Correlation properties of few charged bosons in anisotropic traps

Anna Okopińska, Przemysław Kościk

Jan Kochanowski University in Kielce, Poland





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Outline



- 2 Theoretical description
 - Schrödinger equation
 - Correlation characteristics
 - Quasi-1D system

3 Results

- Effective 1-RDM
- Linear entropy
- von Neumann entropy

Summary



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Experimentally accessible quantum systems

NATURE-MADE: matter built from atoms, molecules, nuclei,...



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Anna Okopińska, Przemysław Kościk Correlation properties of few charged bosons in anisotropic traps

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experimental system \Rightarrow theory has to be derived





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Correlation properties of few charged bosons in anisotropic traps

Artificial quantum systems: interactions

contact interaction



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Artificial quantum systems: interactions

contact interaction

ultracold atoms trapped in optical lattices or optical microtraps



Artificial quantum systems: interactions





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Artificial quantum systems: interactions





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Artificial quantum systems: interactions





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Correlation properties of few charged bosons in anisotropic traps

Schrödinger equation

System of N Coulombically interacting bodies Schrödinger equation

Hamiltonian:

Itonian:

$$\rho_i = \sqrt{y_i^2 + z_i^2}$$

$$H = \sum_{i=1}^N \left[-\frac{\hbar^2 \bigtriangledown_i^2}{2m} + \frac{m}{2} (\omega_x^2 x_i^2 + \omega_\perp^2 \rho_i^2) \right] + \sum_{i < j} \frac{\gamma}{|\mathbf{r}_i - \mathbf{r}_j|},$$



Schrödinger equation Correlation characteristics Quasi-1D system

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after scaling $\mathbf{r} \mapsto \sqrt{\frac{\hbar}{m\omega_x}} \mathbf{r}, E \mapsto \hbar\omega_x E$ Schrödinger equation: $\widehat{H}\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$

$$H = \sum_{i=1}^{N} \left[-\frac{\nabla_i^2}{2} + \frac{1}{2}x_i^2 + \frac{1}{2}\epsilon^2 \rho_i^2 \right] + \sum_{i < j} \frac{g}{|\mathbf{r}_i - \mathbf{r}_j|}.$$



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 $\epsilon = rac{\omega_{\perp}}{\omega_{\star}}$ - anisotropy of the trap



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 $\epsilon = \frac{\omega_{\perp}}{\omega_{x}}$ - anisotropy of the trap $g = \gamma \sqrt{\frac{m}{\omega_{x}\hbar^{3}}}$ - Coulomb / longitudinal trapping energy.

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Schrödinger equation Correlation characteristics Quasi-1D system

Correlation measures

Correlation energy

 $E_{corr} = E_{MF} - E_{exact}$ (Lövdin 1955)



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Statistical correlation coefficient

$$\tau_{ij} = \frac{\langle \mathbf{r}_1 \cdot \mathbf{r}_2 \rangle_{ij} - \langle \mathbf{r} \rangle_i^2}{\langle \mathbf{r}^2 \rangle_i - \langle \mathbf{r} \rangle_i^2}$$
(Kutzelnigg 1968)

expectation values weighted with the probability density

 $|\psi(\mathbf{r}_1,...,\mathbf{r}_N)|^2$ and integrated over the remaining variables.



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Based on one particle reduced density matrix 1-RDM

$$\rho(\mathbf{r}_1, \mathbf{r}_1) = \int \Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) \Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) d^3 r_2 ... d^3 r_N$$



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Based on two particle reduced density matrix 2-RDM

$${}^{2}\rho(\mathbf{r}_{1},\mathbf{r}_{2},\mathbf{r}_{1},\mathbf{r}_{2}) = \int \Psi(\mathbf{r}_{1},\mathbf{r}_{2},...,\mathbf{r}_{N})\Psi(\mathbf{r}_{1},\mathbf{r}_{2},...,\mathbf{r}_{N})d^{3}r_{3}...d^{3}r_{N}$$

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Measures based on 1-RDM

entanglement entropies - global characteristics for pure states

1-RDM admits a Schmidt decomposition

$$\rho = \sum \lambda_k |\mathbf{v}_k\rangle \langle \mathbf{v}_k|, \qquad \sum \lambda_k = \mathbf{1}.$$



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Rényi entropies

$$S(q) = \frac{1}{1-q} \ln \sum \lambda_k^q$$

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Correlation properties of few charged bosons in anisotropic traps



Schrödinger equation Correlation characteristics Quasi-1D system

We consider strong anisotropy case $\epsilon \gg 1$

single transverse-mode approximation

The particles assumed to stay in the lowest state of H_{\perp}



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The particles assumed to stay in the lowest state of H_{\perp}

N-body wave function approximated by: $\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) \approx \psi(x_1, x_2, ..., x_N) \prod_{i=1}^N \varphi(y_i) \varphi(z_i)$

where
$$arphi(z)=(rac{\epsilon}{\pi})^{rac{1}{4}} e^{-rac{\epsilon z^2}{2}}$$
 .


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$$\begin{split} & N-\text{body wave function approximated by:} \\ & \Psi(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N) \approx \psi(x_1,x_2,...,x_N) \Pi_{i=1}^N \varphi(y_i) \varphi(z_i) \\ & \text{where } \varphi(z) = \left(\frac{\epsilon}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\epsilon z^2}{2}}. \\ & \text{Integration over } \bot \text{ gives quasi-1D Schrödinger equation} \\ & H^{1D}\psi(x_1,x_2,...,x_N) = E^{1D}\psi(x_1,x_2,...,x_N) \\ & \text{with } H^{1D} = \sum_{i=1}^N [-\frac{1}{2}\frac{\partial^2}{\partial x_i^2} + \frac{1}{2}x_i^2] + \sum_{i < j} g U^{1D}(x_i,x_j) + N\epsilon \end{split}$$

quasi-1D effective potential:

 $U^{1D}(x_1,x_2) = \sqrt{\frac{\varepsilon\pi}{2}} e^{\frac{\epsilon(x_2-x_1)^2}{2}} (1 - erf[\sqrt{\frac{\varepsilon}{2}}|x_2 - x_1|])$

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Applicability of the single-mode approximation: N = 2

Comparison of E_0^{1D} with exact E_0 from 3D Hamiltonian



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1-RDM in the single-mode approximation

single-mode approximation

1-RDM factorizes to the form

$$\rho(\mathbf{r},\mathbf{r}') = \varphi(\mathbf{y})\varphi(\mathbf{y}')\varphi(\mathbf{z})\varphi(\mathbf{z}')\rho_{1D}(\mathbf{x},\mathbf{x}'),$$

with effective 1D RDM $\rho_{1D}(x, x') = \int \psi(x, x_2, ..., x_N) \psi(x', x_2, ..., x_N) dx_2 ... dx_N = \sum \lambda_l v_l(x) v_l(x')$



Schrödinger equation Correlation characteristics Quasi-1D system

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Linear entropy $L = 1 - tr \hat{\rho}_{1D}^2 = 1 - \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho_{1D}^2(x, x') dx' dx$



Schrödinger equation Correlation characteristics Quasi-1D system

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We calculate the GS wave function of the quasi-1D Hamiltonian $\psi(x_1, x_2, ..., x_N)$ with the quantum diffusion algorithm and use it to determine $\rho_{1D}(x, x')$ and *L*.

Schrödinger equation Correlation characteristics Quasi-1D system

Strictly 1D limit

divergencies

Interaction potential
$$\frac{g}{|x_i-x_j|}$$
 diverges at $x_i = x_j$ for $g \neq 0$.



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Bosonic system fermionized. No divergencies in calculating ψ_F . We determine ψ_F using CI with harmonic oscillator basis $\{\varphi_n^{ho}\}$.



Effective 1-RDM Linear entropy von Neumann entropy

Plot of the effective 1-RDM $\rho_{1D}(x, x')$





Anna Okopińska, Przemysław Kościk

Correlation properties of few charged bosons in anisotropic traps

Effective 1-RDM Linear entropy von Neumann entropy

Plot of the effective 1-RDM $\rho_{1D}(x, x')$



At $\epsilon = 30$ the quasi-1D RDM differs heavily from that of a <u>denuinely 1D system</u>. Big differences at $q \le 5$.

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Jon Hothonouski Universitu

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Ground-state linear entropy



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Asymptotics in the strictly 1D system



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$$\psi(x_1, x_2, ..., x_N) = |\psi_F(x_1, x_2, ..., x_N)| \rightarrow \frac{1}{\sqrt{N!}} |det_{n=0, j=0}^{N-1, N}(\varphi_n^{ho}(x_j))|$$



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$$L_{1D}^{g \to 0} \approx \begin{pmatrix} 0.36 & N = 2\\ 0.51 & N = 3\\ 0.60 & N = 4 \end{pmatrix}$$



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N = 2 analytic result from the harmonic approximation

$$V(x_1, x_2) = \frac{1}{2}x_1^2 + \frac{1}{2}x_2^2 + \frac{g}{|x_2 - x_1|} \approx 3\frac{g^{\frac{3}{4}}}{2^{\frac{3}{4}}} + \frac{1}{4}(x_1 + x_2)^2 + \frac{3}{4}(x_1 - x_2 - \frac{g^{\frac{3}{4}}}{2^{\frac{1}{6}}})^2$$



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Correlation properties of few charged bosons in anisotropic traps

Effective 1-RDM Linear entropy von Neumann entropy

Comparison of the linear and von Neumann entropies



Anna Okopińska, Przemysław Kościk Correlation properties of few charged bosons in anisotropic traps

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 $\epsilon = 30$



Anna Okopińska, Przemysław Kościk

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single-particle density

Comparison $\rho(x) \equiv N\rho(x, x)$ with $\rho_{MF}(x) = N|\phi_{MF}(x)|^2$



Anna Okopińska, Przemysław Kościk Correlation properties of few charged bosons in anisotropic traps

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MF fails to describe the internal structure of the system if $g \gtrsim g_{cr}$

Anna Okopińska, Przemysław Kościk

Correlation properties of few charged bosons in anisotropic traps

Summary and outlook

Systems composed of N=2,3, and 4 Coulombically interacting particles in a harmonic trap of anisotropy ϵ are investigated.



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- an increase in *ϵ* results in an increase in *L*. Entanglement is the largest in the limit of *ϵ* → ∞, when fermionization takes place for any *g* ≠ 0.
- Dependence on *ϵ* is significant only at weak interaction *g* ≤ *g_{cr}*. In this region the entanglement properties of the quasi-1D system differ heavily from a genuinely 1D one.

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