Singlet and triplet pairing in nuclear and cold-atomic systems

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18 Febuary 2023

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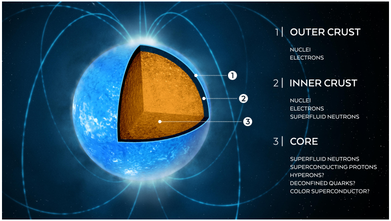
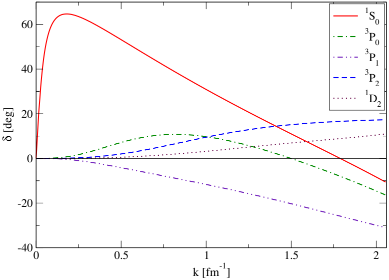
WNPPC 2023

Superfluid neutron matter



Credit: Anna L. Watts

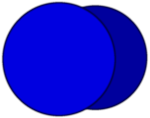


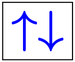
arXiv:1406.6109 [nucl-th]

s-wave (singlet) superfluidity in the inner crust

$10 \text{ km} \lessapprox r \lessapprox 12 \text{ km}$

$\rho \leq \rho_0/2 \quad (k_F \sim 1.4 \text{ fm})$





A new type of superfluidity

Can a mixed-spin (singlet and triplet) pairing state exist?

$$\boxed{\uparrow\downarrow \;\; \downarrow\downarrow \;\; \uparrow\uparrow}$$

The best of both worlds

Two approaches to the nuclear many-body problem for the ground state:

Ab initio (QMC)

- No extra assumptions
- Computationally expensive (only smallish N is feasible)

Phenomenology (BCS)

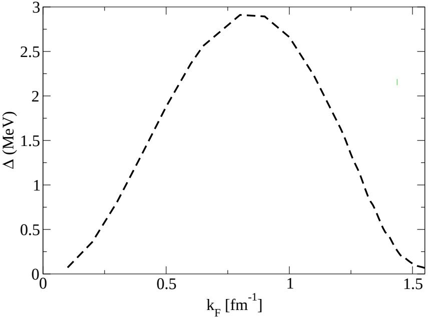
- Easier to implement
- Uncontrolled approximations

Phenomenology can guide *ab initio*
Ab initio can constrain phenomenology

Phenomenology: The BCS theory

$$\hat{\mathcal{H}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{kl}} V^0_{\mathbf{kl}} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \hat{c}_{-\mathbf{l}\downarrow} \hat{c}_{\mathbf{l}\uparrow}$$

$$|\psi\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \right) |0\rangle$$



S. Gandolfi, G. Palkanoglou, J. Carlson, A. Gezerlis, and K. E. Schmidt, Cond. Mat. **7**(1) (2022)

Ab initio: Full Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

AV8' interaction (two body)

$$v_{ij} = \sum_{i=i}^{8} v_p(r_{ij})O^{(p)}(i,j) \ , \quad O^{(p)} = 1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, \ldots$$

UIX interaction (three body)

$$V_{ijk} = V_{2\pi} + V_R \ , \quad \text{two-pion exchange + Remainder}$$

Ab initio: Quantum Monte Carlo (AFDMC)

Based on diffusion in imaginary time

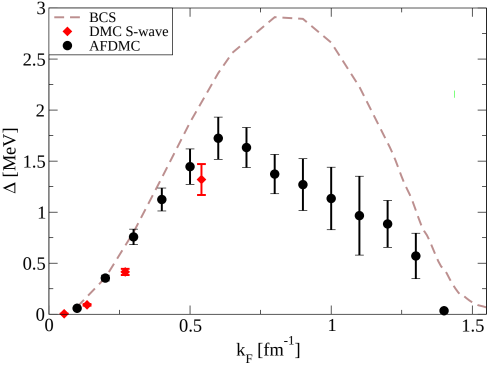
$$\psi(\tau) = e^{-(H-E_0)\tau}\psi_T = e^{-(H-E_0)\tau}\sum_n c_n\psi_n$$

$$\psi(\tau \to \infty) = c_0\psi_0$$

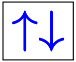
starting from a "physics aware" (i.e., $c_0 \neq 0$) trial state ψ_T

$$\psi_T(R, S) = \left[\prod_{i<j} f(r_{ij})\right]\Phi_{\mathrm{BCS}}(R, S)$$

The pairing gap of superfluid neutrons



Moderately **suppressed** pairing gap up to gap closure



- G. Palkanoglou, F. K. Diakonos, and A. Gezerlis, Phys. Rev. C **102** (2020)
- G. Palkanoglou, A. Gezerlis, Universe 2021, 7(2)
- S. Gandolfi, G. Palkanoglou, J. Carlson, A. Gezerlis, and K. E. Schmidt , Cond. Mat. **7**(1) (2022)

Neutrons and (cold) atoms

Neutron Matter

- In neutron stars and heavy nuclei
- Strongly interacting ($a = -18.5$ fm) close to UFG ($a = -\infty$) $\longrightarrow$
- * MeV scale

Cold atoms

- Experimentally accessible
- Tunable s-wave (now and p-wave) interactions
- * peV scale

Similar E/E_F and Δ/E_F

Mixed spin pairing in cold atoms: Phenomenology

Back to the BCS model

$\uparrow\downarrow$ $\downarrow\downarrow$ $\uparrow\uparrow$

$$\hat{\mathcal{H}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{kl}} V^{0}_{\mathbf{kl}} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \hat{c}_{-\mathbf{l}\downarrow} \hat{c}_{\mathbf{l}\uparrow} + \sum_{\mathbf{kl}} V^{1}_{\mathbf{kl}} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}\uparrow} \hat{c}_{-\mathbf{l}\uparrow} \hat{c}_{\mathbf{l}\uparrow} + \sum_{\mathbf{kl}} V^{1}_{\mathbf{kl}} \hat{c}^{\dagger}_{\mathbf{k}\downarrow} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \hat{c}_{-\mathbf{l}\downarrow} \hat{c}_{\mathbf{l}\downarrow}$$

Mixed spin pairing in cold atoms: Phenomenology

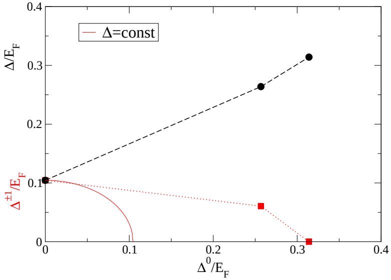
Mixed-spin wavefunction

$$|\psi\rangle = \prod_{\mathbf{k}>0} \Big[u_{\mathbf{k}} + \chi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} + y_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\downarrow} c^{\dagger}_{-\mathbf{k}\uparrow} + \\ + \beta_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\uparrow} + \gamma_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\downarrow} c^{\dagger}_{-\mathbf{k}\downarrow} + z_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c^{\dagger}_{\mathbf{k}\downarrow} c^{\dagger}_{-\mathbf{k}\uparrow} \Big] |0\rangle$$

used before for n-p pairing, e.g., Phys.Lett.B **524** (2002)

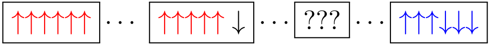
Mixed spin pairing in cold atoms: Phenomenology

We find mixed-spin states but **no** ground-state



The ground-state of an **unpolarized** Fermi gas seems to be of pure pairing

What about spin-imbalance?



Consequences of mixed-spin pairing

- Next step: *Phase diagram, behavior in a trap, possible Sarma phase*
- Next-Next-steps: *Ab initio description*

Conclusions

★ - For s-wave (singlet) pairing of neutrons:

- We have extracted the s-wave pairing gap of neutron matter for all relevant densities of the inner crust of neutron stars

★ - For s and p -wave pairing (mixed-spin) in cold atoms:

- Mixed-spin pairing does not exist in ground-states of unpolarized Fermi gases, but it might exist in spin -imbalanced Fermi gases

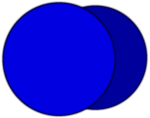
Acknowledgements

Acknowledgements:

- **Alex Gezerlis**
- **Stefano Gandolfi** (LANL)
- **Joe Carlson** (LANL)
- **Kevin Schmidt** (ASU)
- **Dean Lee** (MSU)
- **Caleb Hicks** (MSU)
- **Gabriel Given** (MSU)

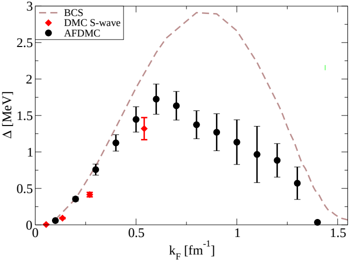
Computational Resources:

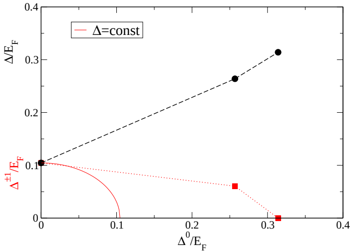
- NERSC
- SHARCNET



Thank you

Thank you & Conclusions





Thank you

BCS Theory and the gap Equations

Gap Distribution

The gap equations are:

$$\begin{aligned} \Delta(\mathbf{k}) &= -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{\sqrt{\xi^2(\mathbf{k}') + \Delta^2(\mathbf{k}')}} \\ \langle N \rangle &= \sum_{\mathbf{k}'} \left(1 - \frac{\xi(\mathbf{k}')}{\sqrt{\xi^2(\mathbf{k}') + \Delta^2(\mathbf{k}')}} \right) \end{aligned}$$

where:

$$\xi(\mathbf{k}) = \frac{\hbar^2}{2m_n}|\mathbf{k}|^2 - \quad \mu$$

BCS Theory and the gap Equations

Gap Distribution

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$$\Delta(\mathbf{k}) = -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{\sqrt{\xi^2(\mathbf{k}') + \Delta^2(\mathbf{k}')}}$$

$$\langle N \rangle = \sum_{\mathbf{k}'} \left(1 - \frac{\xi(\mathbf{k}')}{\sqrt{\xi^2(\mathbf{k}') + \Delta^2(\mathbf{k}')}}\right)$$

Average Particle Number (*Fixed*)

where:

$$\xi(\mathbf{k}) = \frac{\hbar^2}{2m_n}|\mathbf{k}|^2 - \mu$$

BCS Theory and the gap Equations

Gap Distribution

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$$\langle N \rangle = \sum_{\mathbf{k}'} \left(1 - \frac{\xi(\mathbf{k}')}{\sqrt{\xi^2(\mathbf{k}') + \Delta^2(\mathbf{k}')}}\right)$$

Average Particle Number (*Fixed*)

Chemical Potential

where:

$$\xi(\mathbf{k}) = \frac{\hbar^2}{2m_n}|\mathbf{k}|^2 - \mu$$

The solution of the BCS gap Equations

$$u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\xi(\mathbf{k})}{\sqrt{\xi^2(\mathbf{k}) + \Delta^2(\mathbf{k})}}\right)$$
$$v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi(\mathbf{k})}{\sqrt{\xi^2(\mathbf{k}) + \Delta^2(\mathbf{k})}}\right)$$

where:

$$v_{\mathbf{k}}^2 + u_{\mathbf{k}}^2 = 1$$

Odd and even particle numbers

$$\Delta(N) = E(N+1) - \frac{1}{2}\left[E(N) + E(N+2)\right]$$

$$|\psi_\phi\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + e^{i\phi} v_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow}) |0\rangle$$

(even systems)

$$\left|\psi_\phi^{\mathbf{b}\gamma}\right\rangle = \hat{c}^\dagger_{\mathbf{b}\gamma} \prod_{\mathbf{k}\neq\mathbf{b}} (u_{\mathbf{k}} + e^{i\phi} v_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow}) |0\rangle$$

(odd systems)

BCS is formulated in a Grand Canonical Ensemble.

PBCS - the Projected Energy

The energy of the projected states is:

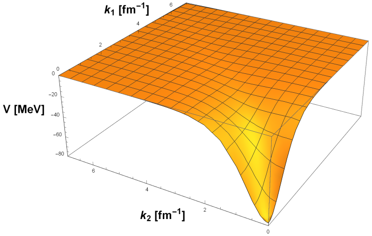
$$
\begin{aligned}
E_N =& 2\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} v_{\mathbf{k}}^2 \frac{R_1^1(\mathbf{k})}{R_0^0} + \sum_{\mathbf{kl}} V_{\mathbf{kl}} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{l}} v_{\mathbf{l}} \frac{R_1^2(\mathbf{kl})}{R_0^0} \ , \\
E_{N+1} =& 2\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} v_{\mathbf{k}}^2 \frac{R_1^2(\mathbf{bk})}{R_0^1(\mathbf{b})} + \\
& + \sum_{\mathbf{kl}} V_{\mathbf{kl}} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{l}} v_{\mathbf{l}} \frac{R_1^3(\mathbf{bkl})}{R_0^1(\mathbf{b})} + \frac{\hbar^2}{2m_n} |\mathbf{b}|^2 \ .
\end{aligned}
$$

The Potential

The **Modified Poschl-Teller Potential**:

$$V(r) = -\lambda(\lambda - 1)\frac{\hbar^2}{m_n}\frac{q^2}{\cosh^2(qr)}$$

- Purely Attractive
- Finite Range



The residuum integrals

The **residuum integrals**:

$$R_n^m(\mathbf{k}_1\mathbf{k}_2\ldots\mathbf{k}_N)(M) = \\ = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-iM\phi} e^{in\phi} \prod_{\mathbf{k}\neq\mathbf{k}_1,\mathbf{k}_2,\ldots,\mathbf{k}_m} (u_{\mathbf{k}}^2 + e^{i\phi} v_{\mathbf{k}}^2)$$

where $M = \dfrac{N}{2}$.

Twisted Boundary Conditions

$$\left|\psi(\mathbf{r}_1 + L\hat{\mathbf{x}}, \ldots, \mathbf{r}_N)\right|^2 = \left|\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)\right|^2$$

Periodic Boundary Conditions

$$\psi(\mathbf{r}_1 + L\hat{\mathbf{x}}, \ldots, \mathbf{r}_N) = \psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

$$\Downarrow$$

$$\mathbf{k} = \frac{2\pi}{L}\mathbf{n}$$

Twisted boundary conditions

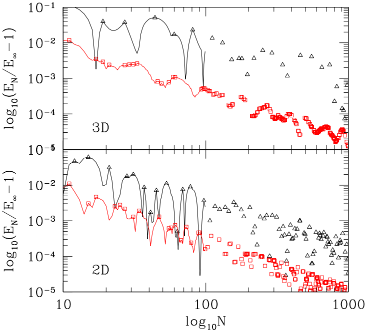
$$\psi\left(\mathbf{r}_1 + L\hat{x}, \mathbf{r}_2, \ldots, \mathbf{r}_{N_0}\right) = e^{i\theta_x}\psi\left(\mathbf{r}_1, \ldots, \mathbf{r}_{N_0}\right)$$

$$\Downarrow$$

$$\mathbf{k} = \frac{2\pi}{L}\left(\mathbf{n} + \frac{\boldsymbol{\theta}}{2\pi}\right)$$

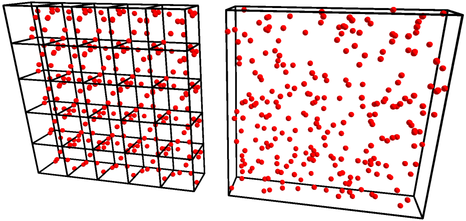
Averaging over $\boldsymbol{\theta}$ can reduce finite-size effects

$$\left\langle \hat{F} \right\rangle = \int \frac{d^3\boldsymbol{\theta}}{(2\pi)^3} \langle \psi(\boldsymbol{\theta}) | \hat{F} | \psi(\boldsymbol{\theta}) \rangle$$



C. Lin, F. H. Zong, and D.M. Ceperley
Phys. Rev. E **64**, 016702 (2001)

Twisted Boundary Conditions

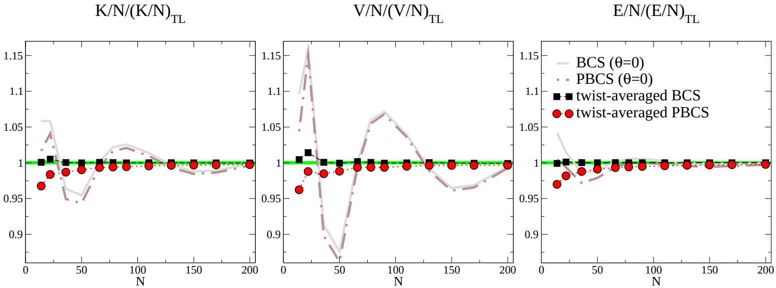


Credit: Nawar Ismail

$$|\psi(\mathbf{r}_1 + L\hat{\mathbf{x}}, \ldots, \mathbf{r}_N)|^2 = |\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2$$

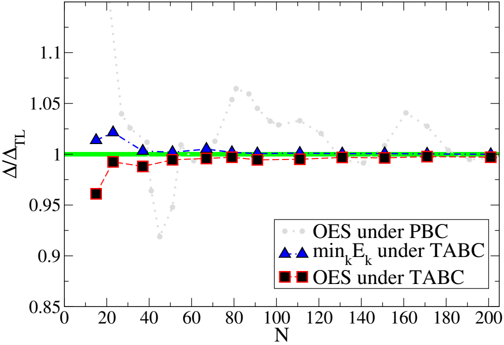
$$\psi(\mathbf{r}_1 + L\hat{\mathbf{x}}, \ldots, \mathbf{r}_N) = e^{i\theta_x}\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

Twist-averaged energy



G. Palkanoglou and A. Gezerlis, Universe **2021**, 7(2), 24

Twist-averaged pairing gap



G. Palkanoglou and A. Gezerlis, Universe **2021**, 7(2), 24

$$\Delta(N) = E(N+1) - \frac{1}{2}\left[E(N) + E(N+2)\right]$$

Phenomenology: The BCS Theory

$$v_{\mathbf{k}}^2 = \frac{1}{2}\left[1 - \frac{\xi(\mathbf{k})}{\sqrt{\xi^2(\mathbf{k}) + \Delta^2(\mathbf{k})}}\right]$$

$$u_{\mathbf{k}}^2 = \frac{1}{2}\left[1 + \frac{\xi(\mathbf{k})}{\sqrt{\xi^2(\mathbf{k}) + \Delta^2(\mathbf{k})}}\right]$$

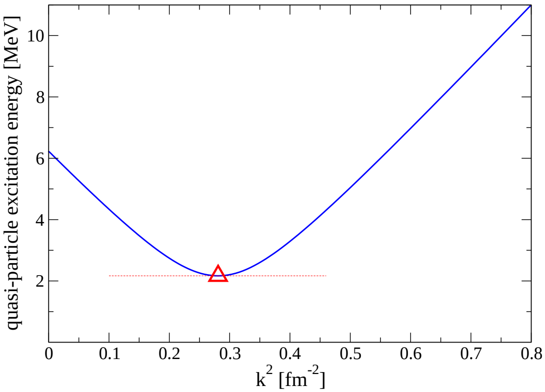
where $\Delta(\mathbf{k})$ satisfies the **gap equation**:

$$\Delta(\mathbf{k}) = -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{\sqrt{\xi^2(\mathbf{k}') + \Delta^2(\mathbf{k}')}}$$

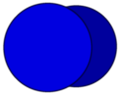
where:

$$\xi(\mathbf{k}) = \frac{\hbar^2}{2m_n}|\mathbf{k}|^2 - \mu$$

Phenomenology: The BCS theory



pairing gap Δ is the pair's binding energy



Phenomenology: The BCS theory

Assume a coherent state of pairs
(resulting in free quasiparticles)

$$|\psi\rangle = \prod_{\mathbf{k}} \left[u(\mathbf{k}) + v(\mathbf{k}) \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \right] |0\rangle$$

where u and v are determined by minimizing the energy of the pairing Hamiltonian

$$\hat{\mathcal{H}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{kl}} V_{\mathbf{kl}} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \hat{c}_{-\mathbf{l}\downarrow} \hat{c}_{\mathbf{l}\uparrow}$$

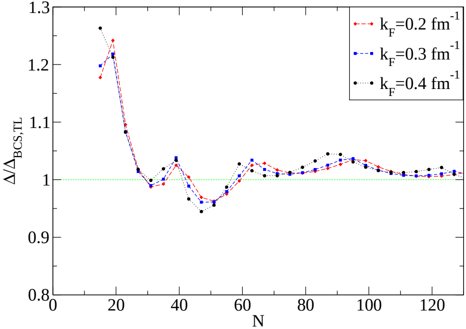
$$\langle\psi| \hat{\mathcal{H}} |\psi\rangle = \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}} v^2(\mathbf{k}) + \sum_{\mathbf{kl}} V_{\mathbf{kl}} u(\mathbf{k}) v(\mathbf{k}) u(\mathbf{l}) v(\mathbf{l})$$

Ab initio: more guidance by phenomenology

Model-independent pairing gap: odd-even staggering

$$\Delta(N) = E(N) - \frac{1}{2}\left[E(N+1) + E(N-1)\right]$$

Finite-size effects



G. Palkanoglou, F. K. Diakonos, and A. Gezerlis, Phys. Rev. C 102, 064324 (2020)

G. Palkanoglou, A. Gezerlis, Universe 2021, 7(2)

Ab initio: Trial state for AFDMC

$$\psi_T(R,S) = \left[\prod_{i<j} f(r_{ij})\right] \Phi(R,S)$$

A symmetric part

$f(r)$: two-body spin-independent only reduces variance

An **anti**symmetric part

$$\Phi(R,S) = \mathrm{Pf}A = \mathcal{A}\left[\phi(1,2), \phi(3,4), \ldots, \phi(N-1,N)\right]$$

$$\phi(i,j) = \sum_{\alpha} c_\alpha \, e^{i\mathbf{k}_\alpha \mathbf{r}_{ij}} \chi(s_i, s_j)$$

c_α → variational

$\left(\text{in BCS } c_\alpha = v_{\mathbf{k}_\alpha}/u_{\mathbf{k}_\alpha}\right)$

Mixed-spin pairing in nuclei: Phenomenology

What we know:

- Pairing in all observed nuclei is spin-singlet
- Predicted spin-triplet in large nuclei $A \sim 100$ at $N = Z$

  G. F. Bertsch and Y. Luo, Phys. Rev. C **81** (2010)

★ Predicted **mixed**-spin pairing in $A \sim 130$ at $N \approx Z$

  A. Gezerlis, G. F. Bertsch, and Y. L. Luo, Phys. Rev. Lett. **106** (2011)

  E. Rrapaj, A. O. Macchiavelli, and A. Gezerlis, Phys. Rev. C **99** (2019)

- Experiment: we expect to see it as:
  - enhanced *np* transfer reaction cross-sections
  - similarities between the spectra of odd-odd and even-even nuclei

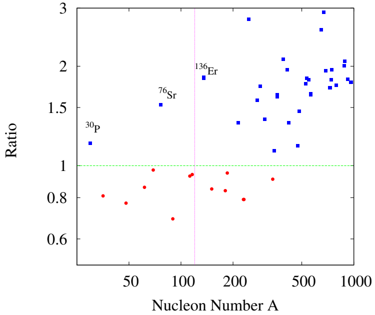
    S. Frauendorf, Rev. Mod. Phys. **73** (2001)

But, **deformation**, neglected in the above, **reduces pairing** by reducing the s.p. level density at mid-shell filling

S. Frauendorf and A. O. Macchiavelli, Prog. Part. Nucl. Phys. **78**, 24 (2014)
G. Hupin and D. Lacroix, Phys. Rev. C **86** (2012)

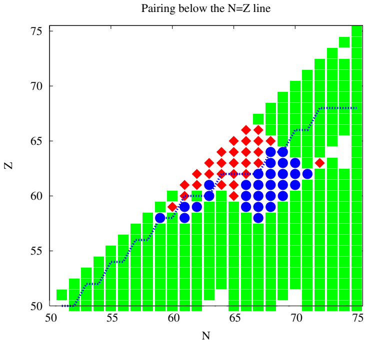
Mixed-spin pairing in nuclei: Phenomenology

singlet and triplet



G. F. Bertsch and Y. Luo, Phys. Rev. C **81** (2010)

singlet, triplet, and mixed



A. Gezerlis, G. F. Bertsch, and Y. L. Luo, Phys. Rev. Lett. **106** (2011)

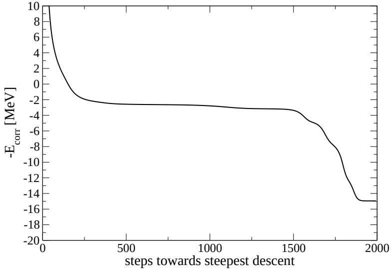
Mixed-spin pairing in nuclei: Phenomenology

HFB treatment (mean-field like BCS) amounts to bi-linearizing the Hamiltonian in quasiparticle (β) space :

$$H = \sum_{ij} \epsilon_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{ijkl} v_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$
$$= H^{00} + \beta^\dagger H^{11} \beta + \frac{1}{2} \beta^\dagger H^{20} \beta^\dagger + \dots$$

The quasiparticles that minimize the energy are found by gradient descent with the state

$$|\Phi(Z)\rangle \propto \exp\left[\sum_{i<j} Z_{ij} \beta_i^\dagger \beta_j^\dagger\right] |0\rangle$$



Mixed-spin pairing in nuclei: Phenomenology

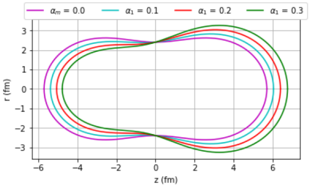
Axially-symmetric deformation in the single-particle states:

$$H_{\rm sp} = \frac{\mathbf{p}^2}{2m} + V^{\rm def}_{\rm WS}(\rho, z) + \kappa \boldsymbol{\nabla} V^{\rm def}_{\rm WS}(\rho, z) \cdot (\mathbf{s} \times \mathbf{p})$$

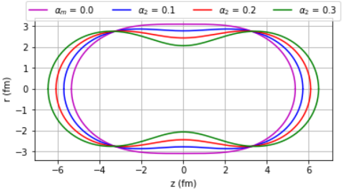
with

$$V^{\rm def}_{\rm WS}(\rho, z) = \frac{V_0}{1 + \exp\left[l(\rho, z)/a\right]} \ , \quad l(\rho, z) = f(\epsilon, a_1, a_2 \ldots ; \rho, z)$$

(see Cassinian ovals: V. V. Pashkevich, Nucl. Phys. A**169** (1971), etc)



(a) Dipole deformations



(b) Quadrupole deformations