From the odd-even staggering to the pairing gap in neutron matter

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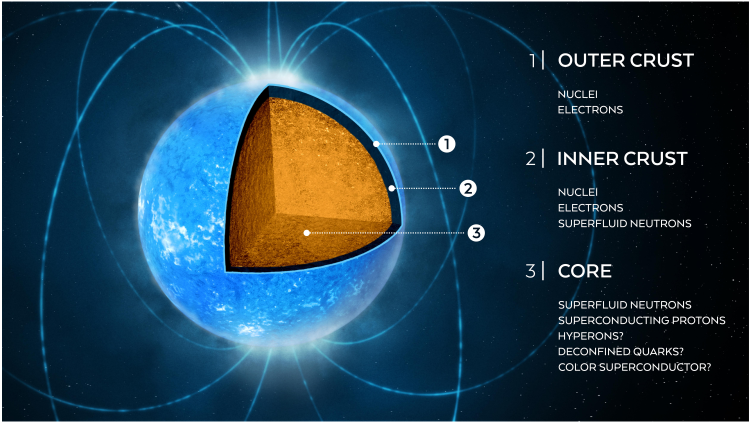
Motivation & Physical System

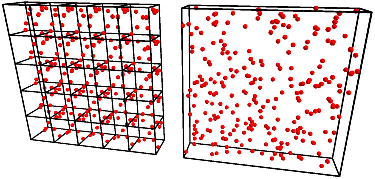


Credit: Anna L. Watts

Motivation & Physical System

Periodic Boundary Conditions

$$|\psi(\mathbf{r}_1 + L\hat{\mathbf{x}}, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2 = |\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2$$



by Nawar Ismail

$$\mathbf{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$$

BCS Theory and The Gap Equations

We describe the system with the Hamiltonian:

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

where:

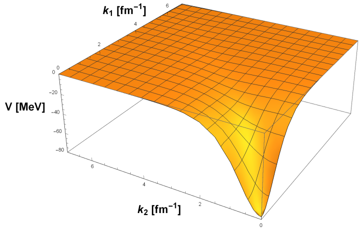
$$\epsilon_{\mathbf{k}} = \frac{\hbar^2}{2m_n} |\mathbf{k}|^2$$

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



BCS Theory and The Gap Equations

The **BCS** ground state is

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

where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ minimize the Free Energy:

$$F = \langle\psi| (\hat{\mathcal{H}} - \mu \hat{N}) |\psi\rangle$$

BCS Theory and The Gap Equations

Gap Distribution

The Gap equations are:

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

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

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

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

Average Particle Number (*Fixed*)

where:

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BCS Theory and The Gap Equations

Gap Distribution

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

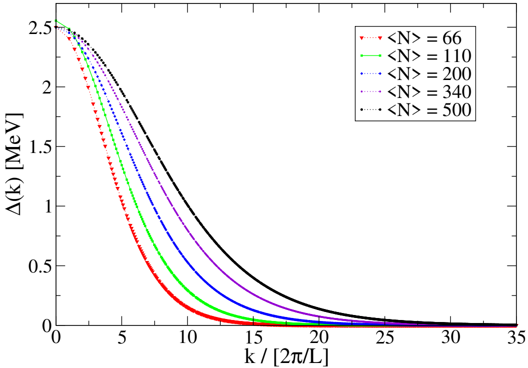
Average Particle Number (*Fixed*)

Chemical Potential

where:

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

The solution of the BCS Gap Equations - $\Delta(\mathbf{k})$ vs $\mathbf{k}$ for different $\langle N \rangle$



The Gap distribution as a function of k for different average particle numbers $\langle N \rangle$

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:

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

The solution of the BCS Gap Equations - Excitation Energy and the Gap

Within BCS we define:

$$\Delta = \min_{\mathbf{k}} E_{\mathrm{q}}(\mathbf{k})$$

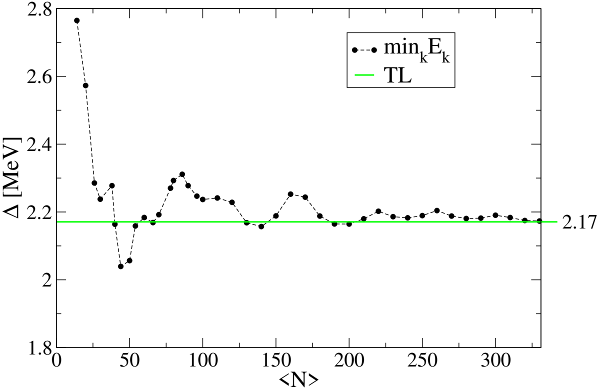
$$\text{where } E_{\mathrm{q}}(\mathbf{k}) = \sqrt{(\frac{\hbar}{2m_n}|\mathbf{k}|^2 - \mu)^2 + \Delta^2(\mathbf{k})}$$

Alternative definition inspired by the odd-even staggering (OES) in nuclear physics:

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

$$\text{for Even } N$$

The solution of the BCS Gap Equations - Δ vs $\langle N \rangle$



The Gap as a function of the average particle number.

The solution of the BCS Gap Equations

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

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

(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 States

Restoring the conservation:

$$|\psi_N\rangle = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i\frac{N}{2}\phi} \prod_{\mathbf{k}} (u_{\mathbf{k}} + e^{i\phi} v_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow}) |0\rangle$$

(even systems)

$$\left|\psi^{\mathbf{b}\gamma}_{N+1}\right\rangle = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-i\frac{N}{2}\phi} \hat{c}^\dagger_{\mathbf{b}\gamma} \prod_{\mathbf{k}\neq\mathbf{b}} (u_{\mathbf{k}} + e^{i\phi} v_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow}) |0\rangle$$

(odd systems)

This is the ground state of the PBCS Theory.

PBCS - the Projected Energy

The energy of the projected states is:

$$E_N = 2\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} v_{\mathbf{k}}^2 \frac{R_1^1(\mathbf{k})}{R_0^0} + \sum_{\mathbf{kl}} V_{\mathbf{kl}} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{l}} v_{\mathbf{l}} \frac{R_1^2(\mathbf{kl})}{R_0^0} \ ,$$

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

The Gap beyond mean-field

BCS definition: mean-field

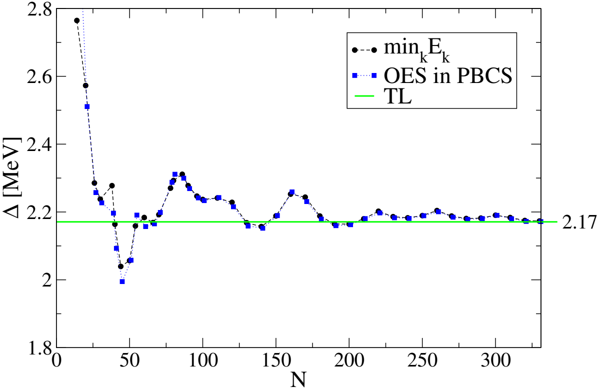
$$\Delta = \min_{\mathbf{k}} E_q(\mathbf{k})$$

OES definition: beyond mean-field

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

for Even N

Δ vs N in BCS & the OES



The Gap in BCS and the OES at $k_{\mathrm{F}}a = -10$.

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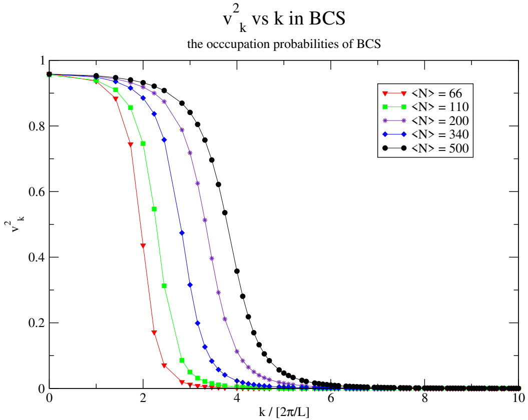
- NERSC
- SHARCNET

Thank you

The solution of the BCS Gap Equations - $v(\mathbf{k})^2$ vs $\mathbf{k}$ for different $\langle N \rangle$



The pair occupation probability as a function of k for different average particle numbers

The BCS Gap Equations at the Thermodynamic Limit (TL)

In the Thermodynamic Limit:

$$\Delta(k) = -\frac{1}{\pi}\int_0^\infty \mathrm{d}k'\,(k')^2 V_0(k,k')\frac{\Delta(k')}{\sqrt{\xi^2(k')+\Delta^2(k')}}$$

$$n = \frac{1}{2\pi^2}\int_0^\infty \mathrm{d}k'\,(k')^2\left(1-\frac{\xi(k')}{\sqrt{\xi^2(k')+\Delta^2(k')}}\right)$$

where $n = \dfrac{k_F^3}{3\pi^2}$ is the number density.

BCS & PBCS - E/N vs N

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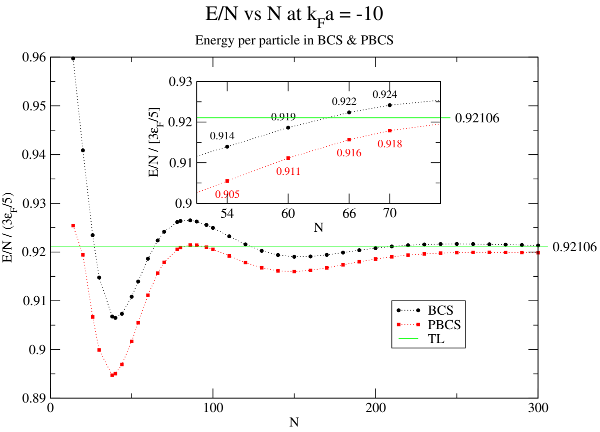

The energy per particle in BCS and PBCS scaled by the energy per particle of the free Fermi gas.

Summary

The Final Step: Twist-Average the results:

$$\int_{-\pi}^{\pi} \frac{\mathrm{d}\boldsymbol{\theta}}{(2\pi)^3} \left(\Delta_{\boldsymbol{\theta}} = E_{\boldsymbol{\theta}}(N+1) - \frac{1}{2}\left[E_{\boldsymbol{\theta}}(N) + E_{\boldsymbol{\theta}}(N+2)\right] \right)$$

Twists

From the odd-even staggering to the pairing gap in neutron matter

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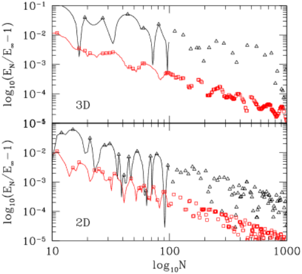
$$\left\langle \hat{A} \right\rangle = (2\pi)^{-d} \int_{-\pi}^{\pi} \mathrm{d}\boldsymbol{\theta} \, \langle \psi(R, \boldsymbol{\theta}) | \, \hat{A} \, | \psi(R, \boldsymbol{\theta}) \rangle$$

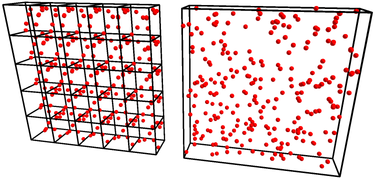


Lin C. et al, *Twist-averaged Boundary Conditions in Continuum Quantum Monte Carlo*

Twists

Periodic Boundary Conditions

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



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Twist

$$\mathbf{k}_n = \frac{2\pi}{L}(n_x, n_y, n_z) + \frac{\boldsymbol{\theta}}{L}$$

Twists

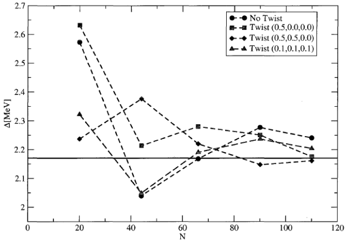


Figure: Gezerlis A. : *Microscopic Simulations of Strongly Paired Systems*

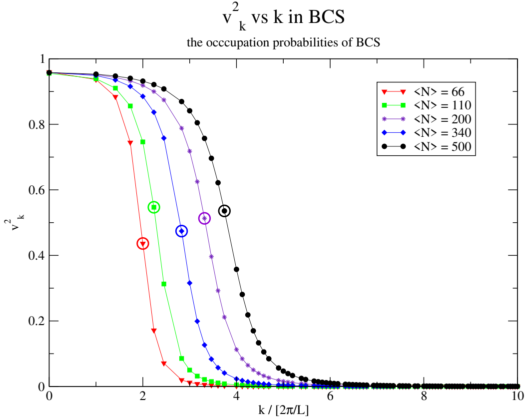
$$\Delta = E(N+1) - \frac{1}{2}\left[E(N) + E(N+2)\right]$$

Solving the BCS Gap Equations

The solution of these equations is found through an iterative scheme:

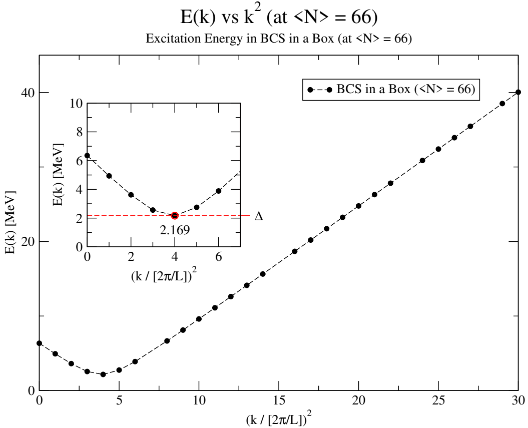
- $\Delta^{(0)}(k) = 1$ & initial guess for μ_{ch}
- $\Delta^{(1)}(k) = -\frac{2\pi}{L^3}\sum_p M(p)V_0(k,p)\frac{\Delta^{(0)}(p)}{\sqrt{\xi^2(p)+(\Delta^{(0)})^2(p)}}$
- $\Delta^{(2)}(k) = -\frac{2\pi}{L^3}\sum_p M(p)V_0(k,p)\frac{\Delta^{(1)}(p)}{\sqrt{\xi^2(p)+(\Delta^{(1)})^2(p)}}$
- ...etc...

The solution of the BCS Gap Equations - $v(\mathbf{k})^2$ vs $\mathbf{k}$ for different $\langle N \rangle$



The pair occupation probability as a function of k for different average particle numbers. Circled are the values of k where $E(k)$ is minimum.

The solution of the BCS Gap Equations-Excitation Energy and the Gap



The excitation energy as a function of k^2. The minimum of the excitation energy is the Gap.

PBCS - The Projected Energy

The **Residuum Integrals**:

$$R_n^N(\mathbf{k}_1\mathbf{k}_2\ldots\mathbf{k}_N)(M) =$$

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

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