Gradient method with application to 4-component fermion condensates

G.F. Bertsch
University of Washington

INT May 5, 2011

Collaborators
Y.L. (Alan) Luo UW
L.M. Robledo Madrid
A. Gezerlis UW

References
Bertsch and Luo, Phys. Rev. C81 064320
Robledo and Bertsch, arXiv:1104.5453
Gezerlis, Bertsch and Luo, arXiv:1103.5793

Textbook
"The Nuclear Many-Body Problem", P. Ring and P. Schuck, Springer 1980

Outline

1. Formalism
   a) reminder HFB/BdG
   b) the gradient method

2. Nuclear Physics
   a) phenomenological Hamiltonian
   b) spin-singlet condensates (!)
   c) spin-triplet condensates (?)
   d) mixed-spin condensates (?)

3. The computer program `hfb_shell`

Formalism for HFB/BdG

$$\beta_k^+ = \sum_l U_{lk} c_l^+ + V_{lk} c_l. \tag{7.1}$$

$$\rho_{ll'} = \langle \Phi | c_{l'}^+ c_l | \Phi \rangle, \qquad \kappa_{ll'} = \langle \Phi | c_{l'} c_l | \Phi \rangle,$$

$$\rho = V^* V^T, \qquad \kappa = V^* U^T = -UV^+.$$

$$\mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}.$$

The W form a unitary group $W^+W = \mathbb{1}$
$2N^2 - N$ independent parameters, homomorphic to $O(N)$ or $SO(N)$, N is the number of states.

$$\hat{H} = \sum_{12} \varepsilon_{12} c_1^+ c_2 + \frac{1}{4} \sum_{1234} v_{1234} c_1^+ c_2^+ c_4 c_3$$

$$\langle \hat{H} \rangle \equiv H^{00} = H(\rho, \kappa) \qquad \text{Wick's theorem.}$$

The two grand strategies to minimize H^{00}

I.) $$\left. \frac{\delta H^{00}}{\delta U_{ij}^*} = 0, \quad \frac{\delta H^{00}}{\delta V_{ij}} = 0 \right|_{W^+W = \mathbb{1}}$$

⇓

$$\begin{bmatrix} h & \Delta \\ -\Delta^* & -h^* \end{bmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

Gradient Method

II)

1) find a set of independent variables Z_{ij}

2) find the gradient

$$\frac{\partial H^{00}}{\partial Z^*_{ij}} \equiv H^{20}_{ij}$$

3) Update $\mathcal{W} \xrightarrow{\eta H^{20}} \mathcal{W}'$

guaranteed to get a lower energy if $|H^{20}| > 0$ and η is small.

1) the form of Z: arbitrary skew-symmetric

$$Z = -Z^t \,, \quad z_{ij} \in \mathbb{C} \,, \quad N^2 - N \text{ parameters}$$

$$\mathcal{W}' = \mathcal{W} \begin{pmatrix} 1 & Z \\ Z^* & 1 \end{pmatrix} \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}$$

$$D = (1 - Z Z^*)^{-\frac{1}{2}}$$

2) Single-particle operators

$$F^{00} = \mathrm{Tr}(\hat{F} \hat{\rho})$$

$$F^{00\prime} = F^{00} - \frac{1}{2}\left[\mathrm{Tr}(F^{20} Z^*) + h.c.\right] + \mathcal{O}(Z^2)$$

$$H^{00\prime} = H^{00} - \frac{1}{2}\left[\mathrm{Tr}(H^{20} Z^*) + h.c.\right] + \mathcal{O}(Z^2)$$

Advantages of the Gradient Method

1. Guaranteed convergence

2. Easy to add constraints

3. Easy to do odd particle numbers

Ring and Schuck, p. 200.

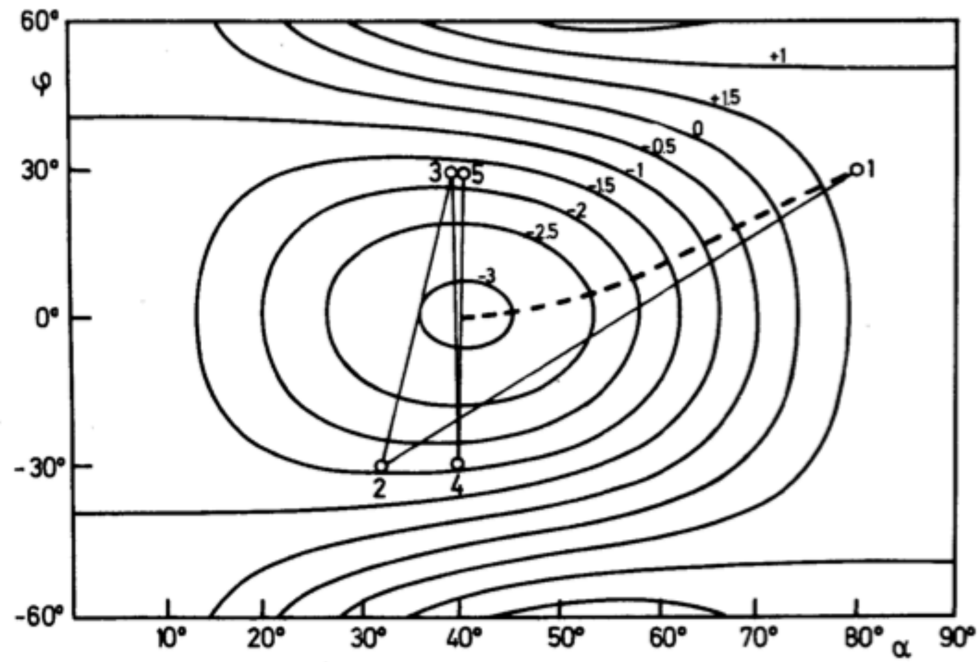
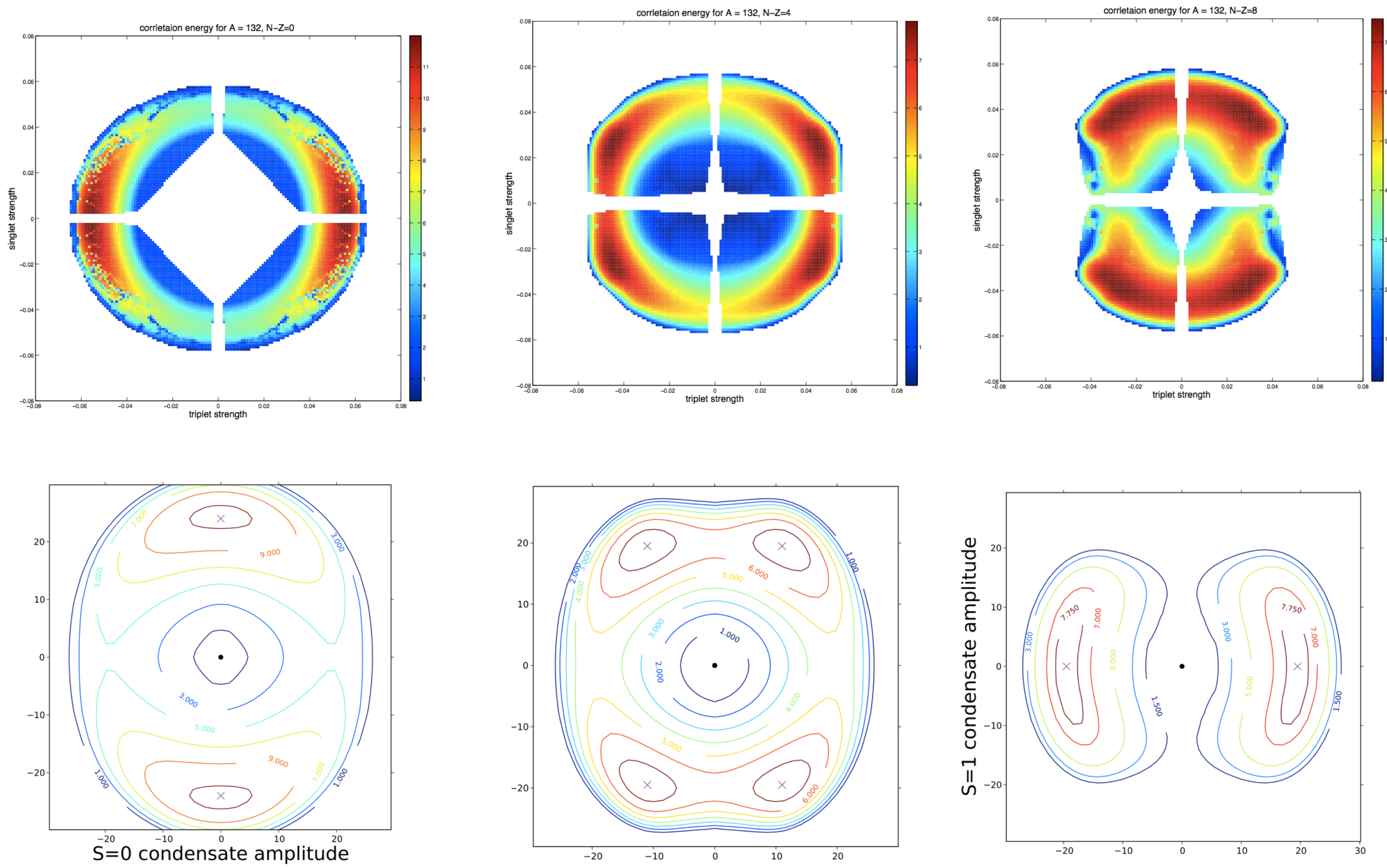


Figure 5.3. Numerical comparison of solution of the HF equations by iterative diagonalization (solid line) and the gradient method (dashed line).


corrletaion energy for A = 132, N−Z=0
corrletaion energy for A = 132, N−Z=4
corrletaion energy for A = 132, N−Z=8
singlet strength
triplet strength
S=0 condensate amplitude
S=1 condensate amplitude

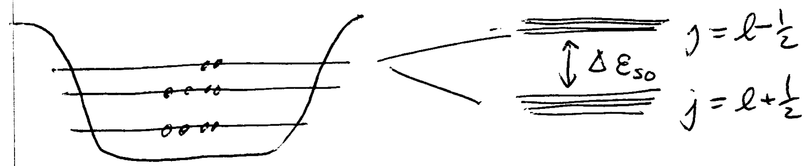
Odd-particle systems

1. The $\mathcal{W}$ transformations have a definite number parity, even or odd.

2. The Z transformation does not change the number parity.

Nuclear Physics

Phenomenological Hamiltonian



spin orbit field $\Delta\varepsilon_{so} \sim \ell \int d^3r \, \frac{dV}{dr} \, |\phi_\ell(r)|^2$

Contact interaction $\langle 12|V|34\rangle = (\text{strength}) \times \int d^3r \, \phi_1^* \phi_2^* \phi_3 \phi_4$

$\langle n\uparrow n\downarrow |V| n\uparrow n\downarrow\rangle$ V_s

$\langle n\uparrow p\uparrow |V| n\uparrow p\uparrow\rangle$ V_t

$\langle n\uparrow p\downarrow |V| n\downarrow p\uparrow\rangle$ $\frac{1}{2}(V_t - V_s)$ etc.

<u>Cases</u>

1) $\Delta\varepsilon_{so}=0$ $V_s = V_t$ $\Rightarrow$ $SU(4)$

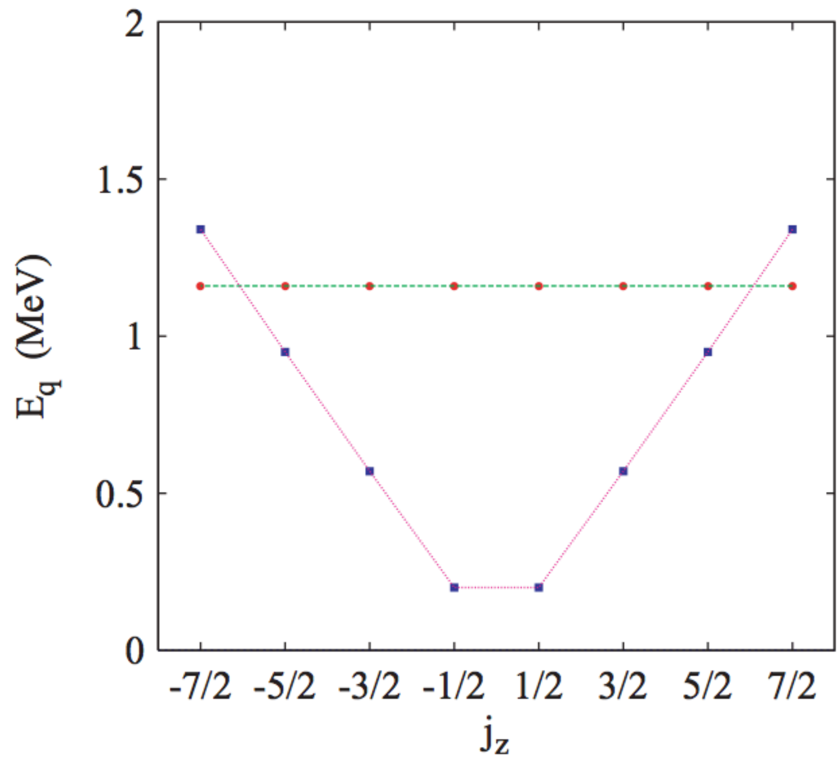
2) $\Delta\varepsilon_{so}$ normal, $V_s \sim \frac{2}{3} V_t$

Identical-particle spin-singlet pairing dominates (Why?)

$\Delta\varepsilon_{so} \sim 5$ MeV $\Delta \sim 1$ MeV

Aside

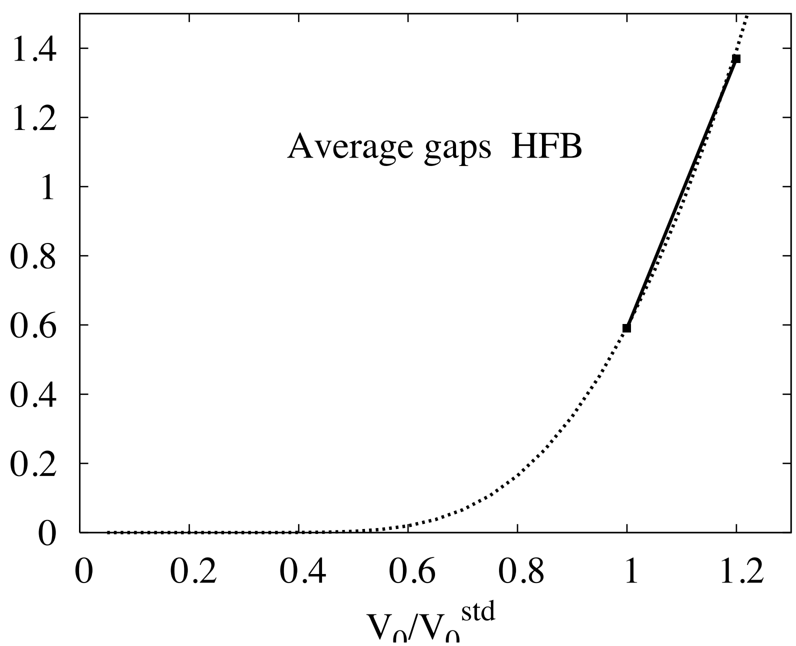
Spin-triplet pairing in a strong spin-orbit field has small gaps.

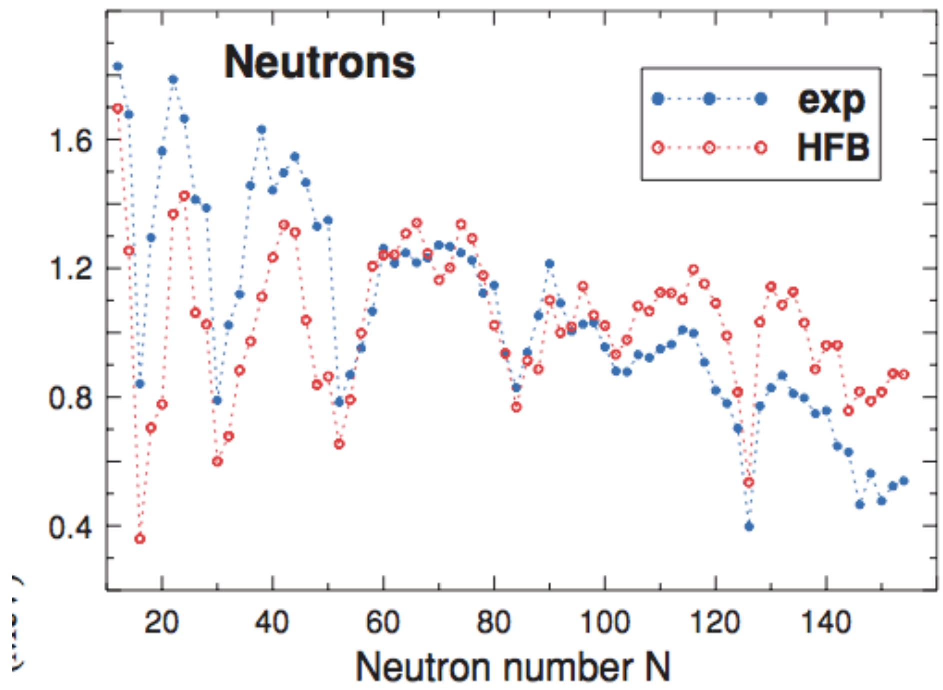


Neutron pairing gaps

$$\Delta_o^{(3)}(N) = \frac{1}{2}\left[B(N+1) + B(N-1) - 2B(N)\right].$$

Phys. Rev. C79 034306 (2009)





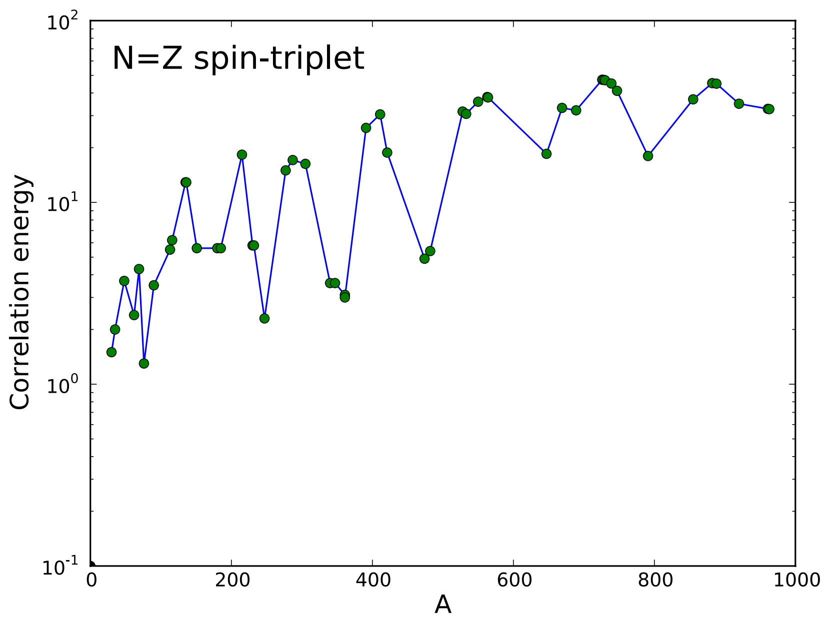
$$\Delta_{BCS} = (E_{max} - E_{min})e^{-1/g}$$

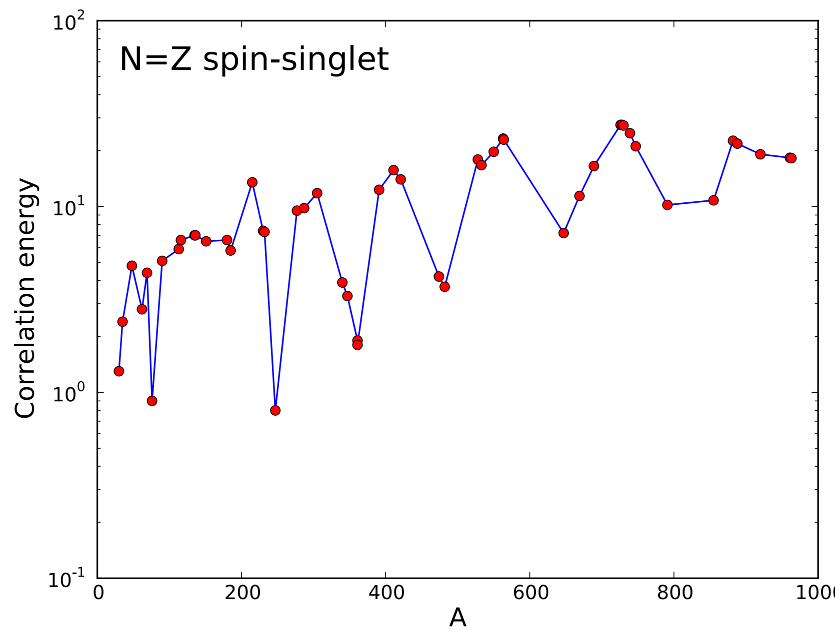
3. Mass Number A very large, N=Z

Phys. Rev. C 81 064320 (2010)

1. There is a large fluctuation of pairing correlation energies, depending on the shells near the Fermi energy.

2. Spin-triplet np pairing is favored in extremely large N=Z nuclei (beyond the proton dripline).





4. Large A, N=Z + a few

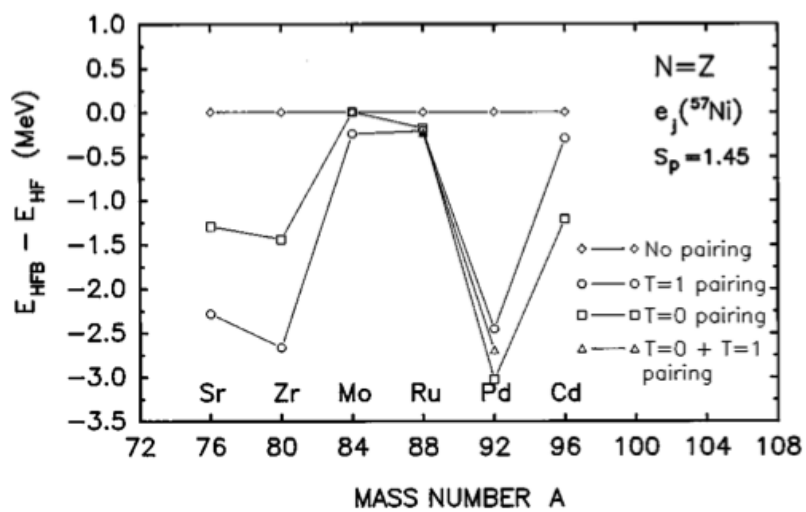
PHYSICAL REVIEW C, VOLUME 60, 014311

Proton-neutron pairing in $Z=N$ nuclei with $A=76-96$

Alan L. Goodman
Department of Physics, Tulane University, New Orleans, Louisiana 70118
(Received 29 December 1998; published 16 June 1999)

The ground states of even-even $Z=N$ nuclei are determined with the isospin generalized BCS equations and the HFB equation. The calculations permit the simultaneous existence of the following Cooper pairs: pp, nn, $pn(T=1)$, and $pn(T=0)$ where the two nucleons in a pair occupy space-spin orbitals which are related by time reversal, as well as $pn(T=0)$ where the two nucleons are in identical space-spin orbitals. There is a transition from $T=1$ Cooper pairs at the beginning of this isotope sequence to $T=0$ Cooper pairs at the end of the sequence. Near the middle of the isotope sequence, there is coexistence of a $T=0$ pair superfluid and a $T=1$ pair superfluid in the same wave function. The fluctuation in the particle number is reduced if the wave function contains proton-neutron pairing. The fluctuation in the isospin is eliminated and isospin is conserved if the wave function contains only $T=0$ pairing. [S0556-2813(99)05407-2]

PACS number(s): 21.60.−n



4. Large A, N=Z + a few

GBL, arXiv:1103.5793

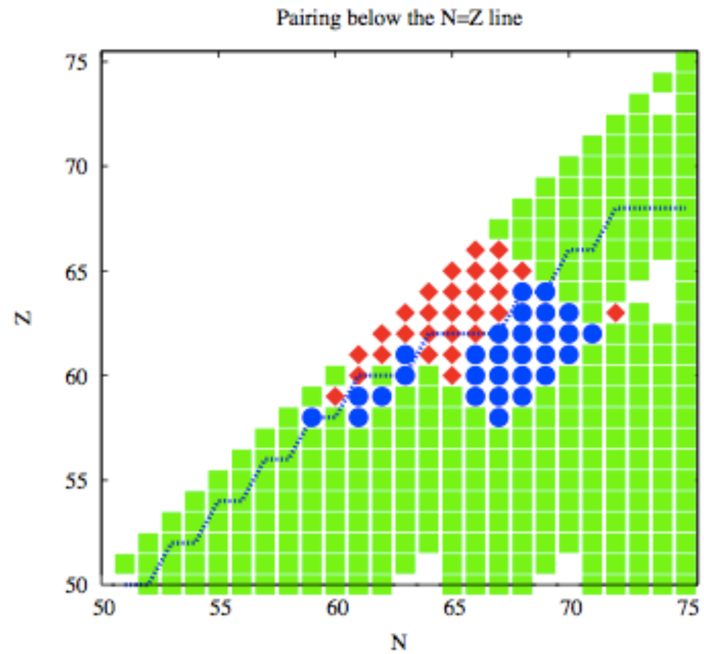


FIG. 1: (color online) Chart of nuclides with $Z \leq N$ for neutron numbers from 50 to 75. Blank squares denote nuclei that exhibit practically no pairing ($E_{corr} < 0.5$), green squares signify the case where the pairing condensate is mostly spin-singlet, red diamonds are used for the nuclei that exhibit spin-triplet, while blue circles denote nuclei for which the pairing is a mixture of spin-singlet and spin-triplet. The blue dashed line is the proton-drip line from Ref. [13].

There need not be a sharp transition between singlet and triplet pairing condensates, as expected from the SU(4)limit. In between the spin-singlet and spin-triplet there may be a mixed spin condensate.

Some open theory questions

1. How can we understand the mixed-spin ground state?
2. Does a trace of the spin-triplet condensate persist in CI-based theory?
3. Do mixed-spin states persist in asymmetric nuclear matter?

The computer program `hfb_shell`

(RB, arXiv:1104.5453)

[2] The code may be downloaded from `http://www.phys.washington.edu/users/bertsch/hfb-shell.21.tar` until it has been published in a journal repository.

Two essential tasks:

1) Compute $h = h(\rho)$, $\Delta = \Delta(\kappa)$
2) Update H^{00}, using $h, \Delta, \mathcal{W}$.

1) depends on the details of the Hamiltonian
2) can be programmed as a universal solver, taking $h(\rho)$ and $\Delta(\kappa)$ as function calls.

```
$ls
README.TXT      hfb.22          sd_data         test_22         uv
$ls hfb.22/
hfb.22.py               hfb_tools.py            hfb_utilities21.py      sd_specific21.py
$grep def hfb.22/hfb_utilities21.py
def check_unitarity(u,v):   #sanity check for u,v matrices
def check_skew(d) :       #sanity check for kappa, Delta, *20 matrices
def Ztransform(Z,uin,vin) :   # Eq. (13)
def F00(rhoL,FopL) :    #
def F20(uL,vL,FopL) :  # Eq. (6)
def F11(uL,vL,FopL) :  #
def G00(kappaL,GopL) :  #
def G11(uL,vL,GopL) :   #
def G20(uL,vL,GopL) :  # Eq. (8)
def G20x(uL,vL,GopL) :  # Eq. (8)
def FG00(FGops,rhoL,kappaL) :
def FG20(FGops,uL,vL) :
def FG11(FGops,uL,vL) :
def write_uv(uL,vL,filename='uv.out'):  #final u,v set is written to uv.out
def read_uv(Ndim,filename):     # read in initial u,v, set
def rho_kappa(uL,vL) :   # Eq. (1)
def H00(rr,kk,vrr,dd,espl) :  # Eq. (2)
def H20(uL,vL,hspL,dd) :    # Eq. (12)
$
```