Nuclear-DFT calculations of nuclear Schiff moment of ^{227}Ac

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EDM and Fundamental Symmetries

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$$\hat{\mathbf{d}} = \sum_a e_a \mathbf{r}_a, \quad a = 1, \ ..., \ Z,$$

in a stationary state of an atom with a certain value $\hat{\boldsymbol{J}}$ of angular momentum requires simultaneous $\hat{\mathscr{P}}$- and $\hat{\mathscr{T}}$- violation.

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★ A nucleus acquires an EDM from either nucleon EDM or $\hat{\mathscr{P}}\hat{\mathscr{T}}$ -violating interaction between nucleons and pions.

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L. I. Schiff, Phys. Rev. **132**, 2194 (1963)

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Electrostatic potential of a nucleus:

$$\varphi(\boldsymbol{R}) = \int \frac{e\rho(\boldsymbol{r})}{|\boldsymbol{R}-\boldsymbol{r}|} d^3r + \frac{1}{Z}(\boldsymbol{d}\cdot\boldsymbol{\nabla}_R)\int \frac{\rho(\boldsymbol{r})}{|\boldsymbol{R}-\boldsymbol{r}|} d^3r$$

$$\int d^3r\ \rho(\boldsymbol{r}) = Z; \qquad \boldsymbol{d} = \int e\boldsymbol{r}\rho(\boldsymbol{r})\ d^3r; \qquad \boldsymbol{R} = \text{electron coordinate}$$

3

Nuclear Schiff Moment

V. Spevak et al., PRC **56**, 1357 (1997)

Nuclear Schiff Moment

Taylor expansion:

$$\frac{1}{|\boldsymbol{R}-\boldsymbol{r}|} = \frac{1}{R} - \boldsymbol{r}\cdot\boldsymbol{\nabla}_R\frac{1}{R} + \frac{1}{2}(\boldsymbol{r}\cdot\boldsymbol{\nabla}_R)^2\frac{1}{R} - \cdots$$

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$$\varphi(\boldsymbol{R}) = \frac{eZ}{R} + 4\pi \boldsymbol{S}\cdot\boldsymbol{\nabla}_R \delta(\boldsymbol{R}) \cdots$$

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Nuclear Schiff moment:

$$\boldsymbol{S} = \frac{1}{10}\left(\int d^3r\ e\rho(\boldsymbol{r})r^2\boldsymbol{r} - \frac{5}{3}\boldsymbol{d}\frac{1}{Z}\int d^3r\ \rho(\boldsymbol{r})r^2\right)$$

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The nuclear Schiff moment induces the nuclear electric dipole moment (EDM) in surrounding electrons.

V. Spevak et al., PRC **56**, 1357 (1997)

4

Nuclear Schiff Moment and Octupole Deformation

J. Dobaczewski et al., PRL **121**, 232501 (2018) and the supplemental material

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$$S = \langle \Psi_0 | \hat{S}_0 | \Psi_0 \rangle \approx \sum_{i \neq 0} \frac{\langle \Psi_0 | \hat{S}_0 | \Psi_i \rangle \langle \Psi_i | \hat{V}_{\mathrm{PT}} | \Psi_0 \rangle}{E_0 - E_i} + \mathrm{c.c.}$$

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$$\hat{V}_{\mathrm{PT}} = \hat{\mathcal{P}}\hat{\mathcal{T}}\text{-violating } NN \text{ interaction}$$

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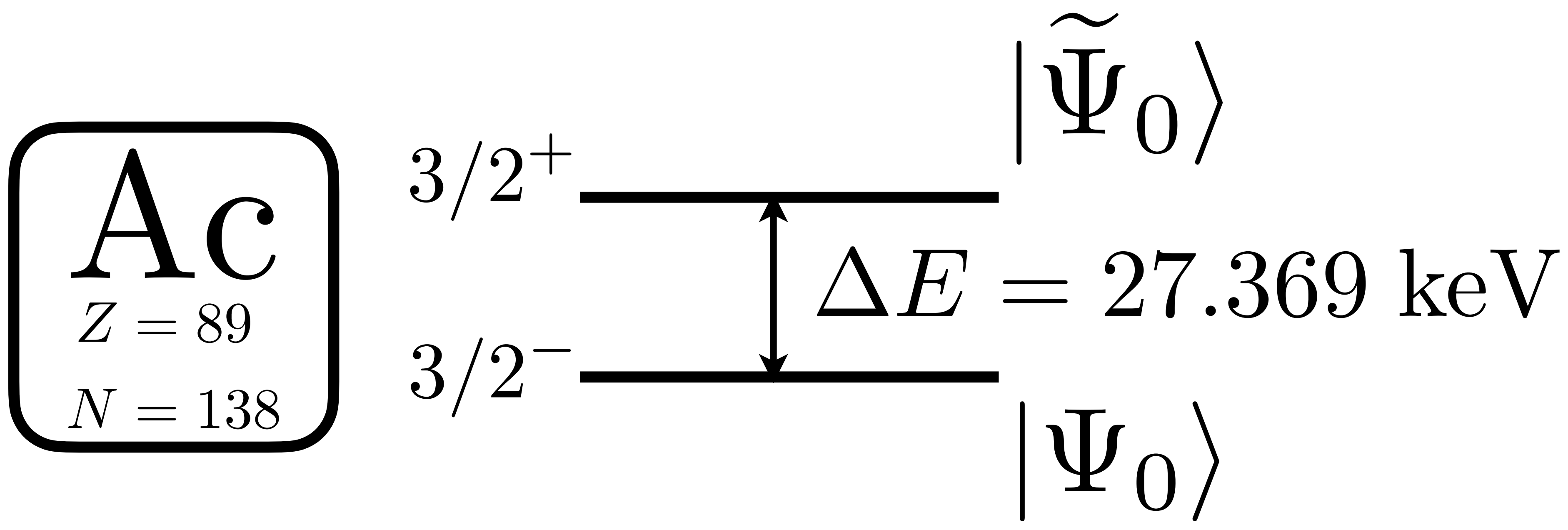

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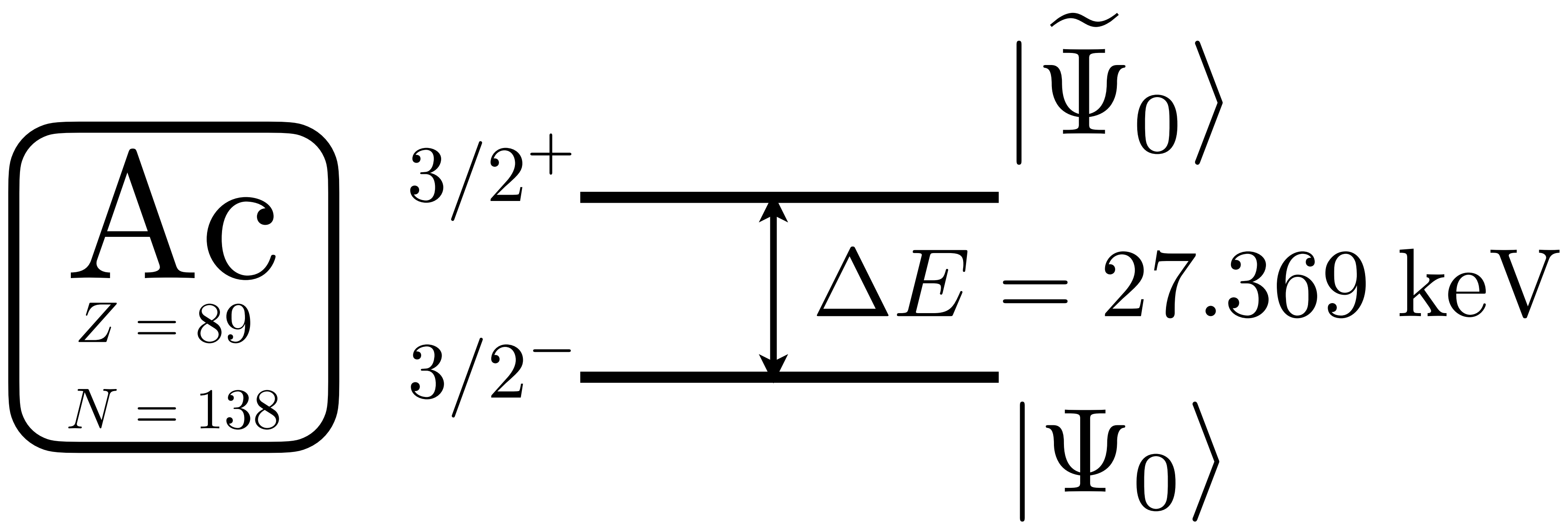

$$S \approx -2 \frac{\langle \Psi_0 | \hat{S}_0 | \widetilde{\Psi}_0 \rangle \langle \widetilde{\Psi}_0 | \hat{V}_{\mathrm{PT}} | \Psi_0 \rangle}{\Delta E}$$

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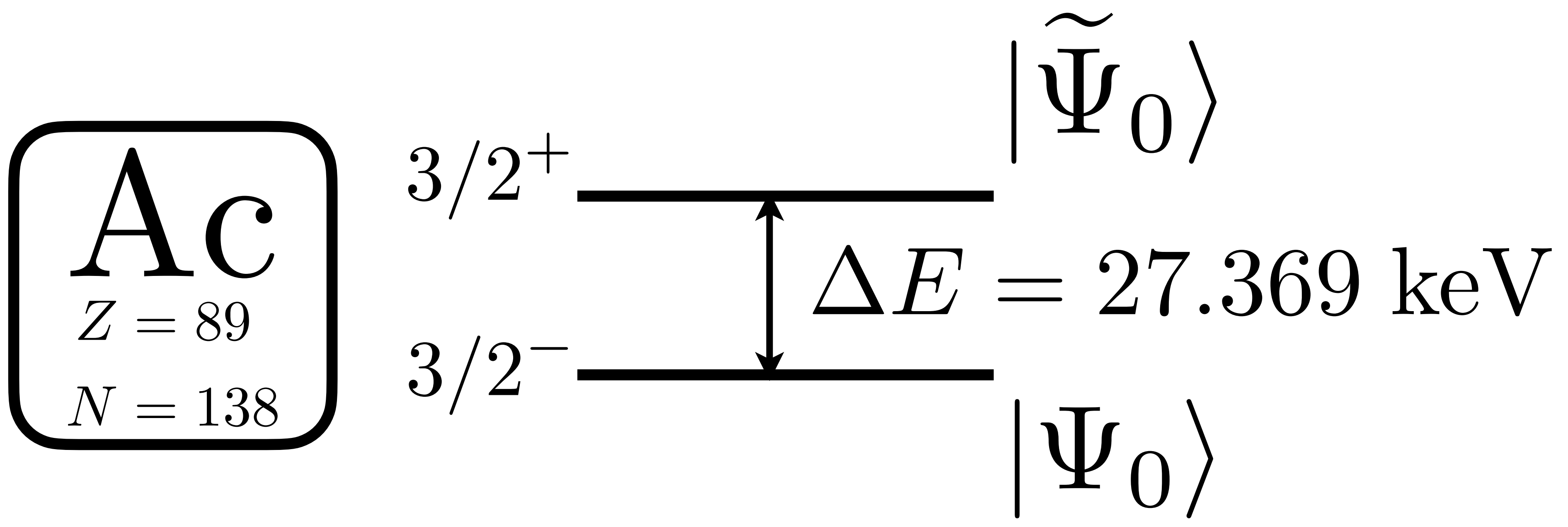

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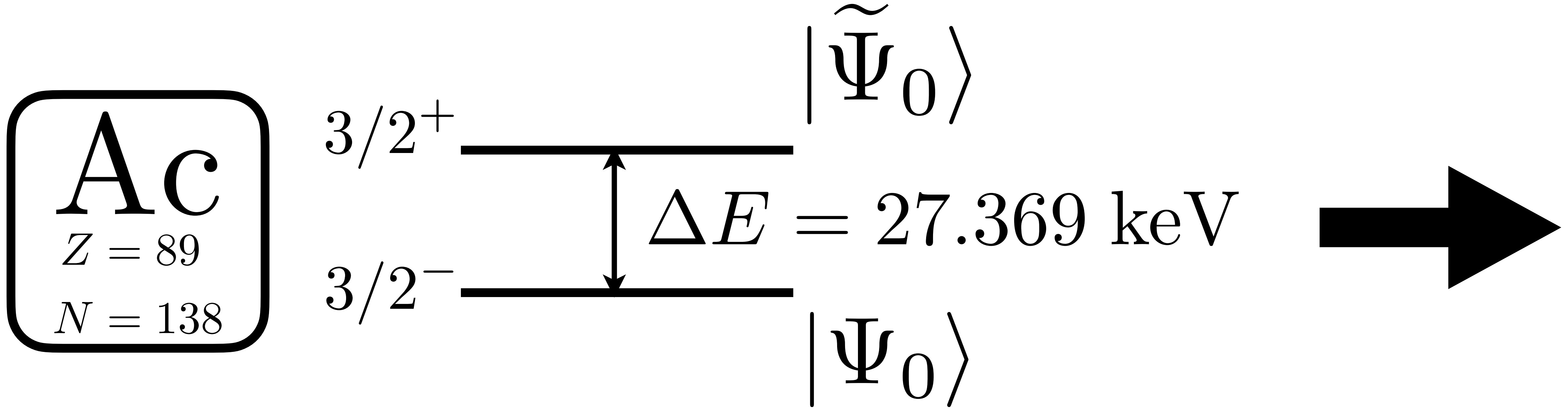

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$$\hat{Q}_0^3 = e \sum_p r_p^3 Y_0^3(\Omega_p) \quad \text{(Octupole operator)}$$

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5 Nuclear Density Functional Theory (Nuclear-DFT)

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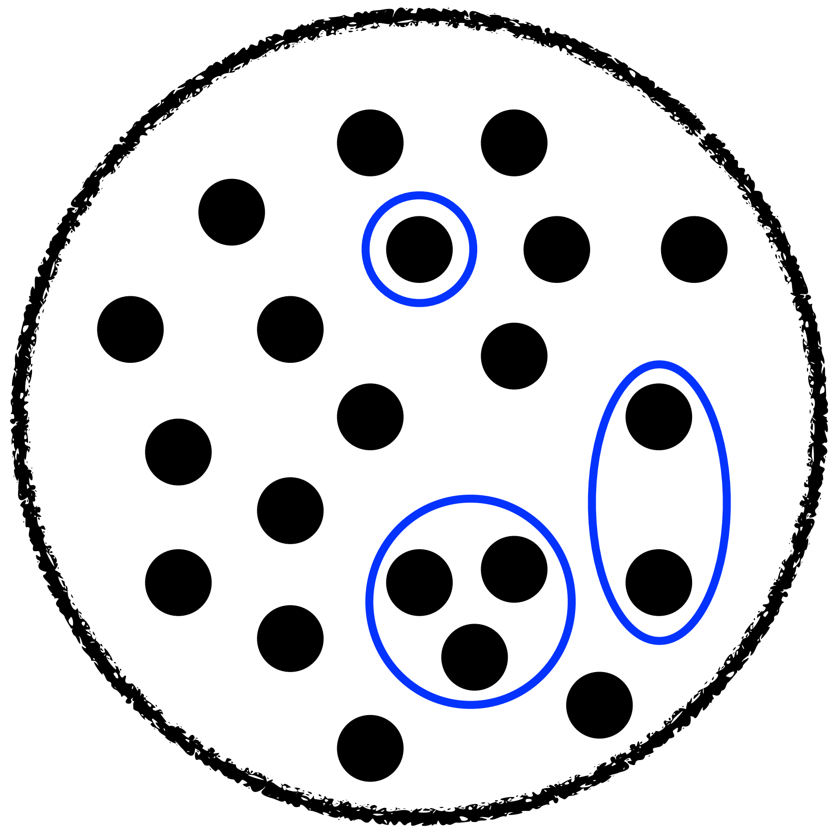

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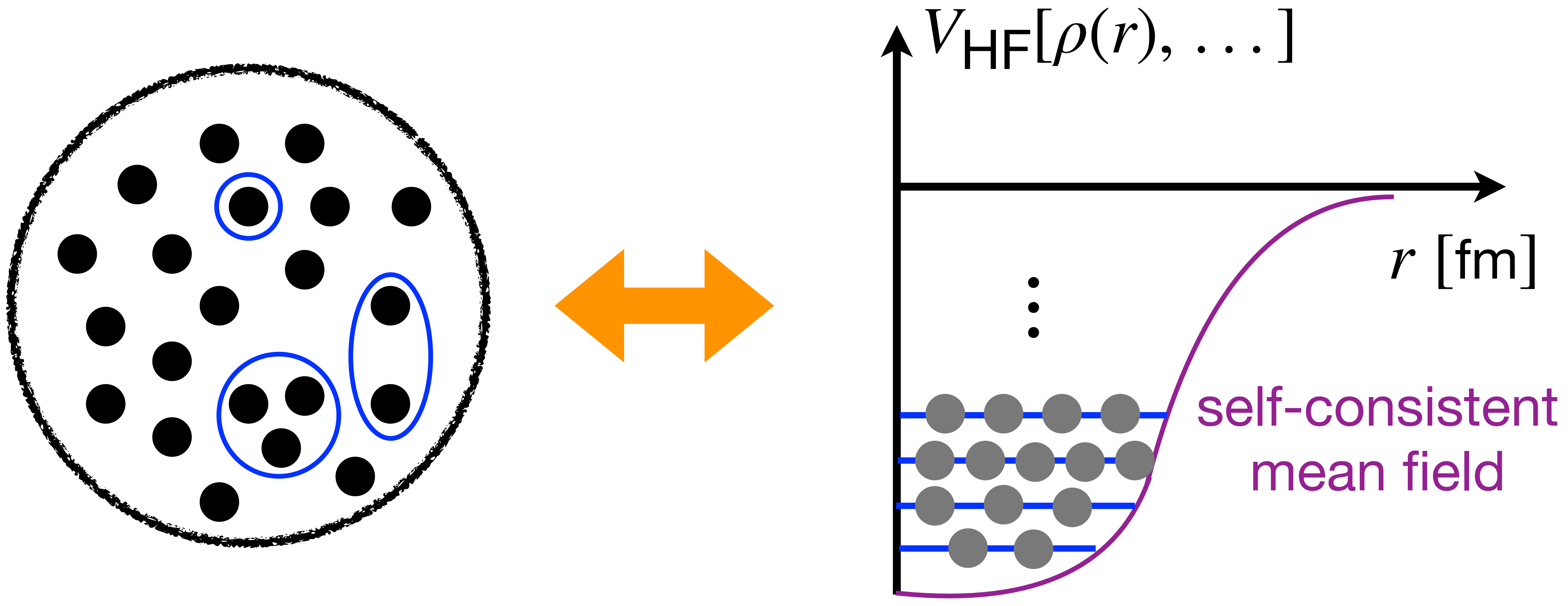

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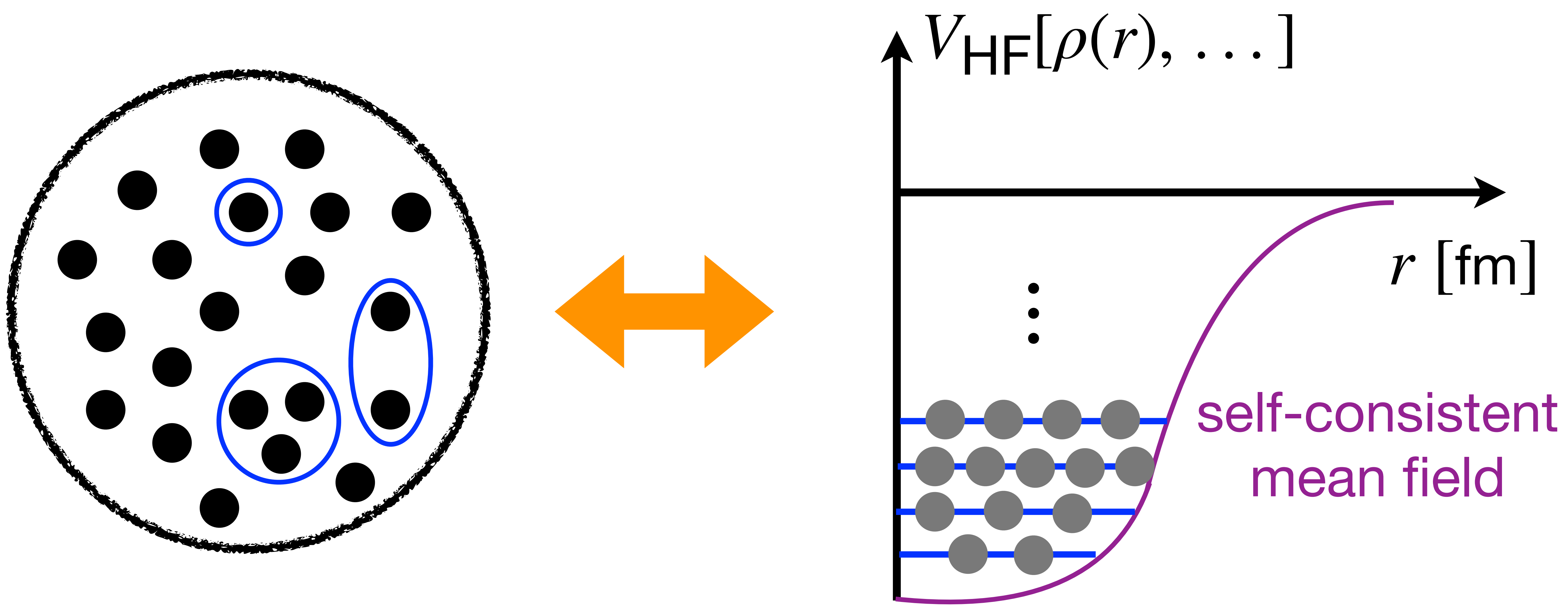

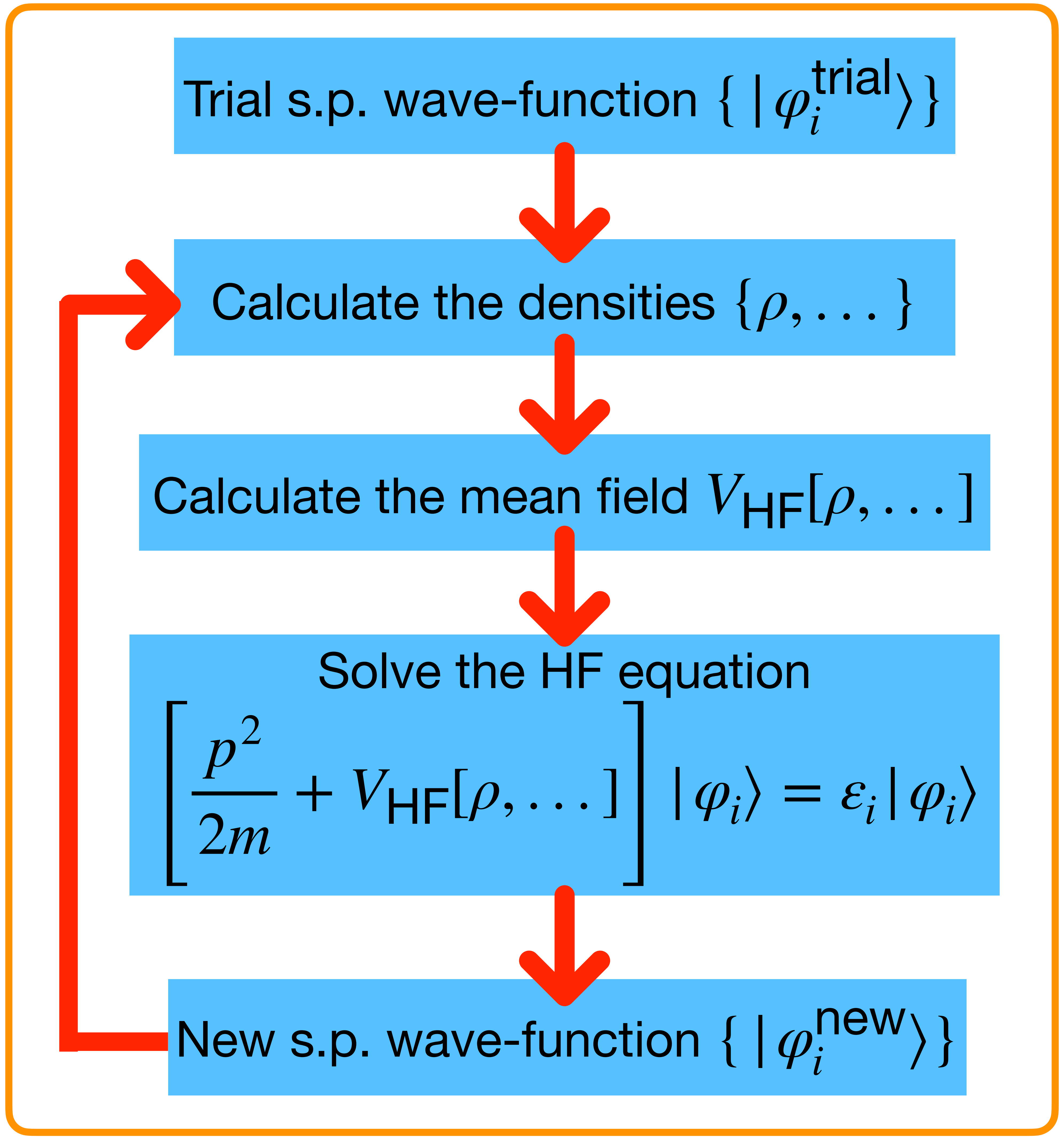

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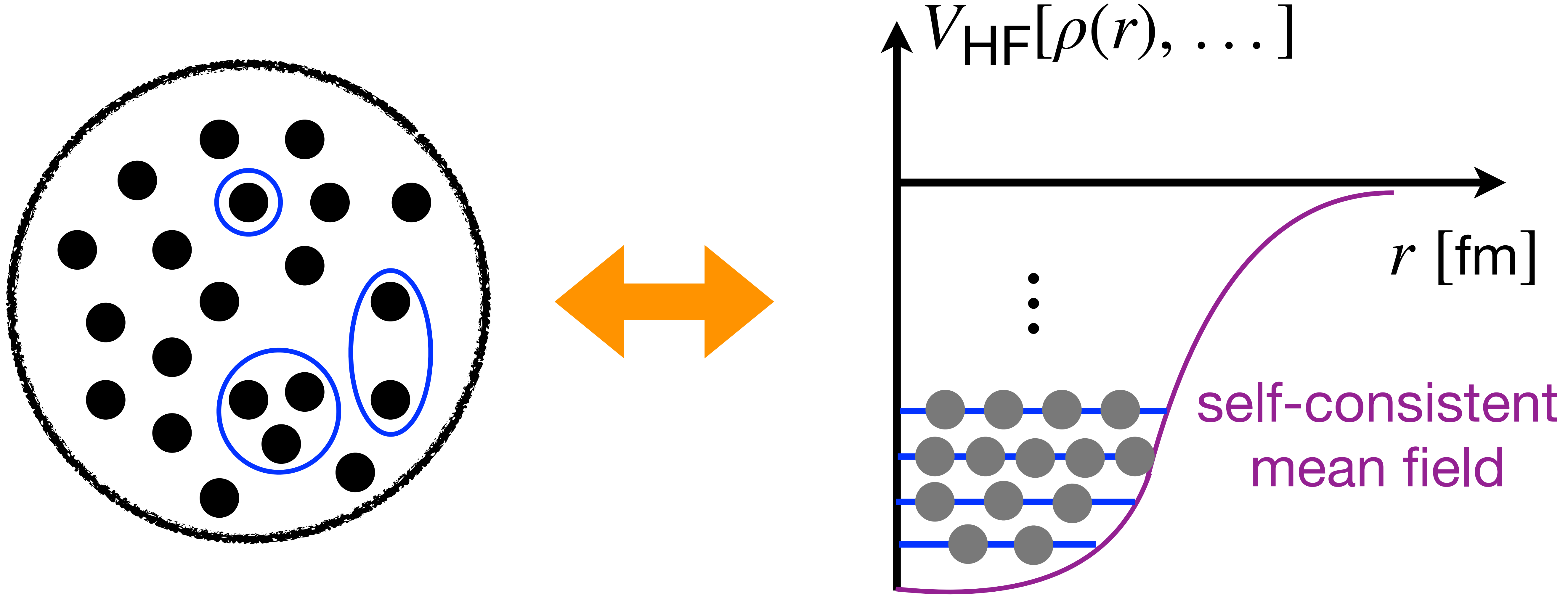

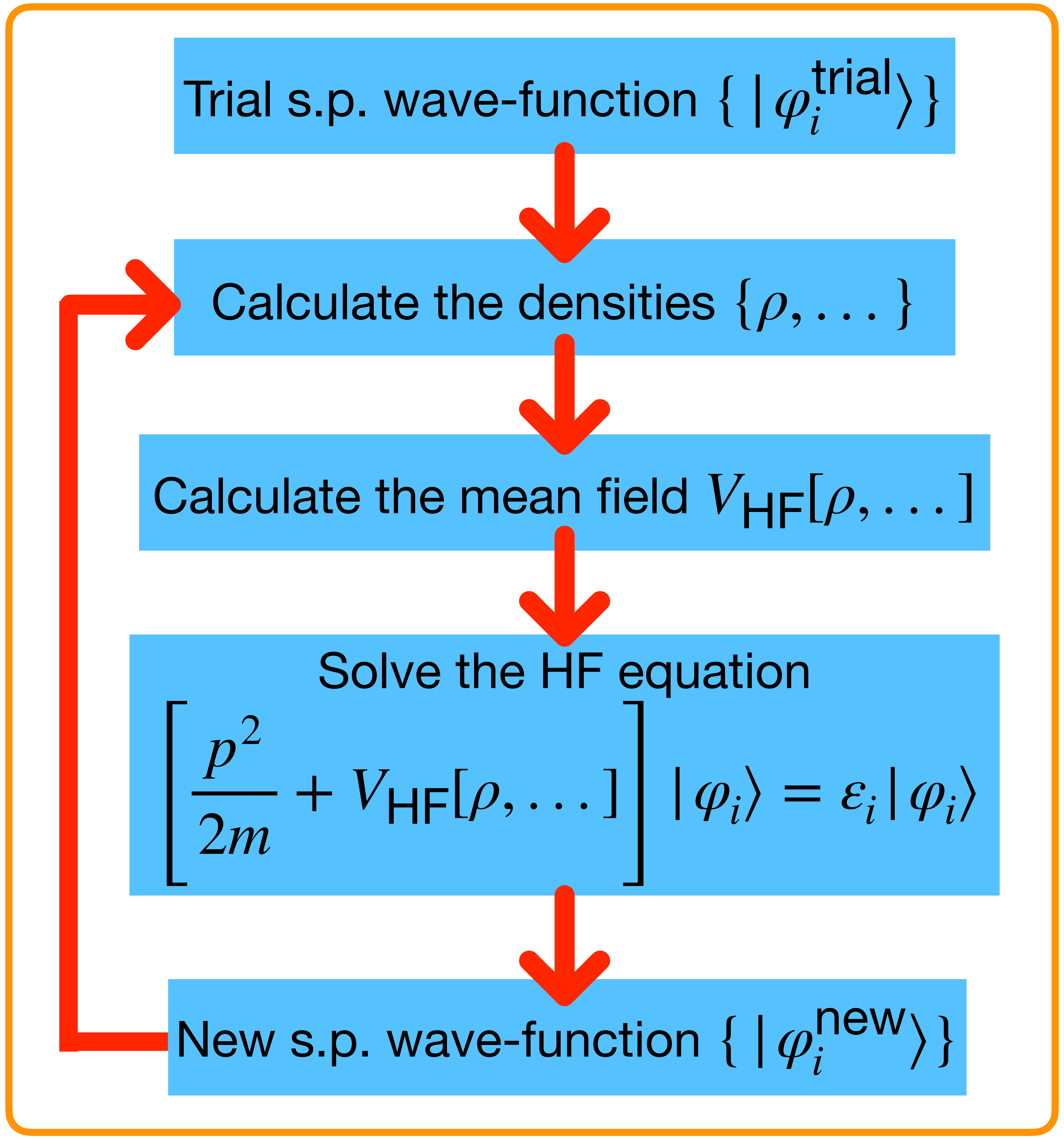

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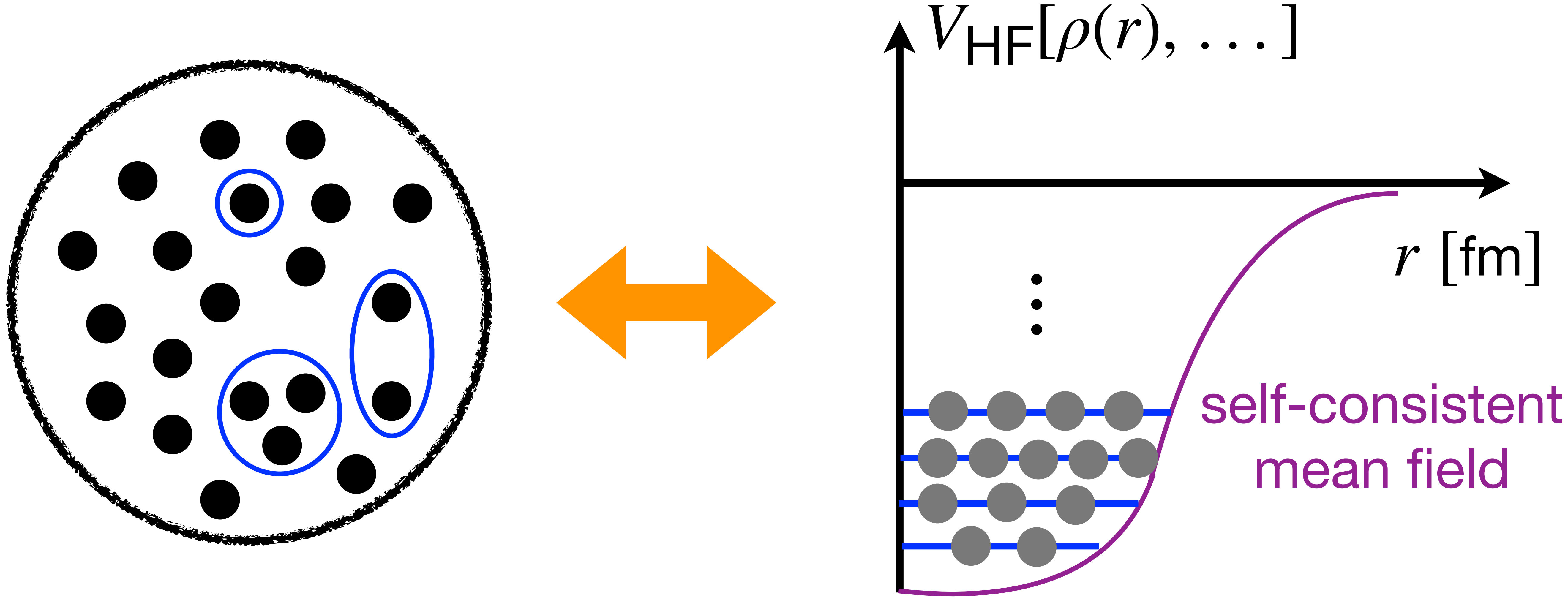

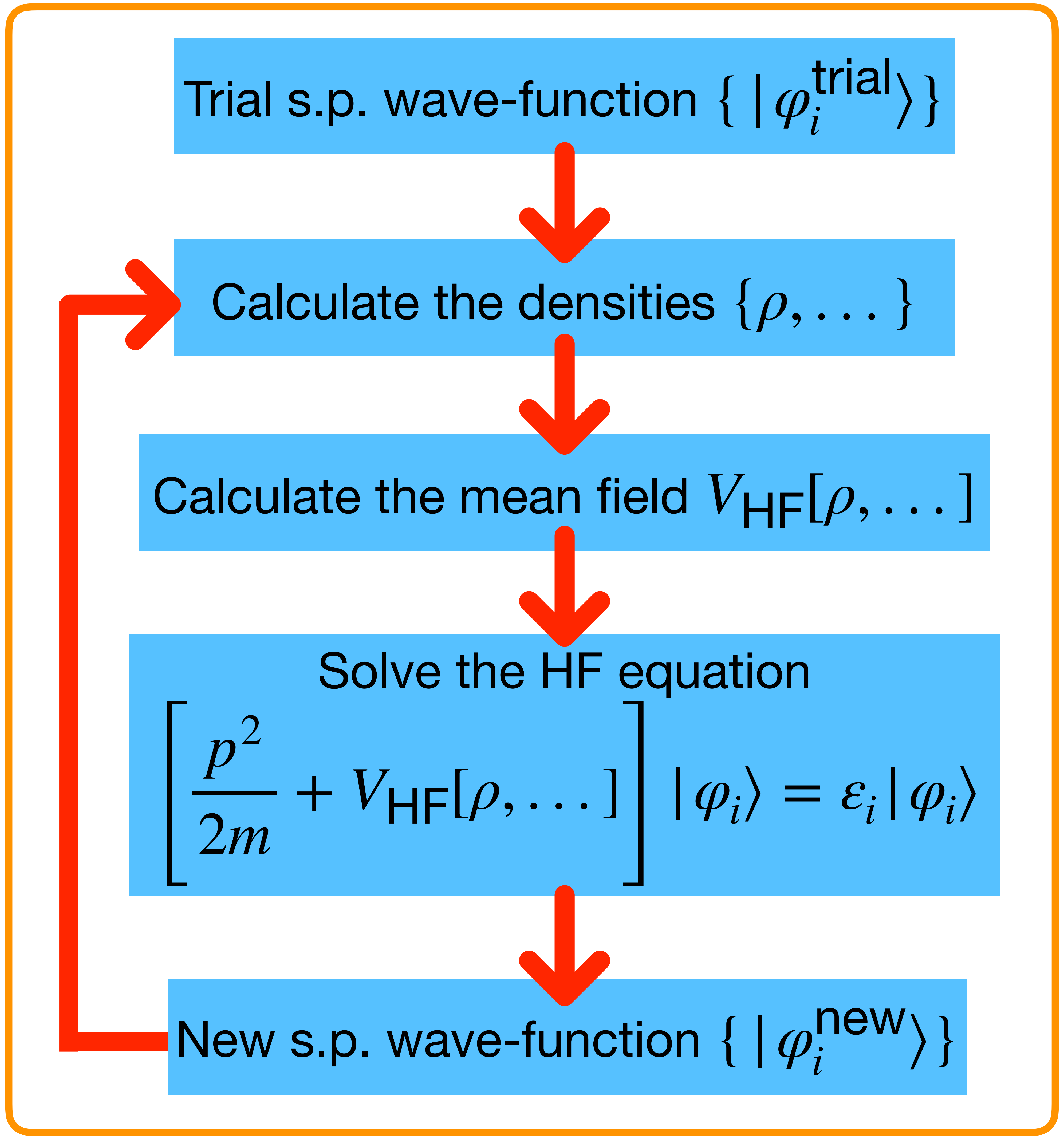

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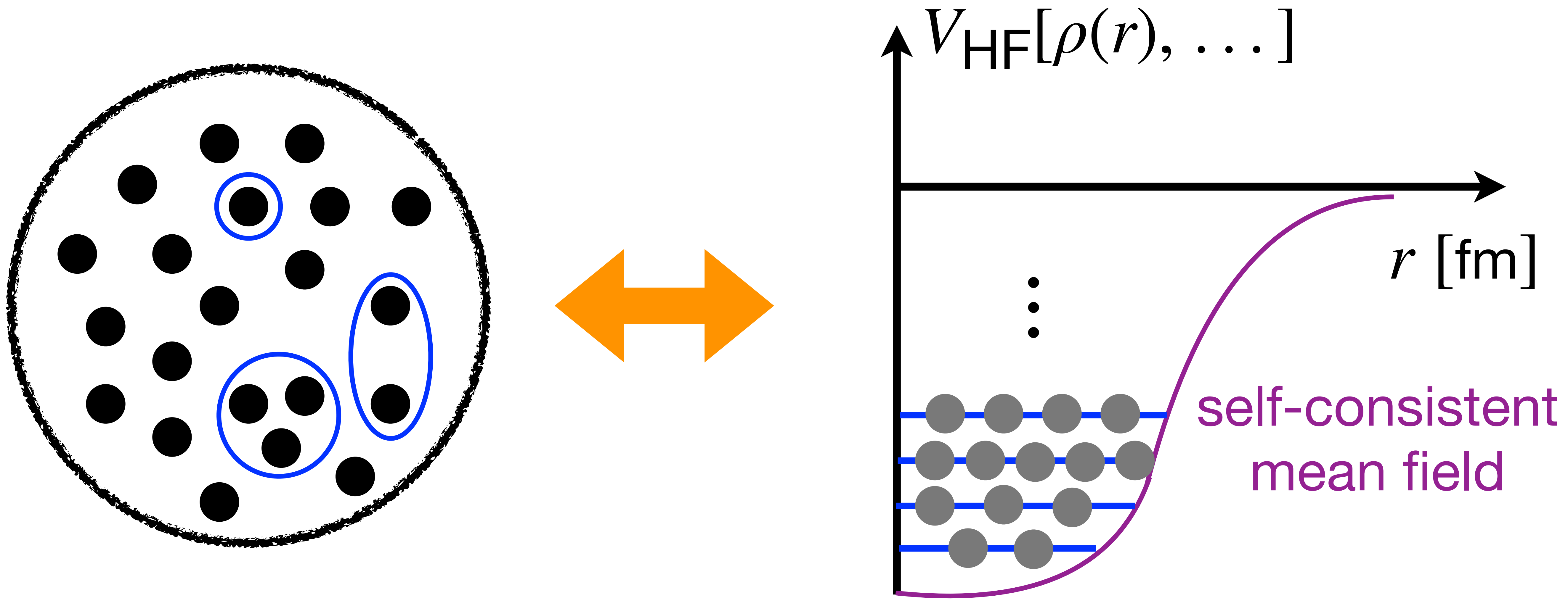

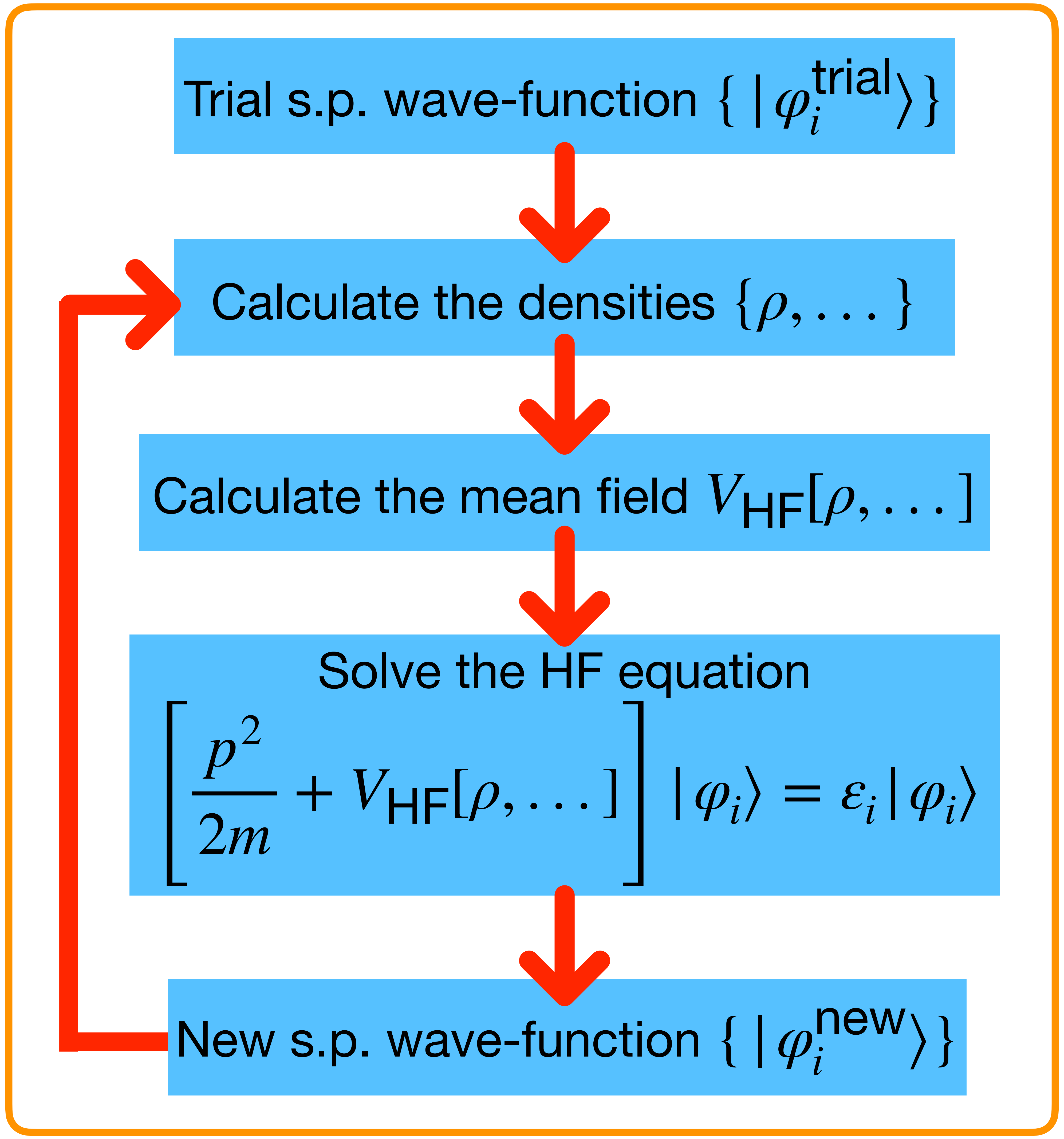

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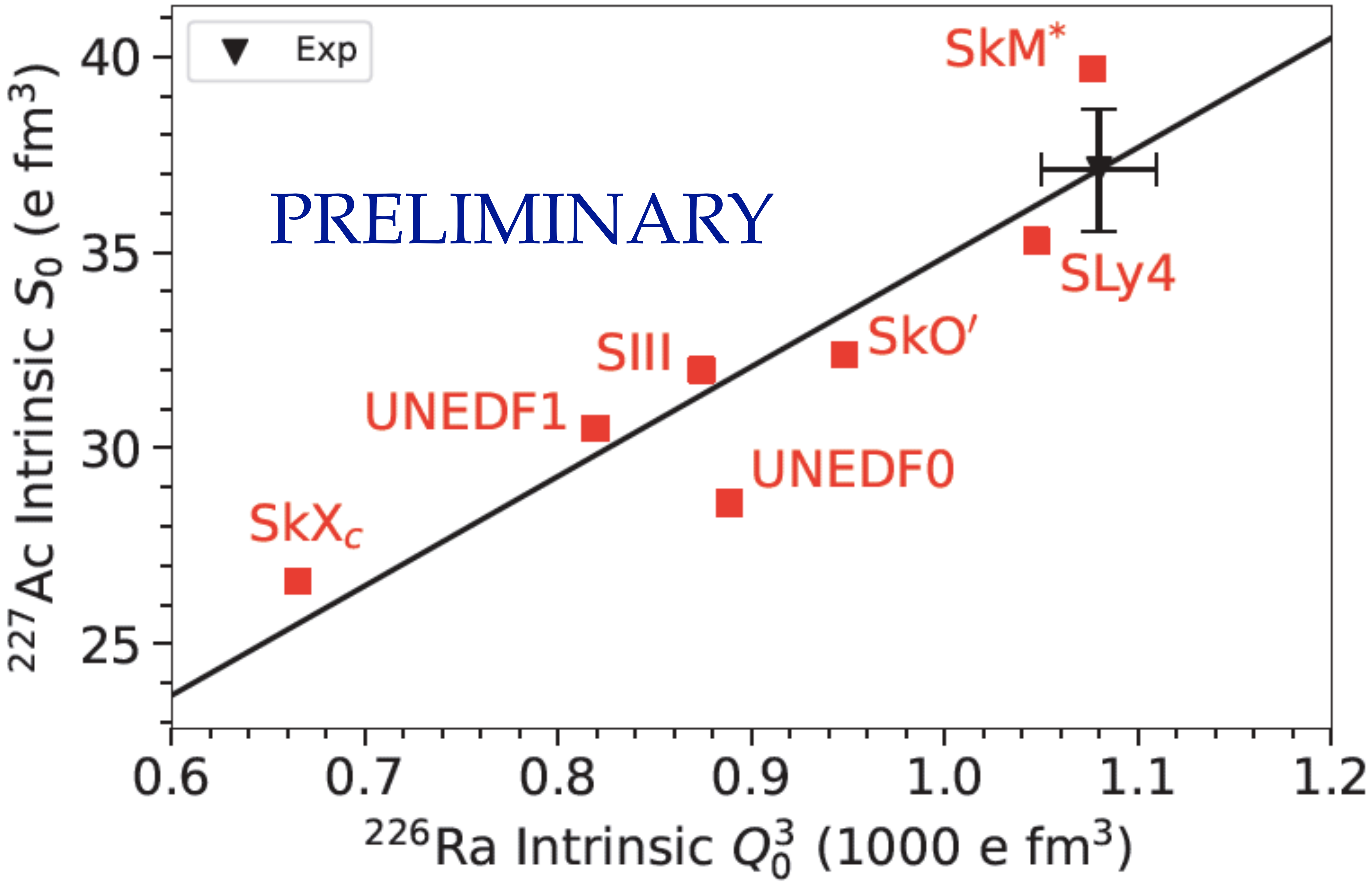
- ★ Quasiparticle blocked state: $\pi[532]3/2^-$

6 Correlation between Octupole and Schiff Moments



Estimated Intrinsic Schiff Moment

H. Wollersheim et al., Nucl. Phys. A **556**, 261 (1993)

J. Dobaczewski et al., PRL **121**, 232501 (2018) and the supplemental material

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$$S_0(^{227}\mathrm{Ac}) = 37.1(1.6)\ \mathrm{e\ fm}^3$$

H. Wollersheim et al., Nucl. Phys. A **556**, 261 (1993)

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Outlook

- We are continuing our calculations to obtain the laboratory Schiff moment.

Acknowledgements

We acknowledge the support from a **Leverhulme Trust Research Project Grant**. This work was partially supported by the **STFC Grant** Nos. ST/P003885/1 and ST/V001035/1 and by the **Polish National Science Centre** under Contract No. 2018/31/B/ST2/02220. We acknowledge the **CSC-IT Center for Science Ltd., Finland**, for the allocation of computational resources. This project was partly undertaken on the **Viking Cluster**, which is a high performance compute facility provided by the **University of York**. We are grateful for computational support from the **University of York High Performance Computing service, Viking and the Research Computing team**.

Back Up Slides

Vector model:

$$\hat{\mathbf{d}} = \frac{\langle aJM'|\hat{\mathbf{d}} \cdot \hat{\mathbf{J}}|aJM\rangle}{J(J+1)}\hat{\mathbf{J}}$$

Using Wigner-Eckart theorem:

$$\langle aJM'|\hat{\mathbf{d}} \cdot \hat{\mathbf{J}}|aJM\rangle = \frac{\delta_{M'M}}{2J+1}\langle aJ||\hat{\mathbf{d}}||aJ\rangle\langle aJ||\hat{\mathbf{J}}||aJ\rangle$$

$$\chi^2 = \sum_i \left[S_0(i) - a - bQ_0^3(i)\right]^2$$

$$\bar{b} = \frac{\langle S_0 Q_0^3\rangle - \langle S_0\rangle\langle Q_0^3\rangle}{\langle [Q_0^3(i)]^2\rangle - \langle Q_0^3\rangle^2}$$

$$\bar{a} = \langle S_0\rangle - \bar{b}\langle Q_0^3\rangle$$

$$\langle S_0 \rangle = \frac{1}{N_d} \sum_i S_0(i), \quad \langle Q_0^3 \rangle = \frac{1}{N_d} \sum_i Q_0^3(i),$$

$$\langle S_0 Q_0^3 \rangle = \frac{1}{N_d} \sum_i S_0(i) Q_0^3(i), \quad \langle [Q_0^3(i)]^2 \rangle = \frac{1}{N_d} \sum_i [Q_0^3(i)]^2$$

$$s = \frac{\chi_0^2}{N_d - N_p} \qquad \mathcal{C} = s\mathcal{M}^{-1} \qquad \mathcal{M}_{ij} = \frac{1}{2} \frac{\partial}{\partial p_i} \frac{\partial}{\partial p_j} \chi^2 \bigg|_{\mathbf{p}=\bar{\mathbf{p}}}$$

$$\mathcal{C}_{aa} = \frac{s}{N_d} \frac{\langle [Q_0^3]^2 \rangle}{\langle [Q_0^3]^2 \rangle - \langle Q_0^3 \rangle^2},$$

$$\mathcal{C}_{ab} = \mathcal{C}_{ba} = -\frac{s}{N_d} \frac{\langle Q_0^3 \rangle}{\langle [Q_0^3]^2 \rangle - \langle Q_0^3 \rangle^2}$$

$$\mathcal{C}_{bb} = \frac{s}{N_d} \frac{1}{\langle [Q_0^3]^2 \rangle - \langle Q_0^3 \rangle^2}.$$

J. Dobaczewski et al., J. Phys. G: Nucl. Part. Phys. **41**, 074001 (2014)

$$\frac{S_{\rm intr}[^{227}{\rm Ac}]}{S_{\rm intr}[^{225}{\rm Ra}]} \propto \frac{[\beta_2 \times \beta_3] \text{ of } {}^{226}{\rm Ra}}{[\beta_2 \times \beta_3] \text{ of } {}^{224}{\rm Ra}} = \frac{0.197 \times 1080}{0.179 \times 0.940} = 1.26$$