Derivation of the time dependent Hartree (Fock) equation

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Dictionary

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2. "Hartree (Fock)": time dependent Hartree (Fock)

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2. Derivation of Hartree (Fock) equations for Fermions
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Mean field for the bosons: The Hartree equation

$$H = \sum_{j=1}^{N} -\Delta_j + \sum_{j=1}^{N} A_t(x_j) + (N-1)^{-1} \sum_{k<j} V(x_j - x_k)$$

Interaction „felt" by each particle of order one

$\Psi_0 = \prod_{j=1}^{N} \phi_0(x_j)$ $\qquad$ $id_t \Psi_t = H_t \Psi_t$

Interaction destroys product structure.

Question:

- In which regimes: $\Psi_t \approx \prod_{j=1}^{N} \phi_t(x_j)$ (in what sense?)
- What is ϕ_t?

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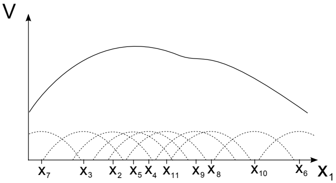
Mean field for "particle 1"



$W(x_1) = (N-1)^{-1}\sum_{j=2}^{N} V(x_1 - x_j)$ for fixed, $|\phi_0|^2$- distributed $x_2, \ldots, x_N$.

Law of large numbers: $|\phi_0|^2$ close to the empirical density ρ_0.

$W(x_1) \approx V \star |\phi_0|^2(x_1)$ ("Mean field").

Effective Dynamics: Hartree equation

$$i d_t \phi_t = \left(-\Delta + A_t + V \star |\phi_t|^2\right)\phi_t \; .$$

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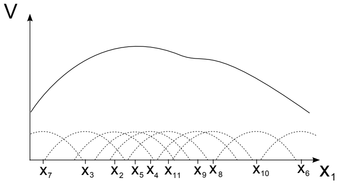

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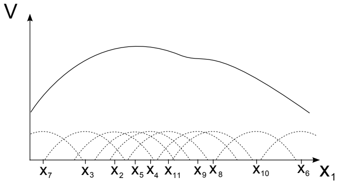

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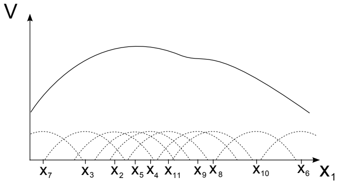

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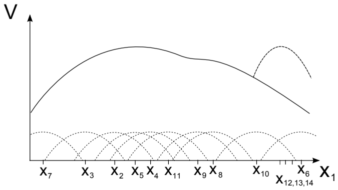
Grönwall argument



Let α_t be a measure for the dirt in the condensate:

$$d_t \alpha_t \leq C(\alpha_t + o(1))$$

Grönwall: α_t stays small if α_0 was small ($\alpha_t \leq e^{Ct}\alpha_0 + o(1)$)

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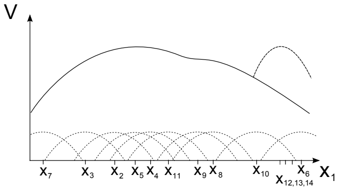

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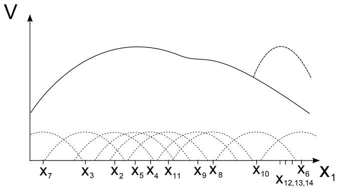

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Usual approach

Control reduced one particle density matrix $\mu_1^{\Psi_t}$
$d_t\mu_1^{\Psi_t}$ depends on $\mu_2^{\Psi_t}$
$d_t\mu_2^{\Psi_t}$ depends on $\mu_3^{\Psi_t}$
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Technically difficult (e.g. Erdös, Schlein, Yau (2009)

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Introduction of a counting measure:

For every $j = 1, \ldots, N$ and $\phi \in L^2(\mathbb{R}^3)$ let p_j^ϕ be the projector given by

$$p_j^\phi = |\phi\rangle\langle\phi|_j \; .$$

Let $q_j^\phi = 1 - p_j^\phi$.
According to Ψ "expected relative number" of particles not in the state ϕ

$$\alpha(\Psi, \phi) = N^{-1} \sum_{j=1}^{N} \langle \Psi, q_j^\phi \Psi \rangle = \langle \Psi, q_k^\phi \Psi \rangle = \| q_k^\phi \Psi \|^2 \; .$$

$\alpha(\Psi, \phi) = 0 \quad \Leftrightarrow \quad \Psi = \prod_{j=1}^{N} \phi(x_j).$

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Example:

$\Psi(x_1,\ldots,x_N) = \left(\chi(x_1,\ldots x_k)\prod_{j=k+1}^{N}\phi(x_j)\right)_{sym}$
with $\chi \in L^2(\mathbb{R}^{3k})$, $p_j\chi = 0$ for all $1 \leq j \leq k$

$\Rightarrow \alpha(\Psi,\phi) = k/N.$

Lemma: $\alpha(\Psi_t,\phi_t) \to 0$ is equivalent to convergence of μ_t to $|\phi_t\rangle\langle\phi_t|$ in operator norm.

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Deriving the mean field equation:

Goal: show that $|d_t\alpha_t| < C(\alpha_t + o(1)) \Rightarrow \alpha_t \ll 1$ by Grönwall
Let

$$h_j := -\Delta_j + A + V \star |\phi_t|^2(x_j) \; .$$

Since

$$d_t q_j^{\phi_t} = -i[h_j, q_j^{\phi_t}]$$

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$$d_t\alpha(\Psi_t,\phi_t) = i\langle\Psi_t,[-\Delta_1 + (N-1)^{-1}\sum_{j=2}^{N} V(x_1 - x_j) - h_1, q_1^{\phi_t}]\Psi_t\rangle$$

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$$= i\Big(\langle\Psi_t,\big(V(x_1 - x_2) - V\star|\phi_t|^2(x_1)\big)\, q_1^{\phi_t}\Psi_t\rangle - c.c.\Big)$$

$$= i\Big(\langle\Psi_t,(p_1^{\phi_t} + q_1^{\phi_t})(p_2^{\phi_t} + q_2^{\phi_t})\big(V(x_1 - x_2) - V\star|\phi_t|^2(x_1)\big)\, q_1^{\phi_t}(p_2^{\phi_t} + q_2^{\phi_t})\Psi_t\rangle - c.c.\Big)\ .$$

All terms $\langle\Psi_t, A_{12}\Psi_t\rangle$ where A_{12} is either selfadjoint or invariant under adjunction plus simultaneous exchange of the variables x_1 and x_2 cancel out.

Only three types remain: $pp \ldots pq$, $pp \ldots qq$ and $pq \ldots qq$

$$I = i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} \left(V(x_1 - x_2) - V \star |\phi_t|^2(x_1) \right) q_1^{\phi_t} p_2^{\phi_t} \Psi_t \rangle$$

$$= i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} V(x_1 - x_2) p_2^{\phi_t} q_1^{\phi_t} \Psi_t \rangle - i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} V \star |\phi_t|^2(x_1) p_2^{\phi_t} q_1^{\phi_t} \Psi_t \rangle$$

$$II = i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} V(x_1 - x_2) q_1^{\phi_t} q_2^{\phi_t} \Psi_t \rangle$$

$$III = i\langle \Psi_t, p_1^{\phi_t} q_2^{\phi_t} \left(V(x_1 - x_2) - V \star |\phi_t|^2(x_1) \right) q_1^{\phi_t} q_2^{\phi_t} \Psi_t \rangle \, .$$

Only three types remain: $pp \dots pq$, $pp \dots qq$ and $pq \dots qq$

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$$III = i\langle \Psi_t, p_1^{\phi_t} q_2^{\phi_t} \left(V(x_1 - x_2) - V \star |\phi_t|^2(x_1) \right) q_1^{\phi_t} q_2^{\phi_t} \Psi_t \rangle \ .$$

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$$I = i\langle\Psi_t, p_1^{\phi_t} p_2^{\phi_t}\left(V(x_1-x_2) - V\star|\phi_t|^2(x_1)\right) q_1^{\phi_t} p_2^{\phi_t}\Psi_t\rangle$$

$$= i\langle\Psi_t, p_1^{\phi_t} p_2^{\phi_t} V(x_1-x_2) p_2^{\phi_t} q_1^{\phi_t}\Psi_t\rangle - i\langle\Psi_t, p_1^{\phi_t} p_2^{\phi_t} V\star|\phi_t|^2(x_1) p_2^{\phi_t} q_1^{\phi_t}\Psi_t\rangle$$

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Only three types remain: $pp\dots pq$, $pp\dots qq$ and $pq\dots qq$

$$I = i\langle\Psi_t, p_1^{\phi_t}p_2^{\phi_t}\left(V(x_1-x_2) - V\star|\phi_t|^2(x_1)\right)q_1^{\phi_t}p_2^{\phi_t}\Psi_t\rangle$$

$$= i\langle\Psi_t, p_1^{\phi_t}p_2^{\phi_t}V(x_1-x_2)p_2^{\phi_t}q_1^{\phi_t}\Psi_t\rangle - i\langle\Psi_t, p_1^{\phi_t}p_2^{\phi_t}V\star|\phi_t|^2(x_1)p_2^{\phi_t}q_1^{\phi_t}\Psi_t\rangle$$

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$$III = i\langle\Psi_t, p_1^{\phi_t}q_2^{\phi_t}\left(V(x_1-x_2) - V\star|\phi_t|^2(x_1)\right)q_1^{\phi_t}q_2^{\phi_t}\Psi_t\rangle\ .$$

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\begin{aligned}
I &= i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} \left(V(x_1 - x_2) - V \star |\phi_t|^2(x_1) \right) q_1^{\phi_t} p_2^{\phi_t} \Psi_t \rangle \\
&= i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} V(x_1 - x_2) p_2^{\phi_t} q_1^{\phi_t} \Psi_t \rangle - i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} V \star |\phi_t|^2(x_1) p_2^{\phi_t} q_1^{\phi_t} \Psi_t \rangle \\
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\end{aligned}
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\begin{aligned}
I &= i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} \left(V(x_1 - x_2) - V \star |\phi_t|^2(x_1) \right) q_1^{\phi_t} p_2^{\phi_t} \Psi_t \rangle \\
&= i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} V(x_1 - x_2) p_2^{\phi_t} q_1^{\phi_t} \Psi_t \rangle - i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} V \star |\phi_t|^2(x_1) p_2^{\phi_t} q_1^{\phi_t} \Psi_t \rangle \\
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\end{aligned}
$$

$$
I : p_2^{\phi_t} V(x_1 - x_2) p_2^{\phi_t} =
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Only three types remain: $pp\dots pq$, $pp\dots qq$ and $pq\dots qq$

$$
\begin{aligned}
I &= i\langle\Psi_t, p_1^{\phi_t}p_2^{\phi_t}\left(V(x_1-x_2) - V\star|\phi_t|^2(x_1)\right)q_1^{\phi_t}p_2^{\phi_t}\Psi_t\rangle\\
&= i\langle\Psi_t, p_1^{\phi_t}p_2^{\phi_t}V(x_1-x_2)p_2^{\phi_t}q_1^{\phi_t}\Psi_t\rangle - i\langle\Psi_t, p_1^{\phi_t}p_2^{\phi_t}V\star|\phi_t|^2(x_1)p_2^{\phi_t}q_1^{\phi_t}\Psi_t\rangle\\
II &= i\langle\Psi_t, p_1^{\phi_t}p_2^{\phi_t}V(x_1-x_2)q_1^{\phi_t}q_2^{\phi_t}\Psi_t\rangle\\
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\end{aligned}
$$

$$
I:\ p_2^{\phi_t}V(x_1-x_2)p_2^{\phi_t} = |\phi_t(x_2)\rangle\langle\phi_t(x_2)|V(x_1-x_2)|\phi_t(x_2)\rangle\langle\phi_t(x_2)|
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Only three types remain: $pp \ldots pq$, $pp \ldots qq$ and $pq \ldots qq$

$$
\begin{aligned}
I &= i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} \left(V(x_1 - x_2) - V \star |\phi_t|^2(x_1) \right) q_1^{\phi_t} p_2^{\phi_t} \Psi_t \rangle \\
&= i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} V(x_1 - x_2) p_2^{\phi_t} q_1^{\phi_t} \Psi_t \rangle - i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} V \star |\phi_t|^2(x_1) p_2^{\phi_t} q_1^{\phi_t} \Psi_t \rangle \\
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\end{aligned}
$$

$$
\begin{aligned}
I : p_2^{\phi_t} V(x_1 - x_2) p_2^{\phi_t} &= |\phi_t(x_2)\rangle \langle \phi_t(x_2)| V(x_1 - x_2) |\phi_t(x_2)\rangle \langle \phi_t(x_2)| \\
&= |\phi_t(x_2)\rangle V \star |\phi_t|^2(x_1) \langle \phi_t(x_2)| = p_2^{\phi_t} V \star |\phi_t|^2 \\
&= p_2^{\phi_t} V \star |\phi_t|^2 p_2^{\phi_t}
\end{aligned}
$$

$\Rightarrow I = 0.$

Only three types remain: $pp \dots pq$, $pp \dots qq$ and $pq \dots qq$

$$I = i\langle \Psi_t, p_1^{\phi_t} p_2^{\phi_t} \left(V(x_1 - x_2) - V \star |\phi_t|^2(x_1) \right) q_1^{\phi_t} p_2^{\phi_t} \Psi_t \rangle$$

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$$I : p_2^{\phi_t} V(x_1 - x_2) p_2^{\phi_t} = |\phi_t(x_2)\rangle \langle \phi_t(x_2)| V(x_1 - x_2) |\phi_t(x_2)\rangle \langle \phi_t(x_2)|$$

$$= |\phi_t(x_2)\rangle V \star |\phi_t|^2(x_1) \langle \phi_t(x_2)| = p_2^{\phi_t} V \star |\phi_t|^2$$

$$= p_2^{\phi_t} V \star |\phi_t|^2 p_2^{\phi_t}$$

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$$= i\langle\Psi_t, p_1^{\phi_t}p_2^{\phi_t}V(x_1-x_2)p_2^{\phi_t}q_1^{\phi_t}\Psi_t\rangle - i\langle\Psi_t, p_1^{\phi_t}p_2^{\phi_t}V\star|\phi_t|^2(x_1)p_2^{\phi_t}q_1^{\phi_t}\Psi_t\rangle$$
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$$I:\ p_2^{\phi_t}V(x_1-x_2)p_2^{\phi_t} = |\phi_t(x_2)\rangle\langle\phi_t(x_2)|V(x_1-x_2)|\phi_t(x_2)\rangle\langle\phi_t(x_2)|$$
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$$
\begin{aligned}
I &= i\langle\Psi_t, p_1^{\phi_t} p_2^{\phi_t} \left(V(x_1 - x_2) - V\star|\phi_t|^2(x_1)\right) q_1^{\phi_t} p_2^{\phi_t}\Psi_t\rangle \\
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\end{aligned}
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I : p_2^{\phi_t} V(x_1 - x_2) p_2^{\phi_t} &= |\phi_t(x_2)\rangle\langle\phi_t(x_2)|V(x_1 - x_2)|\phi_t(x_2)\rangle\langle\phi_t(x_2)| \\
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\begin{aligned}
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$$

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I: p_2^{\phi_t} V(x_1-x_2) p_2^{\phi_t} &= |\phi_t(x_2)\rangle\langle\phi_t(x_2)|V(x_1-x_2)|\phi_t(x_2)\rangle\langle\phi_t(x_2)| \\
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$$I = 0$$
$$II = i\langle\Psi_t, p_1^{\phi_t} p_2^{\phi_t} V(x_1 - x_2) q_1^{\phi_t} q_2^{\phi_t} \Psi_t\rangle$$
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$$|III| \leq \|q_2^{\phi_t}\Psi_t\|^2 2\|V\|_\infty = C\alpha(\Psi_t, \phi_t)$$

$$d_t\alpha(\Psi_t, \phi_t) \leq C(\alpha(\Psi_t, \phi_t) + N^{-1})$$

Only three types remain: $pp \dots pq$, $pp \dots qq$ and $pq \dots qq$

$$
\begin{aligned}
I &= 0 \\
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III &= i\langle \Psi_t, q_2^{\phi_t} p_1^{\phi_t} \left(V(x_1 - x_2) - V \star |\phi_t|^2(x_1) \right) q_1^{\phi_t} q_2^{\phi_t} \Psi_t \rangle \ .
\end{aligned}
$$

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$$
d_t \alpha(\Psi_t, \phi_t) \leq C(\alpha(\Psi_t, \phi_t) + N^{-1})
$$

Fermions

- Microscopic system: $\Psi_0 = \Lambda_{j=1}^N \phi_0^j$
  $H = \sum_{j=1}^N -\Delta_j + \sum_{j=1}^N A_t(x_j) + N^{-2/3} \sum_{k<j} V(x_j - x_k)$
  $N^{-2/3}$-coupling: volume N, Coulomb interaction

$$\int_0^{N^{1/3}} x^{-1} d^3x \sim N^{2/3}$$

- Macroscopic equation: Hartree (Fock)
  $d_t \phi_t^j = \left(-\Delta + A + N^{-1} \sum_{k=1}^N |\phi_t^k|^2 \star V\right) \phi_t^j$
  $-\left(N^{-1} \sum_{k=1}^N \left(\phi_t^{k,*} \phi_t^j\right) \star V\right) \phi_t^k$
- $p = \sum_{j=1}^N |\phi_t^j\rangle\langle\phi_t^j|$
- Difficulties: $I \neq 0$
  $N^{-2/3}$ instead of N^{-1}

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  $- \left(N^{-1} \sum_{k=1}^N \left(\phi_t^{k,*} \phi_t^j \right) \star V \right) \phi_t^k$
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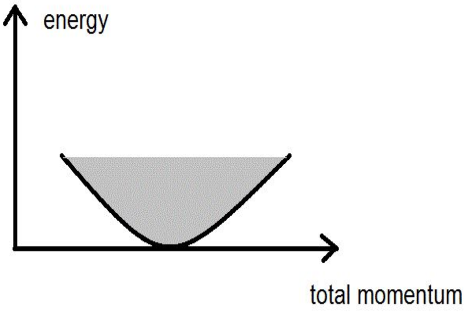
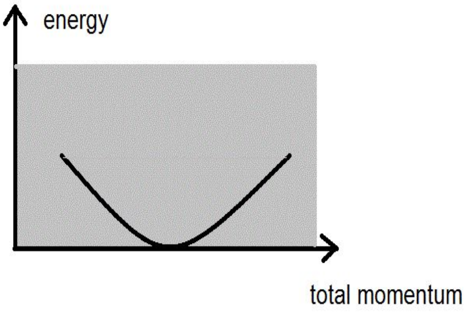
1d: easy: Momentum and energy conservation.



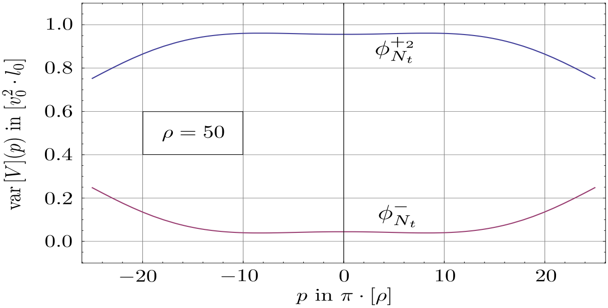
Special situation

Higher dimensions



Estimate of fluctuations

Variance of force at some position y
(fermions: purble, bosons: blue)



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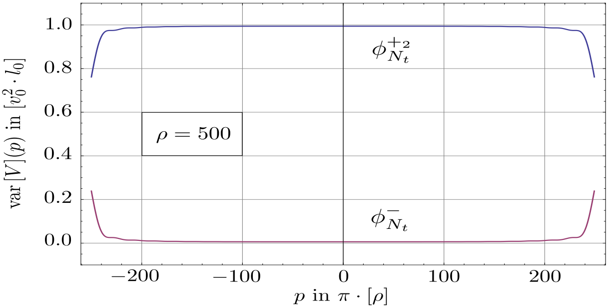

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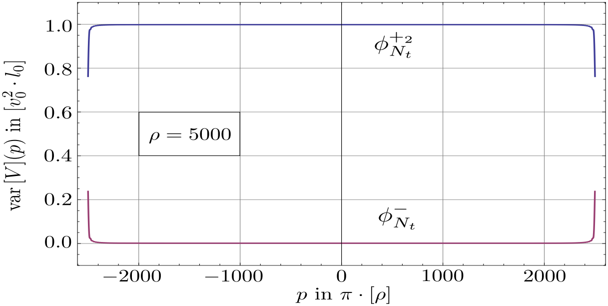

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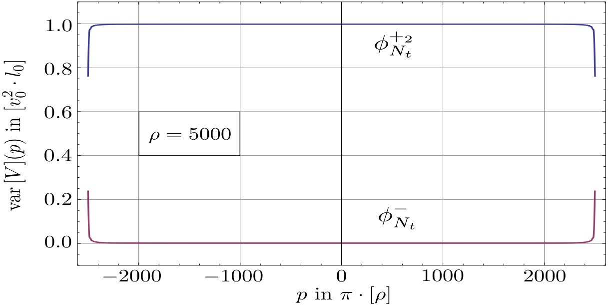

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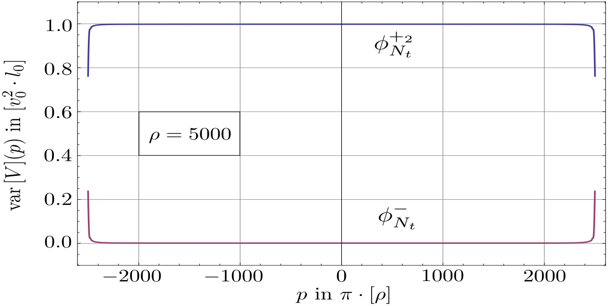

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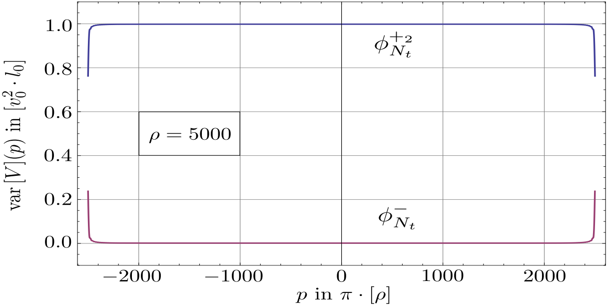

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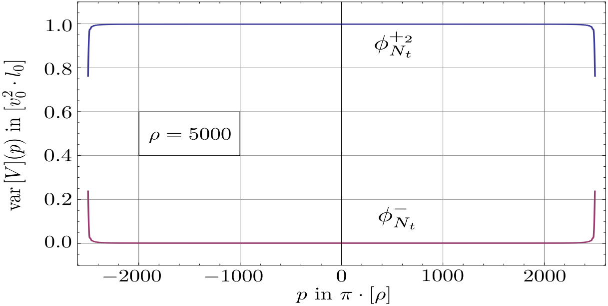

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Thank you!