Superfluid neutron matter with a twist: *From particles to matter*

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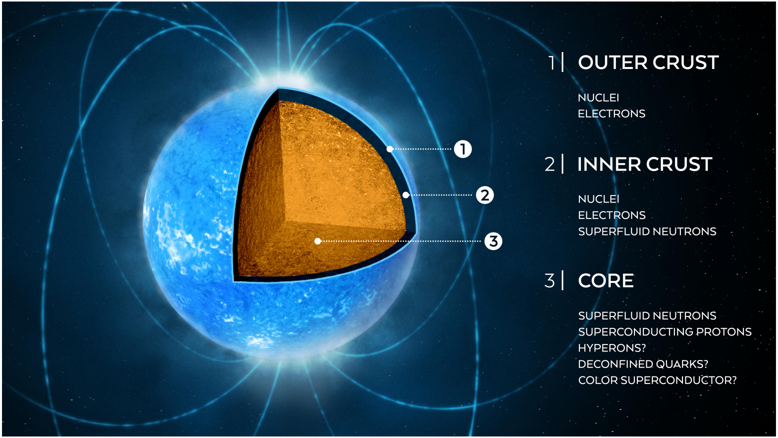
Superfluid neutron matter

- Where to find it & why care about it
- How to study it
- Results: How to study **infinite** superfluid neutron matter with finite systems

Motivation & physical system



Credit: Anna L. Watts

The best of both worlds

Ab initio

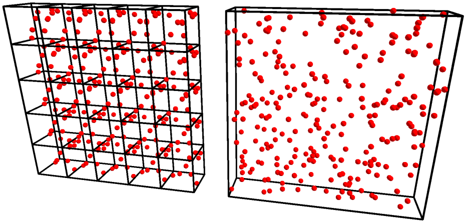
- No extra assumptions
- Computationally expensive (only smallish N is feasible)

Phenomenology

- Easier to implement
- Uncontrolled approximations

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

Twisted Boundary Conditions



Credit: Nawar Ismail

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

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

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

$$\psi(\mathbf{r}_1 + L\hat{\mathbf{x}}, \ldots, \mathbf{r}_N) = \psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$
$$\Downarrow$$
$$\mathbf{k} = \frac{2\pi}{L}\mathbf{n}$$

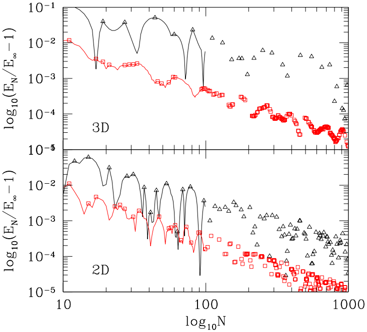
Twisted boundary conditions

$$\psi\left(\mathbf{r}_1 + L\hat{x}, \mathbf{r}_2, \ldots, \mathbf{r}_{N_0}\right) = e^{i\theta_x}\psi\left(\mathbf{r}_1, \ldots, \mathbf{r}_{N_0}\right)$$
$$\Downarrow$$
$$\mathbf{k} = \frac{2\pi}{L}\left(\mathbf{n} + \frac{\boldsymbol{\theta}}{2\pi}\right)$$

Twist-averaged boundary conditions

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

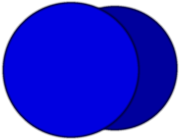
$$\left\langle \hat{F} \right\rangle = \int \frac{d^3\boldsymbol{\theta}}{(2\pi)^3} \left\langle \psi(\boldsymbol{\theta}) \right| \hat{F} \left| \psi(\boldsymbol{\theta}) \right\rangle$$



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

The pairing Hamiltonian

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



BCS and PBCS theories for neutron matter

BCS: *mean-field*

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

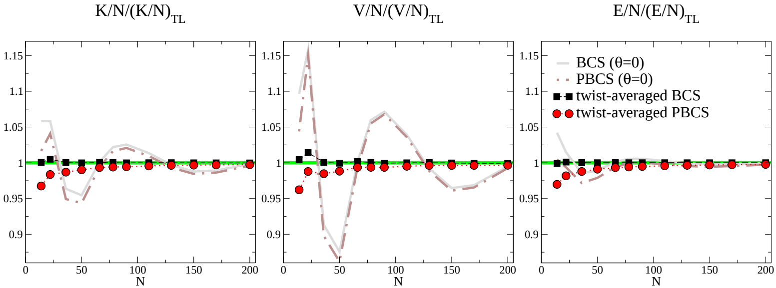
PBCS: *fixed-N*

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

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

for even N

Twist-averaged energy



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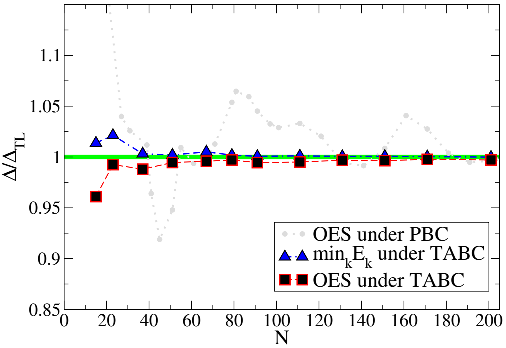
Twist-averaged pairing gap



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

Conclusions

★ - Twist-averaged boundary conditions work well for superfluid systems

★ - We now have a better prescription on how to approximate infinite superfluid neutron matter with a finite system

Acknowledgements

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- **Alex Gezerlis**

Computational Resources:

- NERSC
- SHARCNET

UNIVERSITY of GUELPH

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Thank you

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:

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

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Average Particle Number (*Fixed*)

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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:

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

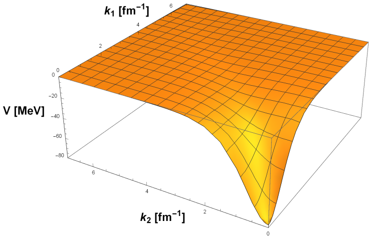
$$E_{N+1} = 2\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} v_{\mathbf{k}}^2 \frac{R_1^2(\mathbf{bk})}{R_0^1(\mathbf{b})} + \\ + \sum_{\mathbf{kl}} V_{\mathbf{kl}} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{l}} v_{\mathbf{l}} \frac{R_1^3(\mathbf{bkl})}{R_0^1(\mathbf{b})} + \frac{\hbar^2}{2m_n} |\mathbf{b}|^2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

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