Pairing correlations, Cooper pairs and exactly solvable pairing models

- Brief historical introduction. 50th anniversary of the BCS paper.
- Richardson exact solution (1963)
- Ultrasmall superconducting grains (1999).
- Cooper pairs and pairing correlations from the exact solution in BCS-BEC crossover (2005) and in atomic nuclei (2007).
- Generalized Richardson-Gaudin Models for r>1 (2006-2007). Exact solution of the T=0,1 p-n pairing model.

# The Cooper Problem

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#### Letters to the Editor

**P**UBLICATION of brief reports of important discoveries in physics may be secured by addressing them to this department. The closing date for this department is five weeks prior to the date of issue. No proof will be sent to the authors. The Board of Editors does not hold itself responsible for the opinions expressed by the correspondents. Communications should not exceed 600 words in length and should be submitted in duplicate.

#### Bound Electron Pairs in a Degenerate Fermi Gas\*

LEON N. COOPER

Physics Department, University of Illinois, Urbana, Illinois (Received September 21, 1956) =  $(1/V) \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2)]$  which satisfy periodic boundary conditions in a box of volume V, and where  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are the coordinates of electron one and electron two. (One can use antisymmetric functions and obtain essentially the same results, but alternatively we can choose the electrons of opposite spin.) Defining relative and center-of-mass coordinates,  $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ ,  $\mathbf{r} = (\mathbf{r}_2 - \mathbf{r}_1)$ ,  $\mathbf{K} = (\mathbf{k}_1 + \mathbf{k}_2)$  and  $\mathbf{k} = \frac{1}{2}(\mathbf{k}_2 - \mathbf{k}_1)$ , and letting  $\mathscr{E}_K + \epsilon_k = (\hbar^2/m)(\frac{1}{4}K^2 + k^2)$ , the Schrödinger equation can be written

$$(\delta_{\mathbf{K}} + \epsilon_{\mathbf{k}} - E) a_{\mathbf{k}} + \sum_{\mathbf{k}'} a_{\mathbf{k}'} (\mathbf{k} | H_1 | \mathbf{k}') \times \delta(\mathbf{K} - \mathbf{K}') / \delta(0) = 0$$
 (1)

where

$$\Psi(\mathbf{k},\mathbf{r}) = (1/\sqrt{V})e^{i\mathbf{k}\cdot\mathbf{k}}\chi(\mathbf{r},K),$$
  

$$\chi(\mathbf{r},K) = \sum_{\mathbf{k}} (a_{\mathbf{k}}/\sqrt{V})e^{i\mathbf{k}\cdot\mathbf{r}},$$
(2)

and

$$(\mathbf{k}|H_1|\mathbf{k}') = \left(\frac{1}{V}\int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}}H_1e^{i\mathbf{k}'\cdot\mathbf{r}}\right)_{0 \text{ phonons}}$$

<u>Problem</u>: A pair of electrons with an attractive interaction on top of an inert Fermi sea.

$$\left|\phi\right\rangle = \sum_{k>k_{F}} \frac{1}{2\varepsilon_{k} - E} c_{k\uparrow}^{+} c_{-k\downarrow}^{+} \left|FS\right\rangle, \quad \frac{1}{G} = \sum_{k>k_{F}} \frac{1}{2\varepsilon_{k} - E}$$

"Bound" pair for arbitrary small attractive interaction. The FS is unstable against the formation of these pairs

If the many-body system could be considered (at least to a lowest approximation) a collection of pairs of this kind above a Fermi sea, we would have (whether or not the pairs had significant Bose properties) a model similar to that proposed by Bardeen which would display many of the equilibrium properties of the superconducting state.

#### Bardeen-Cooper-Schrieffer

PHYSICAL REVIEW

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#### Theory of Superconductivity\*

J. BARDEEN, L. N. COOPER,<sup>†</sup> AND J. R. SCHRIEFFER<sup>‡</sup> Department of Physics, University of Illinois, Urbana, Illinois (Received July 8, 1957)

A theory of superconductivity is presented, based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electrons states involved is less than the phonon energy,  $\hbar\omega$ . It is favorable to form a superconducting phase when this attractive interaction dominates the repulsive screened Coulomb interaction. The normal phase is described by the Bloch individual-particle model. The ground state of a superconductor, formed from a linear combination of normal state configurations in which electrons are virtually excited in pairs of opposite spin and momentum, is lower in energy than the normal state by amount proportional to an average  $(\hbar\omega)^2$ , consistent with the isotope effect. A mutually orthogonal set of excited states in one-to-one correspondence with those of the normal phase is obtained by specifying occupation of certain Bloch states and by using the rest to form a linear combination of virtual pair configurations. The theory yields a second-order phase transition and a Meissner effect in the form suggested by Pippard. Calculated values of specific heats and penetration depths and their temperature variation are in good agreement with experiment. There is an energy gap for individual-particle excitations which decreases from about  $3.5kT_c$  at  $T=0^{\circ}$ K to zero at  $T_c$ . Tables of matrix elements of single-particle operators between the excited-state superconducting wave functions, useful for perturbation expansions and calculations of transition probabilities, are given.

$$\left|\Psi\right\rangle \equiv e^{\Gamma^{+}}\left|0\right\rangle, \quad \Gamma^{+} = \sum_{k} \frac{v_{k}}{u_{k}} c_{k\uparrow}^{+} c_{-k\downarrow}^{+}$$

## **BCS in Nuclear Structure**

PHYSICAL REVIEW

VOLUME 110, NUMBER 4

MAY 15, 1958

#### Possible Analogy between the Excitation Spectra of Nuclei and Those of the Superconducting Metallic State

A. BOHR, B. R. MOTTELSON, AND D. PINES\*

Institute for Theoretical Physics, University of Copenhagen, Copenhagen, Denmark, and Nordisk Institut for Teoretisk Atomfysik, Copenhagen, Denmark

(Received January 7, 1958)

The evidence for an energy gap in the intrinsic excitation spectrum of nuclei is reviewed. A possible analogy between this effect and the energy gap observed in the electronic excitation of a superconducting metal is suggested.

It thus appears that there may exist interesting similarities between the low-energy spectra of nuclei and of the electrons in the superconducting metal. However, it must be stressed that the former are significantly influenced by the finite size of the nuclear system. Thus, the energy gap is observed to decrease

## **Richardson's Exact Solution**

ume 3, number 6

PHYSICS LETTERS

1 February 1963

#### A RESTRICTED CLASS OF EXACT EIGENSTATES OF THE PAIRING-FORCE HAMILTONIAN \*

#### R.W. RICHARDSON

H.M.Randall Laboratory of Physics, University of Michigan, Ann Arbor, Michigan

Received 23 November 1962

# Exact Solution of the BCS Model

$$H_{P} = \sum_{k} \varepsilon_{k} n_{k} + g \sum_{k,k'} c^{\dagger}_{k\uparrow} c_{-k\downarrow} c_{-k\downarrow} c_{k\uparrow\uparrow}$$

Eigenvalue equation:

$$H_{P}\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

Ansatz for the eigenstates (generalized Cooper ansatz)

$$\left|\Psi
ight
angle = \prod_{lpha=1}^{M} \Gamma_{lpha}^{\dagger} \left|0
ight
angle, \quad \Gamma_{lpha}^{\dagger} = \sum_{k} \frac{1}{2\varepsilon_{k} - E_{lpha}} c_{k\uparrow}^{+} c_{-k\downarrow}^{+}$$

# **Richardson equations**

$$1 + g \sum_{k=0}^{M} \frac{1}{2\varepsilon_k - E_\alpha} + 2g \sum_{\beta(\neq \alpha)=1}^{M} \frac{1}{E_\alpha - E_\beta} = 0, \quad E = \sum_{\alpha=1}^{M} E_\alpha$$

#### **Properties**:

This is a set of *M* nonlinear coupled equations with *M* unknowns ( $E_{\alpha}$ ).

The first and second terms correspond to the equations for the one pair system. The third term contains the many body correlations and the exchange symmetry.

The pair energies are either real or complex conjugated pairs.

There are as many independent solutions as states in the Hilbert space. The solutions can be classified in the weak coupling limit ( $g \rightarrow 0$ ).

# What is an exactly solvable model?

.- A model is exactly solvable if we can write explicit expressions for the complete set of eigenstates in terms of a set of parameters, which are in turn solutions of an algebraic problem.

.- The exponential complexity of the many body problem is reduced to a polynomial complexity.

.- Simplest examples of ESM are dynamical symmetry models. The Hamiltonian is a combination of Casimir operators of a Lie algebra. Analytically solvable. Elliot SU(3), IBM SU(3), O(6), U(5). Etc...

# Why are ESM important?

.- They can unveil physical properties that cannot described with existing many-body theories.

.- They could constitute stringent test for many-body theories. Benchmark models.

# Recovery of the Richardson solution: Ultrasmall superconducting grains

•A fundamental question posed by P.W. Anderson in J. Phys. Chem. Solids 11 (1959) 26 :

"at what particle size will superconductivity actually disappear?"

• Since  $d \sim Vol^{-1}$  Anderson argued that for a sufficiently small metallic particle, there will be a critical size  $d \sim \Delta_{\text{bulk}}$  at which superconductivity must disappear.

• This condition arises for grains at the nanometer scale.

• Main motivation from the revival of this old question came from the works:

• D.C. Ralph, C. T. Black y M. Tinkham,

PRL's 74 (1995) 3421 ; 76 (1996) 688 ; 78 (1997) 4087.

The model used to study metallic grains is the reduced BCS Hamiltonian in a discrete basis:

$$H = \sum_{j\sigma} \left( \varepsilon_{j\sigma} - \mu \right) c_{j\sigma}^{+} c_{j\sigma} - \lambda d \sum_{jj'} c_{j+}^{+} c_{j-}^{+} c_{j-} c_{j+}$$

Single particles are assumed equally spaced

$$\varepsilon_{j\sigma} = jd, \quad j = 1, \dots, \Omega$$

where  $\Omega$  is the total number of levels given by the Debye frequency  $\omega_D$  and the level spacing *d* as

$$d\Omega = 2 \omega_D$$

PBCS study of ultrasmall grains:

D. Braun y J. von Delft. PRL 81 (1998)47

 $E_{cond} = \langle \psi | H | \psi \rangle - \langle \psi_0 | H | \psi_0 \rangle$ 



# Condensation energy for even and odd grains

## **PBCS** versus Exact

J. Dukelsky and G. Sierra, PRL 83, 172 (1999)



## Thermodynamic limit of the Richardson equations

M. Gaudin (unpublished). J.M. Roman, G. Sierra and JD, Nucl. Phys. B 634 (2002) 483.

V, N
$$\rightarrow \infty$$
, G=g / V and  $\rho$ =N / V

By using electrostatic techniques and assuming that extremes of the arc are  $2\mu$ +2 i  $\Delta$ , Gaudin derived the BCS equations:

$$Gap \qquad \frac{1}{2}\int d\varepsilon \frac{g(\varepsilon)}{\sqrt{(\varepsilon-\mu)^2 + \Delta^2}} + \frac{1}{G} = 0$$
Number 
$$\rho = \int d\varepsilon g(\varepsilon) \left[ 1 - \frac{\varepsilon - \mu}{\sqrt{(\varepsilon-\mu)^2 + \Delta^2}} \right]$$
The equation for the arc  $\Gamma$  is,  $z = \sqrt{(\varepsilon-\mu)^2 + \Delta^2}$ 

$$D = \operatorname{Re} \left[ \int_{0}^{\infty} d\varepsilon \sqrt{\varepsilon} \left( \frac{z + (\varepsilon-\mu) \ln \left[ \frac{(E-\mu)}{i\Delta} \right]}{\sqrt{(\varepsilon-\mu)^2 + \Delta^2}} - \ln \left[ \frac{\Delta^2 + (E-\mu)(\varepsilon-\mu) + z\sqrt{(\varepsilon-\mu)^2 + \Delta^2}}{i\Delta(E-\varepsilon)} \right] \right] \right]$$

#### Pair energies E for a system of 200 equidistant levels at half filling



For a uniform 3D system in the thermodynamic limit the Gap equation is singular. Leggett (1980) proposed a regularization based on the subtraction the scattering length equation.

$$\frac{m}{4\pi\hbar^2 a_s} = \frac{1}{G} + \frac{1}{2} \int d\varepsilon \frac{g(\varepsilon)}{\varepsilon}$$

Scattering length

The Leggett model describes the BCS-BEC crossover in terms of a single parameter  $\eta = 1/k_F a_s$ . The resulting equations can be integrated (Papenbrock and Bertsch PRC 59, 2052 (1999))

$$\eta = \sqrt[4]{\mu^2 + \Delta^2} P_{1/2} \left( -\frac{\mu}{\sqrt{\mu^2 + \Delta^2}} \right)$$
$$-\frac{4}{3\pi} = \eta \mu + \left( \mu^2 + \Delta^2 \right)^{3/4} P_{3/2} \left( -\frac{\mu}{\sqrt{\mu^2 + \Delta^2}} \right)$$

#### Evolution of the chemical potential and the gap along the crossover



WhatCooper pair in the superfluid is medium? G. Ortiz and JD, Phys. Rev. A 72, 043611 (2005)  $\Psi = A \left[ \varphi_1(r_1) \varphi_2(r_2) \cdots \varphi_{N/2}(r_{N/2}) \right]$  $\varphi(r) = \frac{1}{V} \sum \varphi_k e^{ik \cdot r}$ "Cooper" pair wavefunction  $\varphi_k^{BCS} = C_{BCS} \frac{v_k}{u}$ From MF BCS:  $\varphi_k^P = \langle BCS | c_{k\perp} c_{k\uparrow} | BCS \rangle = C_P u_k v_k$ •From pair correlations:  $\varphi_k^E(E) = \frac{C_E}{2\varepsilon_E - E}$ From Exact wavefuction:

$$\varphi_E(r) = C_E \frac{e^{-r\sqrt{-E/2}}}{r}$$

- E real and <0, bound eigenstate of a zero range interaction parametrized by a.
- E complex and R (E) < 0, quasibound molecule.
- E complex and R (E) > 0, molecular resonance.
- E Real and >0 free two particle state.



## "Cooper" pair wave function



# ODLRO and the fraction of the condensate

For fermions ODLRO occurs in the two-body density matrix

$$\rho_{2}\left(r_{1}', r_{2}', r_{1}, r_{2}\right) = \left\langle \psi_{\uparrow}^{+}\left(r_{1}'\right)\psi_{\downarrow}^{+}\left(r_{2}'\right)\psi_{\uparrow}\left(r_{1}\right)\psi_{\downarrow}\left(r_{2}\right)\right\rangle$$

if it has a macroscopic eigenvalue

$$\rho_{2}\left(r_{1}',r_{2}',r_{1},r_{2}\right) = \left\langle\psi_{\uparrow}^{+}\left(r_{1}'\right)\psi_{\downarrow}^{+}\left(r_{2}'\right)\right\rangle\left\langle\psi_{\uparrow}\left(r_{1}\right)\psi_{\downarrow}\left(r_{2}\right)\right\rangle + \rho_{2}'$$

For a homogeneous system in the thermodynamic limit

$$r_1'-r_1|, |r_2'-r_2| \rightarrow \infty, \quad \langle \psi_{\uparrow}(r_1)\psi_{\downarrow}(r_2)\rangle = \sqrt{\lambda M}\varphi(|r_1-r_2|)$$

$$\lambda = \frac{1}{M} \int dr_1 dr_2 \left| \varphi \left( \left| r_1 - r_2 \right| \right) \right|^2 = \frac{1}{M} \sum_{k} u_k^2 v_k^2$$

# Sizes and Fraction of the condensate

# **Application to Samarium isotopes**

G.G. Dussel, s. Pittel, J. Dukelsky and P. Sarriguren, PRC 76, 011302 (2007)

 ${\color{black} \bullet \hspace{0.1cm} \mathsf{Z} = 62} \ , \ \ 80 \leq N \leq \!\!96$ 

Selfconsistent Skyrme (SLy4) Hartree-Fock plus BCS in 11 harmonic oscillator shells (40 to 48 pairs in 286 double degenerate levels).

• The strength of the pairing force is chosen to reproduce the experimental pairing gaps in <sup>154</sup>Sm ( $\Delta_n$ =0.98 MeV,  $\Delta_p$ = 0.94 MeV)

•  $g_n=0.106$  MeV and  $g_p=0.117$  MeV. A dependence  $g=G_0/A$  is assumed for the isotope chain.

# **Correlations Energies**

Mass	Ec(Exact)	Ec(PBCS	Ec(BCS+H)	Ec(BCS)
142	-4.146	-3.096	-1.214	-1.107
144	-2.960	-2.677	0.0	0.0
146	-4.340	-3.140	-1.444	-1.384
148	-4.221	-3.014	-1.165	-1.075
150	-3.761	-2.932	-0.471	-0.386
152	-3.922	-2.957	-0.750	-0.637
154	-3.678	-2.859	-0.479	-0.390
156	-3.716	-2.832	-0.605	-0.515
158	-3.832	-3.014	-1.181	-1.075

### Fraction of the condensate in mesoscopic systems

$$\lambda = \frac{1}{M\left(1 - M / L\right)} \left( \sum_{\alpha} \left\langle c_{\alpha}^{+} c_{\overline{\alpha}}^{+} c_{\overline{\alpha}} c_{\alpha} \right\rangle - \left\langle c_{\alpha}^{+} c_{\alpha} \right\rangle \left\langle c_{\overline{\alpha}}^{+} c_{\overline{\alpha}} \right\rangle \right)$$
$$\lambda_{BCS} = \frac{1}{M\left(1 - M / L\right)} \sum_{\alpha} u_{\alpha}^{2} v_{\alpha}^{2}$$

From the exact solution f is the fraction of pair energies whose distance in the complex plane to nearest single particle energy is larger than the mean level spacing.



# <sup>154</sup>Sm





# Some models derived from rank 1 RG

BCS Hamiltonian (Fermion and Boson)

Generalized Pairing Hamiltonians (Fermion and Bosons)

Central Spin Model

Gaudin magnets

Lipkin Model

Two-level boson models (IBM, molecular, etc..)

Atom-molecule Hamiltonians (Feshbach resonances)

Generalized Jaynes-Cummings models

Breached superconductivity. LOFF and breached LOFF states.

Reviews: J.Dukelsky, S. Pittel and G. Sierra, Rev. Mod. Phys. 76, 643 (2004); G. Ortiz, R. Somma, J. Dukelsky y S. Rombouts. Nucl. Phys. B 7070 (2005) 401

# Exactly Solvable RG models for simple Lie algebras

## Cartan classification of Lie algebras

rank	$A_n  su(n+1)$	$B_n so(2n+1)$	$C_n sp(2\mathbf{n})$	$D_n so(2n)$
1	su(2), su(1,1) pairing	so(3)~ $su(2)$	$sp(2) \sim su(2)$	$so(2) \sim u(1)$
2	<i>su</i> (3) Three level Lipkins	so(5), so(3,2) pn-pairing	$sp(4) \sim so(5)$	so(4) ~ $su(2)xsu(2)$
3	su(4) Wigner	so(7) FDSM	sp(6) FDSM	so(6)~su(4)
4	su(5)	so(9)	<i>sp</i> (8)	so(8) pairing T=0,1. Ginnocchio. 3/2 fermions

# **Exactly Solvable Pairing Hamiltonians**

1) SU(2), Rank 1 algebra

$$\begin{split} H &= \sum_{i} \mathcal{E}_{i} n_{i} - g \sum_{ij} P_{i}^{+} P_{j} \\ 1 + g \sum_{k=0}^{M} \frac{1}{2\mathcal{E}_{k} - E_{\alpha}} + 2g \sum_{\beta(\neq \alpha)=1}^{M} \frac{1}{E_{\alpha} - E_{\beta}} = 0, \quad E = \sum_{\alpha=1}^{M} E_{\alpha} \end{split}$$

2) SO(5), Rank 2 algebra

$$H = \sum_{i} \varepsilon_{i} n_{i} - g \sum_{ij\tau} P_{i\tau}^{+} P_{j\tau}$$

J. Dukelsky, V. G. Gueorguiev, P. Van Isacker, S. Dimitrova, B. Errea y S. Lerma H. PRL 96 (2006) 072503.

3) SO(8), Rank 4 algebra  $H = \sum_{i} \varepsilon_{i} n_{i} - g_{T} \sum_{ij\tau} P_{i\tau}^{+} P_{j\tau} - g_{S} \sum_{ij\sigma} D_{i\sigma}^{+} D_{j\sigma}$ 

S. Lerma H., B. Errea, J. Dukeslky and W. Satula. PRL 99, 032501 (2007).

# The exact solution



80 Nucleons in L=50 equidistant levels







 $J_T$ : iso-MoI,  $\lambda$ : Wigner energy ,  $\Delta E$ : 2qp excitation (V=2)



FIG. 2: (a) Inverse of the iso-MoI  $(1/J_T)$ , (b) signature splitting  $\delta e_T$  and (c) linear term enhancement factor  $\lambda$  versus Tfor pure T=0 model (circles), pure T=1 model (diamonds) and the SO(8) model (triangles). Filled (open) symbols refer to even-(odd-)T branches of E(T). The calculations were done for g = 0.16 except for gray triangles in the lowest panel which mark the SO(8) solution for g = 0.22.

# Summary

- From the analysis of the exact BCS wavefunction we proposed a new pictorial view to the nature of the Cooper pairs
- Alternative definition of the fraction of the condensate. Consistent with change of sign of the chemical potential.
- For finite system, PBCS improves significantly over BCS but it is still far from the exact solution. Typically, PBCS misses of order 1 MeV in binding energy.
- •The T=0,1 pairing model could be a benchmark to study different approximations like the isocranking model or approximations dealing with alpha correlations and alpha condensation. It can be also describe the Ginnocchio model with non-degenerate orbits or spin 3/2 cold atom models.
- SP(6) RG model: A deformed-superfluid benchmark model?