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Local Quantum Cooling for Large Fermi Systems with Pairing

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Outline

- Motivation
- Method: Quantum cooling, DFT, TDDFT, and Tests
- Applications: Spin imbalanced systems, Protonic clusters, and Nuclear Pasta
- Conclusions
- Outlook

Motivation

Motivation

- For large superfluid fermionic systems (cold atoms, nuclear matter), **numerical ground-state preparation** is a **bottleneck** with the current standard approaches.
- We want a dynamical description of finite-temperature effects via dissipation and stochastic models.
- Both of these are achieved by dissipative dynamics

Standard Approaches

The majority of many-body techniques used to study fluctuations and dissipation of large quantum systems operate directly on wave functions:

$$i\hbar\frac{\partial\varphi_k}{\partial t} = \underline{\boldsymbol{H}}\varphi_k + (\underline{\boldsymbol{S}}_k - i\underline{\boldsymbol{W}}_k\varphi_k) + \sum_l \lambda_{kl}\varphi_l. \tag{1}$$

$\underline{\boldsymbol{W}}_k \longrightarrow$ Dissipation (Breaks orthonormality)

$\underline{\boldsymbol{S}}_k \longrightarrow$ Fluctuations

$\lambda_{kl} \longrightarrow$ Lagrangian multiplier that enforce $\langle\varphi_k|\varphi_l\rangle = \delta_{kl}$

A. Bulgac, *Phys. Rev. C* **100**, 014615 (2019).

Why It's Difficult (with the current immplementations)?

Consider a single time step of the form (using $\underline{\boldsymbol{S}}_k = 0$)

$$\varphi_k(t + \Delta t) = e^{-i(\underline{\boldsymbol{H}} - i\underline{\boldsymbol{W}}_k)\Delta t/\hbar}\varphi_k(t), \tag{2}$$

applied to all M evolved wave functions, each of length N

- $e^{-i(\underline{\boldsymbol{H}} - i\underline{\boldsymbol{W}}_k)\Delta t/\hbar} \to \mathscr{O}(MN \log N)$ operations with spectral methods.
- Gram–Schmidt process $\to \mathscr{O}(M^2 N)$.

For large many-body systems, where $M \gg \log N$, this orthogonalization stage dominates the computational cost, often by orders of magnitude.

Goal

To have a method that evolves an initial condition in time, and it:

- Keeps orthonormality
- Local in coordinate space so it can be seamlessly integrated into time-dependent density functional theory frameworks. **Independently of the density functional**.
- Selective on dissipation channel

Method

Quantum cooling

Consider a system evolving with a single wavefunction: $\hat{H}\psi = E\psi$
We evolve the system with a "cooling" Hamiltonian $\hat{H}_c = \hat{H}_c^\dagger$,

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle \equiv i\hbar|\dot{\psi}\rangle = \hat{H}_c|\psi\rangle \tag{3}$$

The change in energy is:

$$\begin{aligned}\dot{E} &= \langle\dot{\psi}|\hat{H}|\psi\rangle + \langle\psi|\hat{H}|\dot{\psi}\rangle + \cancel{\langle\psi|\dot{\hat{H}}|\psi\rangle} \\ &= \frac{-\langle\psi|\hat{H}_c\hat{H}|\psi\rangle + \langle\psi|\hat{H},\hat{H}_c|\psi\rangle}{i\hbar} = \frac{\langle\psi|[\hat{H},\hat{H}_c]|\psi\rangle}{i\hbar} \\ &= -\langle\psi|\psi\rangle\mathrm{Tr}\left(i[\hat{R},\hat{H}]\hat{H}_c\right)/\hbar; \quad \hat{R} \equiv \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}\text{: normalized density operator}\end{aligned} \tag{4}$$

Quantum cooling

Why not choose $\hat{H}_c = \left(i[\hat{R}, \hat{H}]\right)^\dagger = -i[\hat{R}, \hat{H}]$?
This would lead to

$$\hbar \dot{E} = -\langle\psi|\psi\rangle \mathrm{Tr}\left(i[\hat{R}, \hat{H}]\hat{H}_c\right) = -\langle\psi|\psi\rangle \mathrm{Tr}\left(\hat{H}_c^\dagger \hat{H}_c\right) \leq 0 \qquad (5)$$

We can even improve this by doing it locally in time and adding a proportionality factor:

$$\hat{H}_c = -i\alpha[\hat{R}(t), \hat{H}]$$

Quantum cooling: Bosonic Case

Consider the case of a macroscopic wavefunction Ψ_t and $\hat{H} = -\hbar^2\nabla^2/2m + V(\mathbf{x})$, then:
$\hat{H}_c = -2\alpha \mathrm{Im}(\Psi_t^* \hat{H} \Psi_t) = -2\alpha\hbar\nabla \cdot \vec{j} = \alpha\hbar\dot{\rho}$

$$\hbar\dot{E} = 2\mathrm{Im}\langle\Psi_t|\hat{H}\hat{H}_c|\Psi_t\rangle = -2\alpha(\mathrm{Im}\langle\Psi_t|\hat{H}|\Psi_t\rangle)^2 < 0 \qquad (6)$$

Quantum cooling: Fermionic Case

$\hat{R}$ is changed for the generalized density matrix

$$\mathscr{R} = \begin{pmatrix} \underline{\boldsymbol{\rho}} & \underline{\boldsymbol{\kappa}} \\ -\underline{\boldsymbol{\kappa}}^* & \underline{\mathbf{1}} - \underline{\boldsymbol{\rho}}^* \end{pmatrix}; \quad \rho_{\mu\nu} = \langle \hat{a}_\nu^\dagger \hat{a}_\mu \rangle, \kappa_{\mu\nu} = \langle \hat{a}_\nu \hat{a}_\mu \rangle \tag{7}$$

$$\mathscr{H}_{td} = \mathscr{H} + \mathscr{H}_c \tag{8}$$

One can do dynamical evolution with energy dissipation taking into account:
$\mathscr{H}$: the **intrinsic (TD-DFT) Hamiltonian**, specific of the problem.
$\mathscr{H}_c \propto [\mathscr{R}(t), \mathscr{H}] = \dot{\mathscr{R}}(t)$ the **cooling potential** (huge matrix) that can be separately divided into:

- Diagonal terms (mean field)
- Non-diagonal (pairing terms) { Particle conserving / Non-Particle conserving

Intiution of quantum cooling

Intuitive picture similar to that in laser cooling of atoms or *optical molasses*[1]: the introduced cooling potential is large where the generalized density changes, thereby mitigating large changes and cooling the system.

$$\dot{\mathscr{R}} \Longrightarrow \dot{E} \lll 0$$

$$\dot{\mathscr{R}} \Longrightarrow \dot{E} \sim 0$$

$$\dot{\mathscr{R}} = 0 \Longrightarrow \dot{E} = 0$$

C. N. Cohen-Tannoudji and W. D. Phillips, *Physics Today*. **43**, 33 (1990).

DFT Framework

We work with Superfluid Local Density Approximation (SLDA)-type functionals where densities are **parametrized** via Bogoliubov quasiparticle functions

$$\varphi_{n,\sigma}(\mathbf{r},t) = [u_{n,\sigma}(\mathbf{r},t),\ v_{n,\sigma}(\mathbf{r},t)]^T\,, \qquad \int \varphi^\dagger_\eta(\mathbf{r},t)\varphi_{\eta'}(\mathbf{r},t) = \delta_{\eta,\eta'}, \quad \sigma = \{\uparrow,\downarrow\},\{\mathrm{p},\mathrm{n}\}.$$

Quasiparticle (hole and particle)+ orthonormality condition (Pauli)

(9)

$$E_0[\rho,\tau,\nu] = \int \mathscr{E}(\rho_\sigma,\tau_\sigma,\mathbf{j}_\sigma,\nu_\sigma)d^3r \tag{10}$$

$$\rho_\sigma = \sum_{|E_c|<E_n} |v_{n,\sigma}|^2 f_{\beta'}(-E_n) \qquad \nu_\sigma = \tfrac{1}{2}\sum_{|E_c|<E_n} u_{n,\sigma}v^*_{n,\sigma}(f_{\beta'}(-E_n) - f_{\beta'}(E_n))$$

$$\tau_\sigma = \sum_{|E_c|<E_n} |\nabla v_{n,\sigma}|^2 f_{\beta'}(-E_n) \qquad \mathbf{j}_\sigma = \sum_{|E_c|<E_n} \mathrm{Im}\,[v_{n,\sigma}\nabla v^*_{n,\sigma}] f_{\beta'}(-E_n)$$

Minimization of the SLDA-type functional leads to equations that are mathematically equivalent to BdG or HFB equations

$$\begin{pmatrix} \underline{\boldsymbol{h}}_\sigma(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -\underline{\boldsymbol{h}}_\sigma(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_{n,\sigma}(\mathbf{r}) \\ v_{n,\sigma}(\mathbf{r}) \end{pmatrix} = \varepsilon_n \begin{pmatrix} u_{n,\sigma}(\mathbf{r}) \\ v_{n,\sigma}(\mathbf{r}) \end{pmatrix}, \tag{11}$$

$$\underline{\boldsymbol{h}}_\sigma = \nabla \frac{\delta E_0}{\delta \tau_\sigma} \nabla + \frac{\delta E_0}{\delta \rho_\sigma} - \frac{1}{2} \left\{ \frac{\delta E_0}{\delta \tau_\sigma} \right\}, \quad \Delta = -\frac{\delta E_0}{\delta \tau_\sigma^*} \tag{12}$$

Adiabatic approximation

$$\begin{pmatrix} \underline{\boldsymbol{h}}_\sigma(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -\underline{\boldsymbol{h}}_\sigma(\mathbf{r}) \end{pmatrix} \begin{pmatrix} u_{n,\sigma}(\mathbf{r}) \\ v_{n,\sigma}(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} u_{n,\sigma}(\mathbf{r}) \\ v_{n,\sigma}(\mathbf{r}) \end{pmatrix}$$

$$\Downarrow \qquad (13)$$

$$\begin{pmatrix} \underline{\boldsymbol{h}}_\sigma(\mathbf{r},t) & \Delta(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & -\underline{\boldsymbol{h}}_\sigma(\mathbf{r},t) \end{pmatrix} \begin{pmatrix} u_{n,\sigma}(\mathbf{r},t) \\ v_{n,\sigma}(\mathbf{r},t) \end{pmatrix} = i\hbar\frac{\partial}{\partial t} \begin{pmatrix} u_{n,\sigma}(\mathbf{r},t) \\ v_{n,\sigma}(\mathbf{r},t) \end{pmatrix}$$

Dynamics depend on **densities** (easier to manage than multiple wave functions)

Explicit formula for Quantum Cooling

$$\mathscr{H}_{td} = \begin{pmatrix} \underline{\boldsymbol{h}}_\sigma - \mu_\sigma - \alpha\frac{\hbar\vec{\nabla}\cdot\vec{j}_\sigma(\vec{r})}{\rho_0} & \Delta + \beta\tilde{\Delta}_1 + i\gamma\tilde{\Delta}_2 \\ \left(\Delta + \beta\tilde{\Delta}_1 + i\gamma\tilde{\Delta}_2\right)^* & -(\underline{\boldsymbol{h}}_\sigma - \mu_\sigma - \alpha\frac{\hbar\vec{\nabla}\cdot\vec{j}_\sigma(\vec{r})}{\rho_0}) \end{pmatrix}, \quad \alpha, \beta > 0 \tag{14}$$

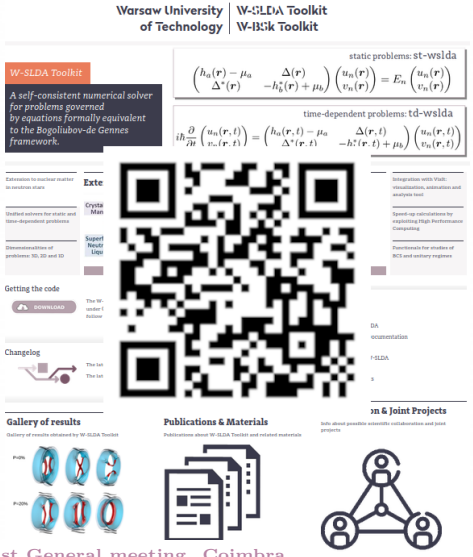
$$\tilde{\Delta}_1 = -\Delta\sin(\theta_{B'} - \arg\Delta), \quad \theta_{B'} = \arg B',$$

$$\tilde{\Delta}_2 = \Delta\frac{N(t) - N_{req}(t)}{N_{req}(t)},$$

$$B' = -\frac{\hbar^2}{2m}\sum_n \left(v^*_{n,b}\nabla^2 u_{n,a} + u_{n,a}\nabla^2 v^*_{n,b}\right)\left(f_{\beta'}(-E_n) - f_{\beta'}(E_n)\right),$$

- Scheme 1: $\alpha > 0, \beta = 0, \gamma = 0$ Kills non rotational currents.
- Scheme 2 $\alpha = 0, \beta > 0, \gamma = 0$ Minimizes excitations on the pairing field (PC).
- Scheme 3 $\alpha = 0, \beta = 0, \gamma > 0 (< 0)$ Eliminates (adds) particles up to N_{req}

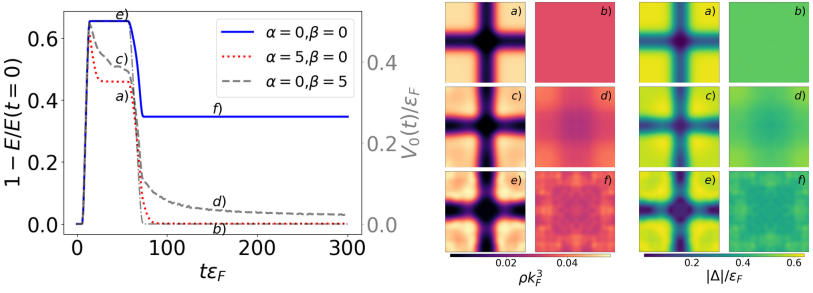
W-SLDA Toolkit



- Static solver (self consistent)
- Dynamic solver
- Different functionals incorporated: Bogoliubov-deGenes, Spin Imbalanced configurations, Nuclear matter

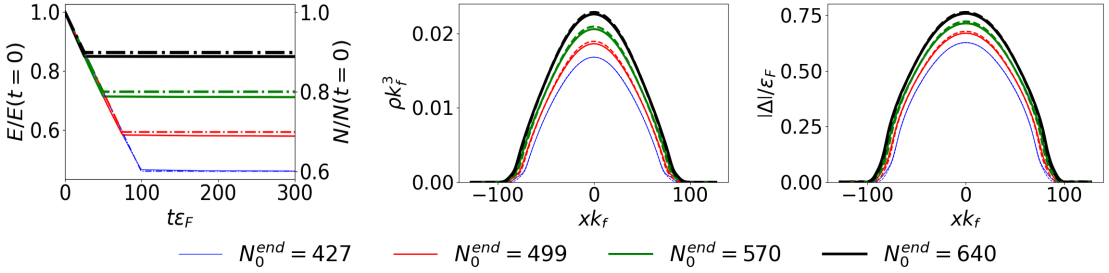
Test 1: Quench Setup $\mathcal{E}_{SLDA}$

- Uniform UFG. $N_\uparrow = N_\downarrow = 277$
- Strong perturbation applied, System far from equilibrium.



Test 2: Particle Number Evolution $\mathcal{E}_{SLDA}$

- UFG in a 1D harmonic trap $\omega_z/\varepsilon_F(0) = 1.23 \times 10^{-2}$. $N(t=0) = 475$
- Using $\alpha = 10, \beta = 5, \gamma = 0.1$ at a constant rate $\dot{N}_{req} = -2.86\epsilon_F$
- Evaporative cooling-like

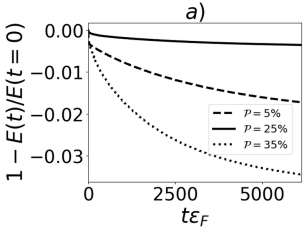


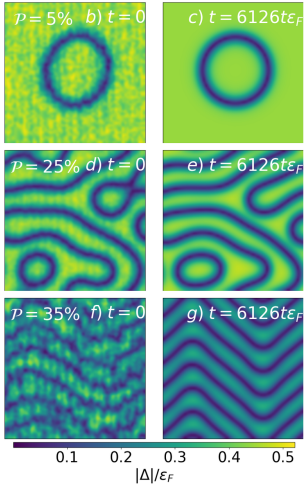
Applications

Application 1: Spin-Imbalanced $\mathcal{E}_{ASLDA}$

2D UFG $N_\uparrow = 1215 > N_\downarrow$.

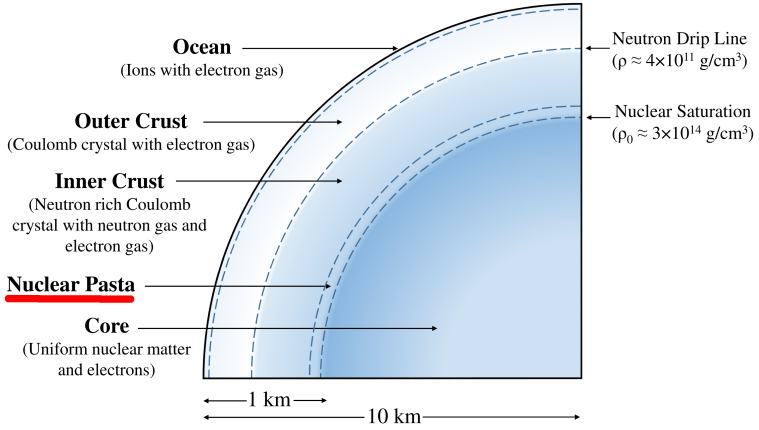
Initial configurations obtained after a few SC iterations.





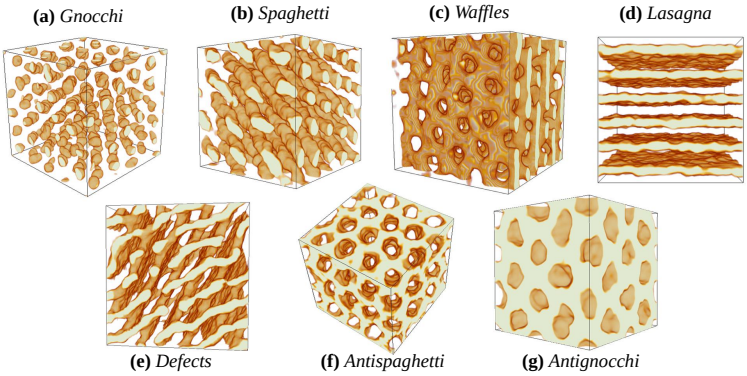
[2] B. Tüzemen, et. al. , New J. Phys. 25, 033013 (2023).

Neutron stars



M.E. Caplan and C.J. Horowitz. Rev. Mod. Phys. 89, 041002 (2017)

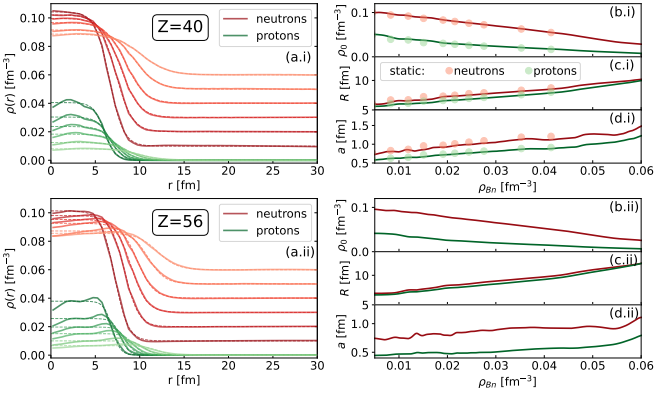
Pasta phases



M.E. Caplan and C.J. Horowitz. Rev. Mod. Phys. 89, 041002 (2017)

Application 2: Density Scan $\mathscr{E}_{BSK}$

Protonic clusters in neutron star inner crust: Evolution of a single static solution, but changing the background density ρ_{Bn}

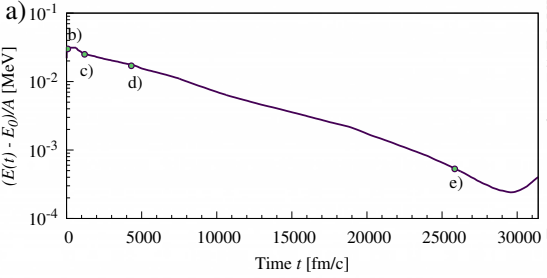


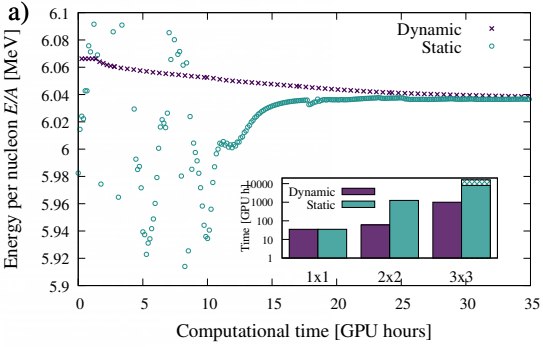
$$\rho_\sigma(r) = \frac{\rho_{0\sigma}}{1+\exp\left(\frac{r-R_\sigma}{a_\sigma}\right)} + \rho_{B\sigma}$$

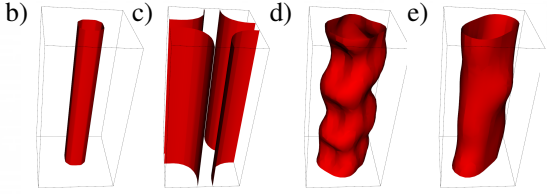
[3] D. Pęcak et al., *Phys. Rev. X 14, 041054* (2024)

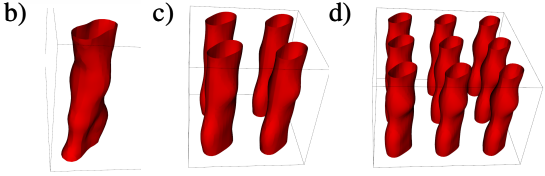
Application 3:Nuclear Pasta $\mathscr{E}_{BSK}$

Uniform system + a brief cylindrical potential (breaks the symmetry) → one strand.









Conclusions

- **Takeaway message**: Quantum cooling is an evolution scheme that tracks energy minima states dynamically.
- Local quantum cooling is efficient for large systems.
- Pairing-channel cooling is essential, particularly for strongly paired systems.
- Enables particle-number control and density scans.
- The generality of the method permits its use in any desired functional within TDDFT.

Outlook

- Vorticity in nuclear pasta
- Real-time dynamics with dynamical temperature description.
- Model particle–particle scattering processes that are otherwise absent in mean-field approaches.

Aknowledgments

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Thank you for your attention!

JEAA, D. Pęcak, M.M. Forbes, and G. Wlazłowski *Phys. Rev. C* 113, 065805 (2026).

Backup Slides

DFT Framework: different formulae

For the Unitary Fermi Gas

$$\mathscr{E}_{SLDA}(\rho,\tau,\nu)=\left(A\frac{\tau(\mathbf{r})}{2}+B\frac{3}{5}\rho(\mathbf{r})\varepsilon_F(\mathbf{r})+\frac{C}{\rho(\mathbf{r})^{1/3}}|\nu(\mathbf{r})|^2\right), \tag{15}$$

For spin-imbalanced systems, this is extended to

$$\mathscr{E}_{ASLDA}(\rho_\uparrow,\rho_\downarrow,\tau,\nu)=\frac{\hbar^2}{2m}\left(A_\uparrow(\rho_\uparrow,\rho_\downarrow)\frac{\tau_\uparrow(\mathbf{r})}{2}+A_\downarrow(\rho_\uparrow,\rho_\downarrow)\frac{\tau_\downarrow(\mathbf{r})}{2}+D(\rho_\uparrow,\rho_\downarrow)\right)+g|\nu(\mathbf{r})|^2, \tag{16}$$

For interacting nuclear matter, this is extended to $q=p,n$

$$\begin{aligned}\mathscr{E}_{WBSK}(\rho_p,\nabla\rho_p,\tau_q,\nu_q,\vec{j}_q)&=\frac{\hbar^2}{2m_n}\tau_n+\frac{\hbar^2}{2m_p}\tau_p+\mathscr{E}_\tau(\rho_q,\tau_q,\vec{j}_q)+\\&\mathscr{E}_\rho(\rho_q)+\mathscr{E}_{\Delta_\rho}(\rho_q,\nabla\rho_q)\\&+\mathscr{E}_\pi(\rho_q,\nabla\rho_{q\nu q})+\mathscr{E}_{Coul}(\rho_p),\end{aligned} \tag{17}$$

$$\mathscr{H}_c = \alpha \mathscr{U}_U + \beta \mathscr{U}_{c\delta} + \gamma \mathscr{U}_{nc\delta} \tag{18}$$

$$\mathscr{U}_U = -\tilde{\alpha} \begin{pmatrix} \text{diag}(\underline{\mathbf{A}}) & \underline{\mathbf{0}} \\ \underline{\mathbf{0}} & \text{diag}(\underline{\boldsymbol{A}})^* \end{pmatrix}, \tag{19}$$

with

$$\text{diag}(\underline{\boldsymbol{A}}) = \begin{pmatrix} \text{diag}\Big([\underline{\boldsymbol{h}}_{\uparrow,\uparrow}, \underline{\boldsymbol{\rho}}_{\uparrow\uparrow}] \Big) & \underline{\mathbf{0}} \\ \underline{\mathbf{0}} & \text{diag}\Big([\underline{\boldsymbol{h}}_{\downarrow,\downarrow}, \underline{\boldsymbol{\rho}}_{\downarrow\downarrow}] \Big) \end{pmatrix} = \begin{pmatrix} U_{\uparrow}^{(d)} & \underline{\mathbf{0}} \\ \underline{\mathbf{0}} & U_{\downarrow}^{(d)} \end{pmatrix}, \tag{20}$$

In the spatial coordinates, we have that $U_{\sigma}^{(d)}(\mathbf{r}) = -\frac{\tilde{\alpha}}{m} \nabla \cdot \mathbf{j}_{\sigma}(\mathbf{r})$

In practice, this modifies the single-particle Hamiltonian as

$$(\underline{\boldsymbol{h}}_{td})_{\sigma} = \underline{\boldsymbol{h}}_{\sigma} - \frac{\alpha}{m\rho_0} \underbrace{\nabla \cdot \mathbf{j}_{\sigma}(r)}_{-\dot{\rho}_{\sigma}(r)}; \text{ with } \rho_0 \text{ a characteristic density} \tag{21}$$

Main new contribution of this work

$$\mathscr{U}_{\Delta} = -i \begin{pmatrix} \underline{\mathbf{0}} & \underline{\boldsymbol{B}}_{td} \\ \underline{\boldsymbol{B}}_{td}^{*} & \underline{\mathbf{0}} \end{pmatrix}, \tag{22}$$

where

$$\underline{\boldsymbol{B}}_{td} = \tilde{\beta}(r) \begin{pmatrix} \underline{\mathbf{0}} & B(r) \\ -B(r) & \underline{\mathbf{0}} \end{pmatrix}. \tag{23}$$

Here, $\tilde{\beta}(r)$ is a position-dependent proportionality coefficient. The corresponding pairing cooling potential is then

$$\Delta^{(d)}(\mathbf{r}) \equiv -i\tilde{\beta}(\mathbf{r})B(\mathbf{r}),$$

the choice of B can make the evolution particle-conservative or not.

$$B = (\underbrace{\mathrm{Re}(B)}_{\dot{N}=0} + \underbrace{\mathrm{Im}(B)}_{\dot{N}\neq 0})e^{i\arg(B)} \tag{24}$$

In practice, this modifies the pairing field as

$$\Delta_{td}(\mathbf{r}) = \Delta(\mathbf{r})\Big(1 - \beta\sin\big(\theta_{B'}(\mathbf{r}) - \arg(\Delta(\mathbf{r}))\big) + \tilde{\gamma}\Big), \tag{25}$$

$\theta_{B'} = \arg\left(-\frac{1}{2m}\sum_n \left[u_n\nabla^2 v_n^* + v_n^*\nabla^2 u_n\right]\right)$,
$\tilde{\gamma} = \gamma\frac{N(t)-N_{req}(t)}{N_{req}(t)} \Longrightarrow$ Controlled changes in particle number (or densities)