# Semiclassical Fermion Densities for Many-Fermion Systems

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- Many-fermion system
  - Schrödinger equation
  - Not exactly solvable in general for large N

- DFT: particle density $n(\boldsymbol{r})$ is enough

- Solution: Approximation of $n(\boldsymbol{r})$

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- Ribeiro et al. [PRL **114**, 050401 (2015)]
  - Modified WKB approximation

$$n^{SC}(x) = \underbrace{\frac{p_\mu(x)}{\hbar\sqrt{z}}\left[z\,\mathrm{Ai}^2(-z) + \mathrm{Ai}'^2(-z)\right]}_{n_0(x)}\Bigg|_{z=z_\mu(x)} + \text{(1st order correction)}$$

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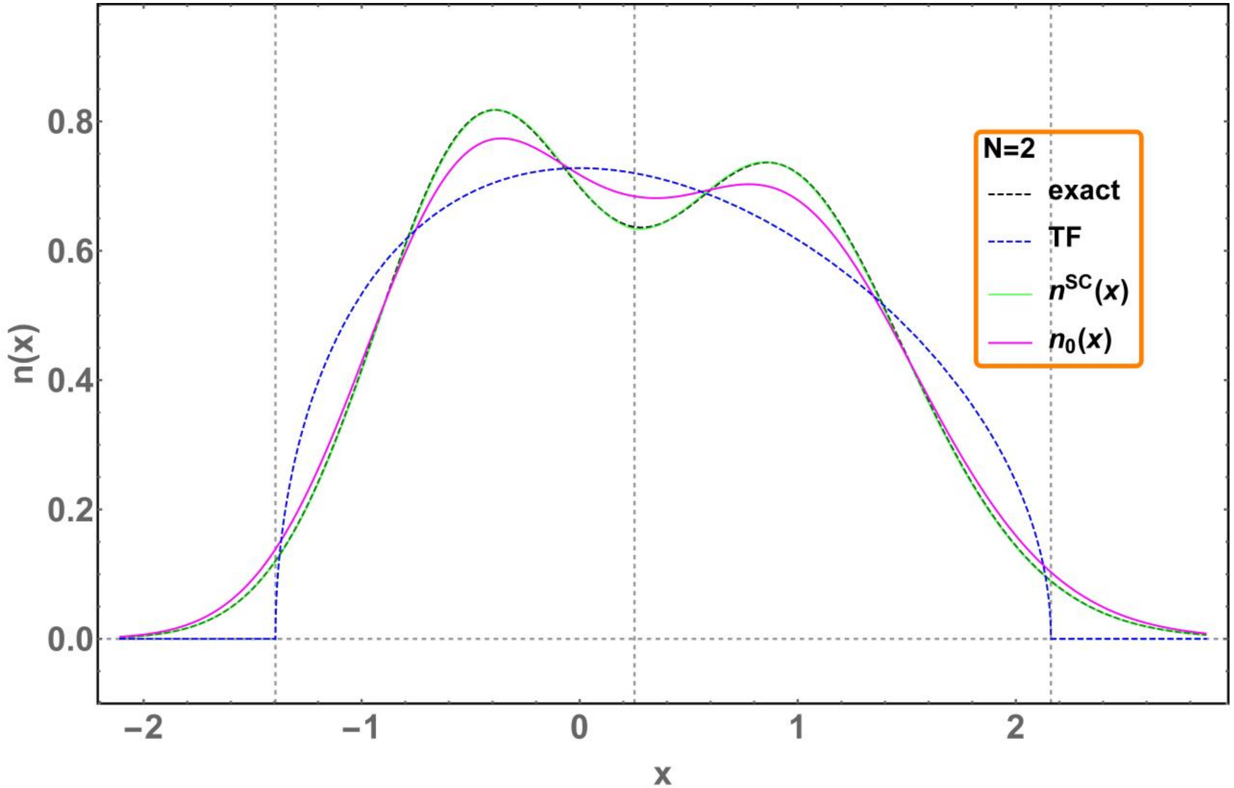
- Ribeiro et al. [PRL **114**, 050401 (2015)]




1D Morse Potential
2 fermions
Spin-polarised

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- Ribeiro et al. [PRL **114**, 050401 (2015)]
  - Difficult to extend to higher dimensions

- Aim: Semiclassical approximation
  - Extendable to higher dimensions
  - Applicable to non-isotropic potentials
  - Include interactions

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- Particle density:

$$n(\boldsymbol{r}) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\mu} \mathrm{d}E \int_{-\infty}^{\infty} \mathrm{d}T\ \mathrm{e}^{\frac{\mathrm{i}ET}{\hbar}} \underbrace{\langle \boldsymbol{r}| \mathrm{e}^{-\frac{\mathrm{i}HT}{\hbar}} |\boldsymbol{r}\rangle}_{K(\boldsymbol{r},\boldsymbol{r};T)}$$

- Suzuki-Trotter (ST) decomposition:

I. $e^{-\frac{iHT}{\hbar}} \cong e^{-\frac{iT}{\hbar}\frac{P^2}{4m}} e^{-\frac{iT}{\hbar}V(R)}\ e^{-\frac{iT}{\hbar}\frac{P^2}{4m}}$

II. $e^{-\frac{iHT}{\hbar}} \cong e^{-\frac{iT}{\hbar}\left(\frac{1}{2}+\frac{1}{\sqrt{6}}\right)\frac{\boldsymbol{P}^2}{2m}}\ e^{-\frac{iT}{\hbar}V(\boldsymbol{R})} e^{-\frac{iT}{\hbar}\left(\frac{1}{2}-\frac{1}{\sqrt{6}}\right)\frac{\boldsymbol{P}^2}{2m}}$

III. $e^{-\frac{iHT}{\hbar}} \cong e^{-\frac{iT}{\hbar}\frac{1}{6}\frac{\boldsymbol{P}^2}{2m}}\ e^{-\frac{iT}{\hbar}\frac{V(\boldsymbol{R})}{2}}\ e^{-\frac{iT}{\hbar}\frac{2}{3}\frac{\boldsymbol{P}^2}{2m}}\ e^{-\frac{iT}{\hbar}\frac{V(\boldsymbol{R})}{2}}\ e^{-\frac{iT}{\hbar}\frac{1}{6}\frac{\boldsymbol{P}^2}{2m}}$

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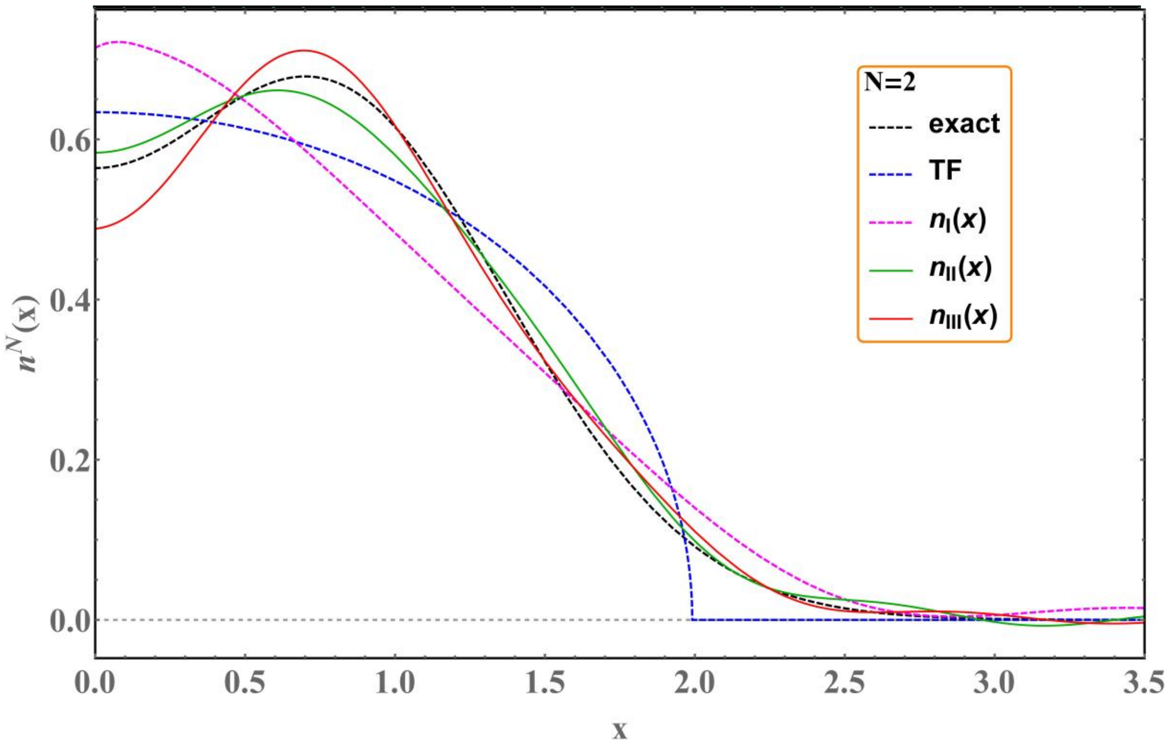
- Suzuki-Trotter decomposition:




1D Harmonic Oscillator
2 fermions
Spin-polarised

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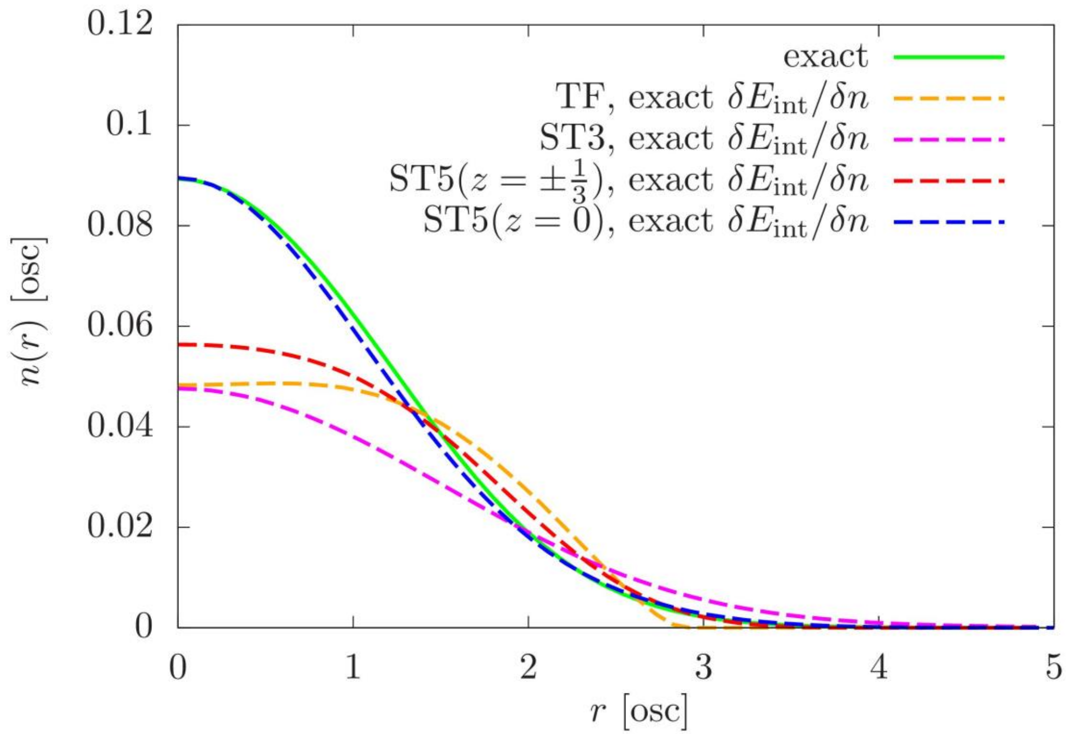
- Suzuki-Trotter decomposition:
  - Preliminary results




3D Hooke's atom

2 fermions

$$H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + \frac{1}{8}(r_1^2 + r_2^2) + \frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

# Upcoming tasks

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- Self-consistent Hooke's atom
- Other ST decomposition
- Average over different ST decomposition
- Benchmark with other exact results

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# Thank you