The ν Jastrow factor

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Marios Michael
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Outline

1. The Jastrow factor
    - u
    - p
    - Problems
2. The ν Jastrow factor
    - Proposal
    - Features
3. Tests
    - Accuracy
    - Local energy
    - Efficiency
4. Summary

The Hamiltonian

- Hamiltonian:

$$H = -\frac{1}{2}\sum_{i}\nabla_i^2 + \sum_{i>j}\frac{1}{r_{ij}}$$

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- Non-interacting Hamiltonian:

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- Non-interacting Hamiltonian:

$$H = -\frac{1}{2}\sum_i \nabla_i^2$$

- Solution:

$$D_\uparrow(\mathbf{r}_1,\ldots,\mathbf{r}_M) = \begin{vmatrix} \mathrm{e}^{\mathbf{k}_1\mathbf{r}_1} & \mathrm{e}^{\mathbf{k}_2\mathbf{r}_1} & \ldots & \mathrm{e}^{\mathbf{k}_M\mathbf{r}_1} \\ \mathrm{e}^{\mathbf{k}_1\mathbf{r}_2} & \mathrm{e}^{\mathbf{k}_2\mathbf{r}_2} & \ldots & \mathrm{e}^{\mathbf{k}_M\mathbf{r}_2} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{e}^{\mathbf{k}_1\mathbf{r}_M} & \mathrm{e}^{\mathbf{k}_2\mathbf{r}_M} & \ldots & \mathrm{e}^{\mathbf{k}_M\mathbf{r}_M} \end{vmatrix}$$

Correlations

- Wavefunction including Jastrow factor:

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_M) = \mathrm{e}^{J(\mathbf{r}_1, \ldots, \mathbf{r}_M)} D_\uparrow D_\downarrow$$

- Slater determinant captures statistics
- Jastrow factor captures correlations

Kato cusp conditions

- Divergent potential energy at coalescence must be cancelled by diverging kinetic energy, which sets the condition

$$\left.\frac{\partial J}{\partial r_{ij}}\right|_{r_{ij}=0} = \Gamma$$

- For opposite spins

$$\Gamma = \frac{1}{2}$$

u term

- Polynomial term

$$J(\mathbf{r}_1, \ldots, \mathbf{r}_M) = \sum_{i>j} \mathrm{u}(r_{ij})$$

where*

$$\mathrm{u}(r_{ij}) = \left(\qquad \sum_{n=1}^{N} \alpha_n r_{ij}^n \right)$$

*P. López Ríos, P. Seth, N.D. Drummond, and R.J. Needs, Phys. Rev. E **86**, 036703 (2012)

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where*

$$\mathrm{u}(r_{ij}) = \left(\sum_{n=1}^{N} \alpha_n r_{ij}^n \right) \left(1 - \frac{r_{ij}}{L}\right)^C \Theta(L - r_{ij})$$

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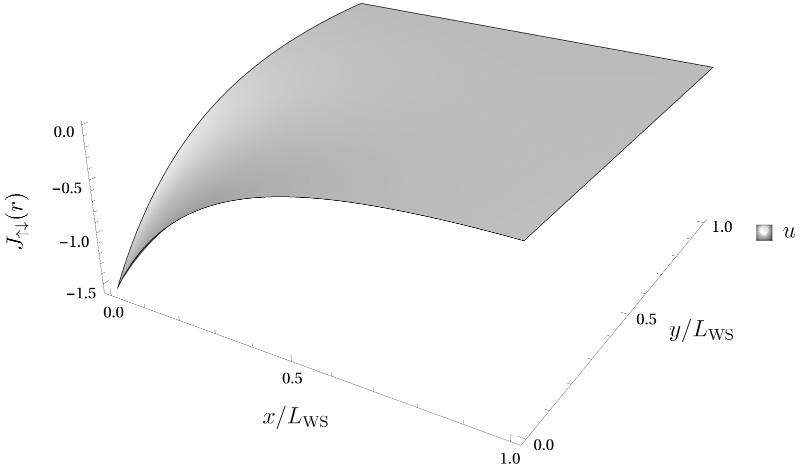
u term


0.0
−0.5
−1.0
−1.5
$J_{\uparrow\downarrow}(r)$
0.0
0.5
1.0
x/L_{WS}
0.0
0.5
1.0
y/L_{WS}
u

p term

- Sinusoidal term

$$J(\mathbf{r}_1, \ldots, \mathbf{r}_M) = \sum_{i>j} \mathrm{p}(\mathbf{r}_{ij})$$

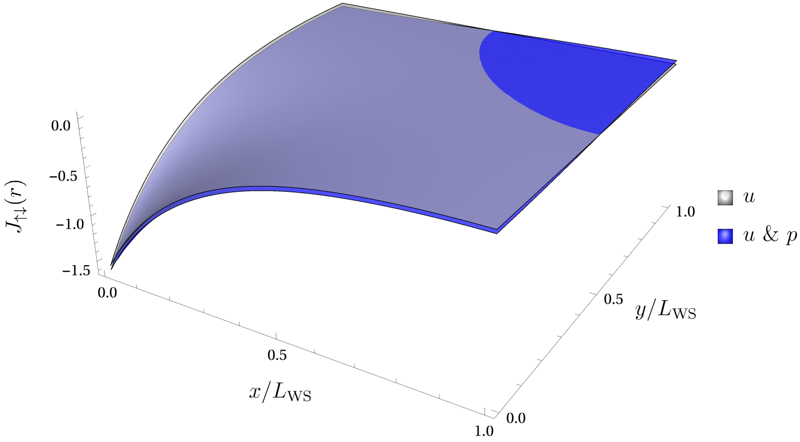
where*

$$\mathrm{p}(\mathbf{r}_{ij}) = \sum_P a_P \sum_{\mathbf{G}_P^+} \cos(\mathbf{G}_P \cdot \mathbf{r}_{ij})$$

for simulation cell reciprocal lattice vectors $\mathbf{G}_P$.

*N.D. Drummond, M.D. Towler, and R.J. Needs, Phys. Rev. B **70**, 235119 (2004)

u & p terms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u & p

Problems

- How many u vs how many p terms?
- p terms expensive to calculate
- Cutoff length enters nonlinearly

The ν Jastrow factor

- We propose a new Jastrow factor

$$J(\mathbf{r}_1, \ldots, \mathbf{r}_M) = \sum_{i>j} \nu(\mathbf{r}_{ij})$$

where

$$\nu(\mathbf{r}) = \sum_{n=1}^{N} c_n \left| f^2(\mathbf{x}) + f^2(\mathbf{y}) + f^2(\mathbf{z}) \right|^{n/2}$$

$$f(\mathbf{x}) = |\mathbf{x}| \left(1 - \frac{|\mathbf{x}/L_x|^N}{N+1} \right)$$

Features

$$\nu(\mathbf{r}) = \sum_{n=1}^{N} c_n \left| f^2(\mathbf{x}) + f^2(\mathbf{y}) + f^2(\mathbf{z}) \right|^{n/2}$$

$$f(\mathbf{x}) = |\mathbf{x}| \left(1 - \frac{|\mathbf{x}/L_x|^N}{N+1} \right)$$

- Small radius:

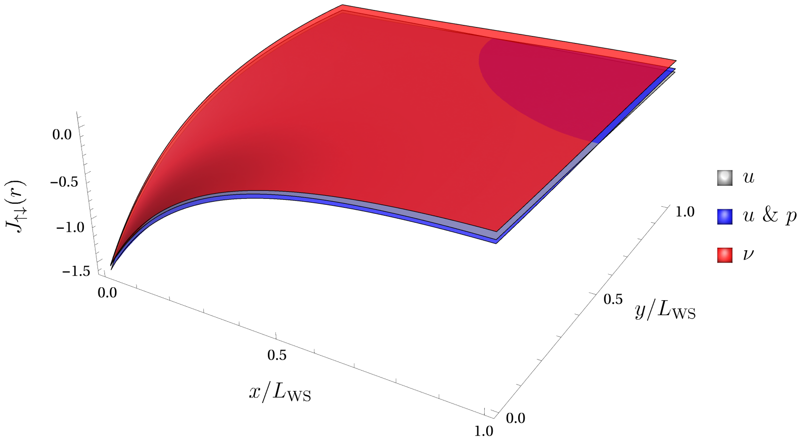
$$f(\mathbf{x}) = |\mathbf{x}| + \ldots$$

$$\Rightarrow \nu(\mathbf{r}) = \sum_{n=1}^{N} c_n r^n + \ldots$$

so Kato cusp condition simply

$$c_1 = \Gamma$$

ν term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Features

$$\nu(\mathbf{r}) = \sum_{n=1}^{N} c_n \left| f^2(\mathbf{x}) + f^2(\mathbf{y}) + f^2(\mathbf{z}) \right|^{n/2}$$

$$f(\mathbf{x}) = |\mathbf{x}| \left(1 - \frac{|\mathbf{x}/L_x|^N}{N+1} \right)$$

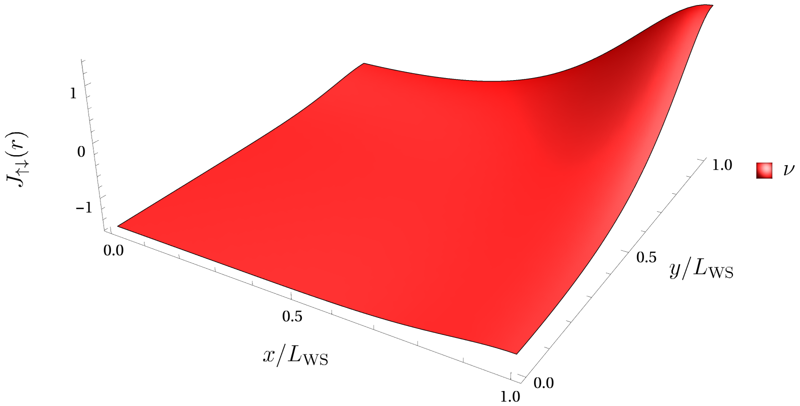
- Large radius:

$$f(\mathbf{x}) = \mathrm{const.} - \frac{N}{2} \left(\frac{x}{L_x} - 1 \right)^2 + \ldots$$

$$\Rightarrow \nu(\mathbf{r}) = \sum_{n=1}^{N} c_n \left(\mathrm{const.} - \frac{n}{2} \frac{N^n}{(N+1)^{n-1}} \left(\frac{x}{L_x} - 1 \right)^2 \right) + \ldots$$

so $n = N$ term has most effect at cell boundary

ν term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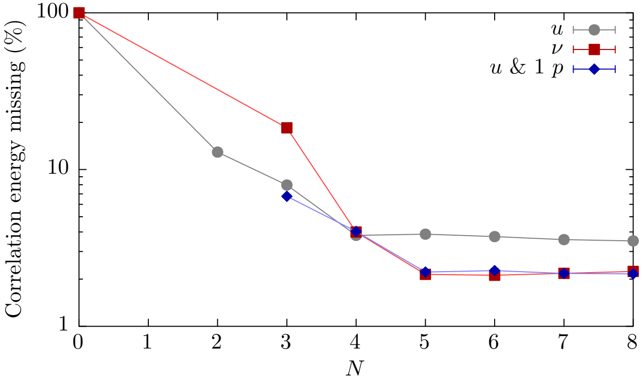
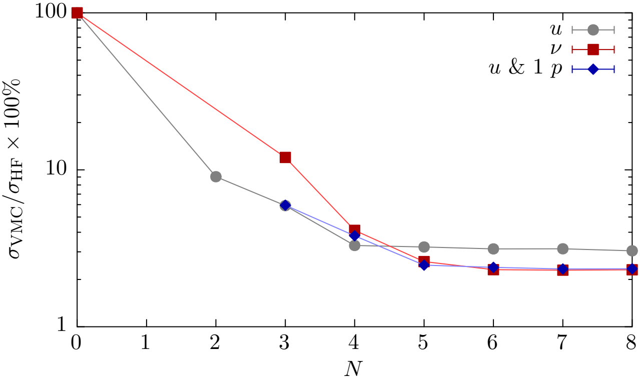
    - ν term captures effect of both together
- p terms expensive to calculate
    - ν term comparable to u term
- Cutoff length enters nonlinearly
    - No cutoff length!
    - All coefficients linear

Correlation energy



Local energy variance



Summary

- New Jastrow factor
  - Easier to use
  - Easier to optimise
  - Cheaper than p term
  - Captures same amount of correlation energy of HEG
- Future progress
  - Test in inhomogeneous system
  - Three-body version

Local energy