.5031	2.6511

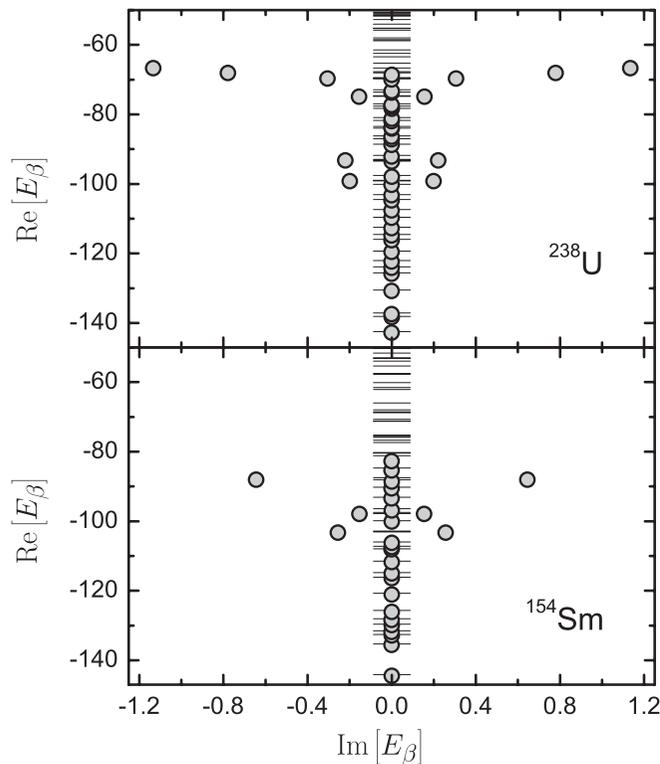


FIG. 3. Pair energies (gray circles) of the exact ground-state solution for protons in ^{238}U and ^{154}Sm . The horizontal segments in the real axis represent the parameters $\eta_i = 2(\epsilon_i - \alpha)$.

obtain the exact solution by solving numerically the set of M nonlinear coupled Richardson equations (6) using the method described in [13]. The exact correlation energy shown in Table I is, in both nuclei, considerably greater than the mean-field results, reflecting the importance of beyond-mean-field

quantum correlations and number fluctuations. The exact ground-state wave function is completely determined by the position of the M pairons in the complex plane. Figure 3 shows the exact ground states for both nuclei. Considering the structure of the pair wave functions (2), we may argue that ^{238}U has four correlated Cooper pairs, while ^{154}Sm has only two. Further analysis of the Cooper-pair wave function from the exact solutions, as was carried out in [14] for cold atoms and in [13] for nuclei within the rational model, is straightforward but beyond the scope of this Rapid Communication.

In summary, we have presented a new, exactly solvable Hamiltonian with separable pairing interaction and nondegenerate single-particle energies (4), which arises as a particular linear combination of the hyperbolic integrals of motion (1). The separable form of the pairing matrix elements could be derived from a novel Thomas-Fermi approximation for a contact interaction in a square-well potential [15]. We have shown that the separable Hamiltonian (4) with two free parameters is able to reproduce qualitatively the general trend of the state-dependent gaps, as described by the Gogny force in the HF basis. At the same time, it reproduces accurately the HFB wave function represented by the pairing tensor. As such, our exactly solvable Hamiltonian is an excellent benchmark for testing approximations beyond HFB in realistic situations for even and odd nuclei. Moreover, a self-consistent HF plus exact pairing approach could be set up along the lines of Ref. [16] for well-bound nuclei. The inclusion of exact $T = 1$ proton-neutron pairing within this self-consistent approach is also possible [17].

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