Symmetry-breaking wave functions from similarly-transformed propagators

: applications to the fermion problem in 2D quantum dots

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INT, Aug.14, 2018

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Similarity transformation

The partition function

$$Z(\tau) = \int d\mathbf{x}\, G(\mathbf{x}, \mathbf{x}; \tau) \qquad G(\mathbf{x}, \mathbf{x}'; \tau) = \langle \mathbf{x} | \mathrm{e}^{-\tau H} | \mathbf{x}' \rangle$$

is invariant under the similarity transformation

$$Z(\tau) = \int d\mathbf{x} \langle \mathbf{x} | \phi \mathrm{e}^{-\tau H} \phi^{-1} | \mathbf{x} \rangle = \int d\mathbf{x} \phi(\mathbf{x}) G(\mathbf{x}, \mathbf{x}; \tau) \phi^{-1}(\mathbf{x})$$
$$= \int d\mathbf{x}\, G(\mathbf{x}, \mathbf{x}; \tau)$$

provide that $\phi(\mathbf{x}) \neq 0$ at all $\mathbf{x}$. This suggests that $\phi(\mathbf{x})$ should be a bosonic wave function.

Similarity transformed Hamiltonian

The partition function can therefore be obtained from the transformed (Fokker-Planck) propagator

$$\tilde{G}(\mathbf{x}, \mathbf{x}'; \tau) = \langle \mathbf{x} | \mathrm{e}^{-\tau \tilde{H}} | \mathbf{x}' \rangle$$

where the transformed Hamiltonian is

$$\tilde{H} = \phi(\mathbf{x}) H \phi^{-1}(\mathbf{x}) = K + D + E_L$$

with $K = -\frac{1}{2}\nabla^2$, $E_L(\mathbf{x}) = \dfrac{H\phi(\mathbf{x})}{\phi(\mathbf{x})}$ and

$$D\psi = \nabla \cdot (-\nabla S \, \psi \,) \qquad \phi(\mathbf{x}) = e^{-S(\mathbf{x})}$$

This is DMC with importance sampling.

Similarity transformed propagator

The First-order approximation is

$$\tilde{G}_1(\mathbf{x}, \mathbf{x}_0; \tau) = \langle \mathbf{x} | \mathrm{e}^{-\tau K} \mathrm{e}^{-\tau D} \mathrm{e}^{-\tau E_L} | \mathbf{x}_0 \rangle$$

$$= \frac{1}{(2\pi\tau)^{D/2}} \exp\left[-\frac{1}{2\tau} (\mathbf{x} - \mathbf{x}(\tau))^2 \right] \mathrm{e}^{-\tau E_L(\mathbf{x}_0)}$$

where $\mathbf{x}(\tau)$ is the trajectory of the drift equation

$$\frac{d\mathbf{x}}{d\tau} = v(\mathbf{x}) = -\nabla S(\mathbf{x})$$

with initial position $\mathbf{x}_0$.

Transformed harmonic propagator

For a D-dimension harmonic oscillator

$$H = -\frac{1}{2}\nabla^2 + \frac{1}{2}\mathbf{x}^2$$

can take $\phi(\mathbf{x}) = \psi_0(\mathbf{x})$, so that $S(\mathbf{x}) = \frac{1}{2}\mathbf{x}^2$ $E_L = \frac{D}{2}$

$$\frac{d\mathbf{x}}{d\tau} = -\nabla S(\mathbf{x}) = -\mathbf{x} \quad \rightarrow \quad \mathbf{x}(\tau) = \mathbf{x}_0 \mathrm{e}^{-\tau}$$

giving $$\tilde{G}_1(\mathbf{x}, \mathbf{x}_0; \tau) = \frac{1}{(2\pi\tau)^{D/2}} \exp\left[-\frac{1}{2\tau}(\mathbf{x} - \mathbf{x}_0 \mathrm{e}^{-\tau})^2\right] \mathrm{e}^{-\tau E_L}$$

vs exact $$\tilde{G}(\mathbf{x}, \mathbf{x}_0; \tau) = \frac{1}{[2\pi T(\tau)]^{D/2}} \exp\left[-\frac{1}{2T(\tau)}(\mathbf{x} - \mathbf{x}_0 \mathrm{e}^{-\tau})^2\right] \mathrm{e}^{-\tau E_L}$$

Orstein-Uhlenbeck

$$T(\tau) = \frac{1}{2}(1 - \mathrm{e}^{-2\tau})$$

Exact partition function

The first order transformed propagator gives,

$$
\begin{aligned}
Z &= \int d\mathbf{x}\tilde{G}_1(\mathbf{x},\mathbf{x};\tau) \\
&= \frac{1}{(2\pi\tau)^{D/2}}\int d\mathbf{x}\exp\left[-\frac{1}{2\tau}\mathbf{x}^2(1-\mathrm{e}^{-\tau})^2\right]\mathrm{e}^{-\tau E_L} \\
&= \frac{1}{(2\pi\tau)^{D/2}}[2\pi\tau(1-\mathrm{e}^{-\tau})^{-2}]^{D/2}\mathrm{e}^{-\tau D/2} \\
&= \left(\frac{\mathrm{e}^{-\frac{1}{2}\tau}}{1-\mathrm{e}^{-\tau}}\right)^D = [2\sinh(\tau/2)]^{-D}
\end{aligned}
$$

the exact partition function! Independent of T(τ).

Exact ground state wave function

In the limit of $\tau \to \infty$ the exact FP-propagator gives,

$$\tilde{G}(\mathbf{x}, \mathbf{x}_0; \tau) \to \frac{1}{\pi^{D/2}} \exp\left[-\mathbf{x}^2\right] \mathrm{e}^{-\tau E_0} = \psi_0^2(\mathbf{x}) \mathrm{e}^{-\tau E_0}$$

the first-order propagator gives,

$$\tilde{G}_1(\mathbf{x}, \mathbf{x}_0; \tau) \to \frac{1}{(2\pi\tau)^{D/2}} \exp\left[-\frac{1}{2\tau}\mathbf{x}^2\right] \mathrm{e}^{-\tau E_L}$$

However, after letting $\tau \to \infty$ in the trajectory $\mathbf{x}(\tau)$, if we now let τ be a free parameter and set τ=1, then

$$\tilde{G}_1(\mathbf{x}, \mathbf{x}_0; \tau = 1) \propto \exp\left[-\frac{1}{2}\mathbf{x}^2\right] \propto \psi_0(\mathbf{x})$$

This seems contrived, but wait!

Free fermions in the harmonic oscillator

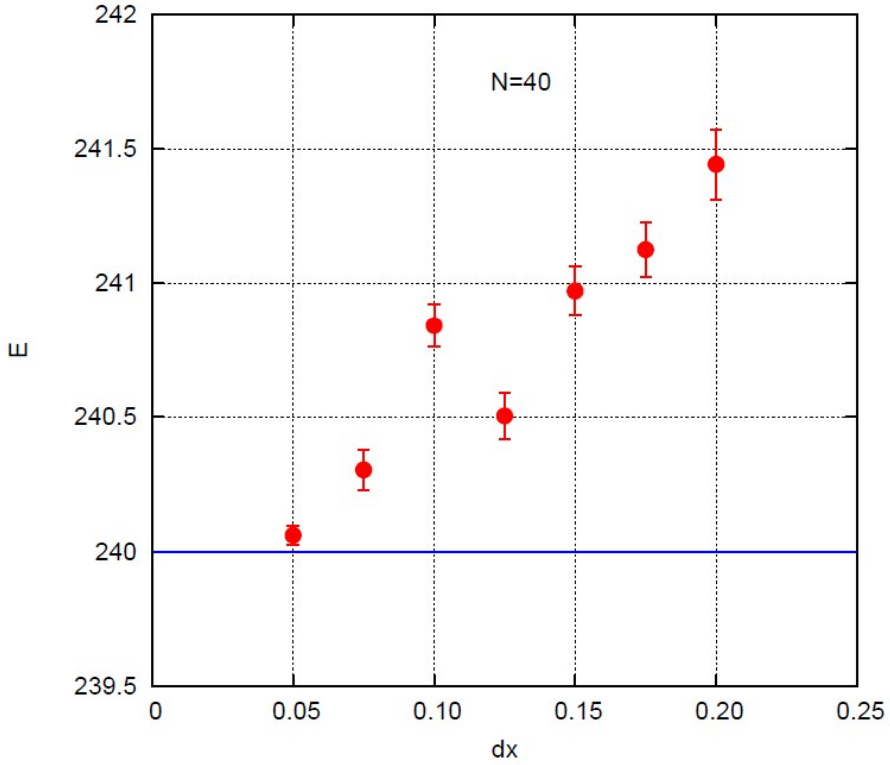
For N fermions (spin-polarized electrons), construct the determinant wave function

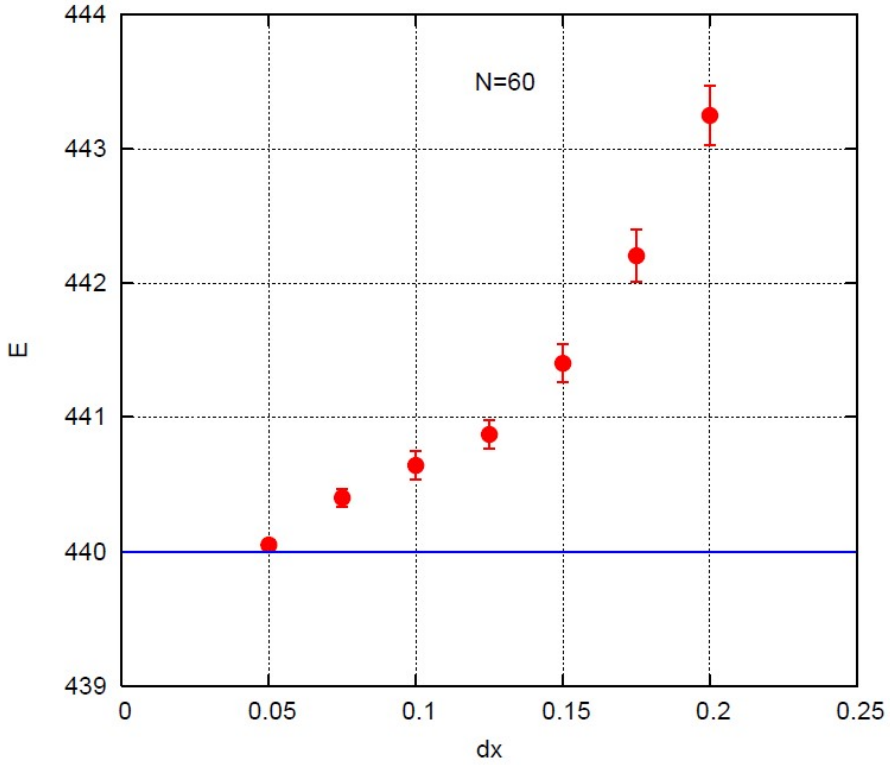
$$\Psi(\mathbf{x}_1, \mathbf{x}_2 \ldots \mathbf{x}_N) = \det\left|\exp[-\frac{1}{2}(\mathbf{x}_i - \mathbf{s}_j)^2]\right|$$

where $\mathbf{s}_i = \mathbf{x}_i(\tau \to \infty)$ →0, but we will just let it be close to but not zero. The resulting energy of this wave function is then exact for N non-interacting fermions in the harmonic oscillator. No explicit excited states needed.

GS energy of N free fermions in HO

For N=40 and 60





Exact energy: 240 and 440

Calculation: 240.06(4), 440.05(3)

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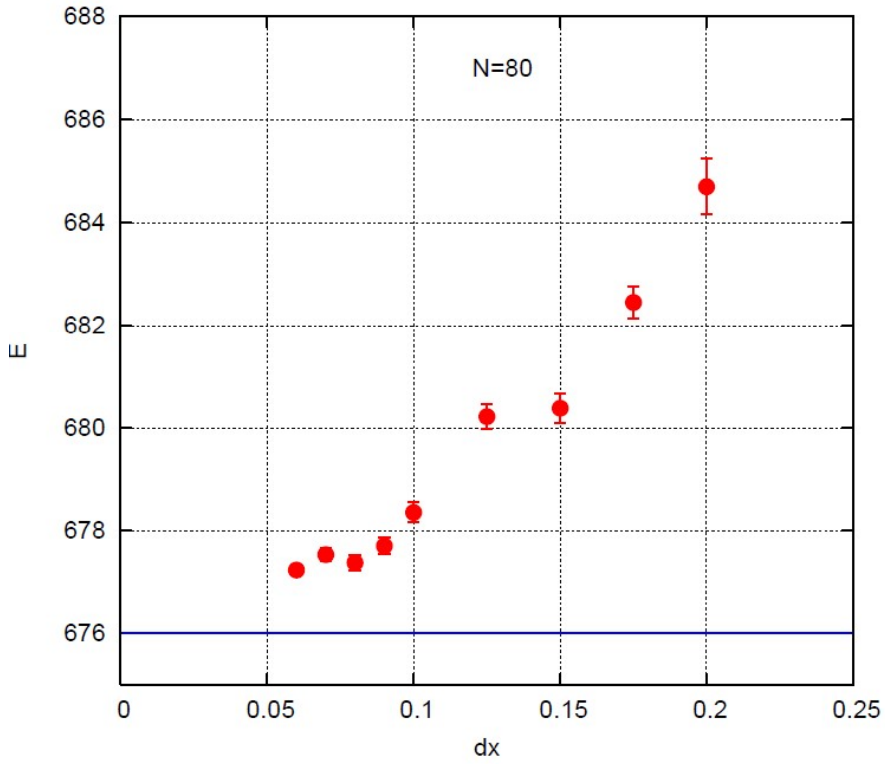
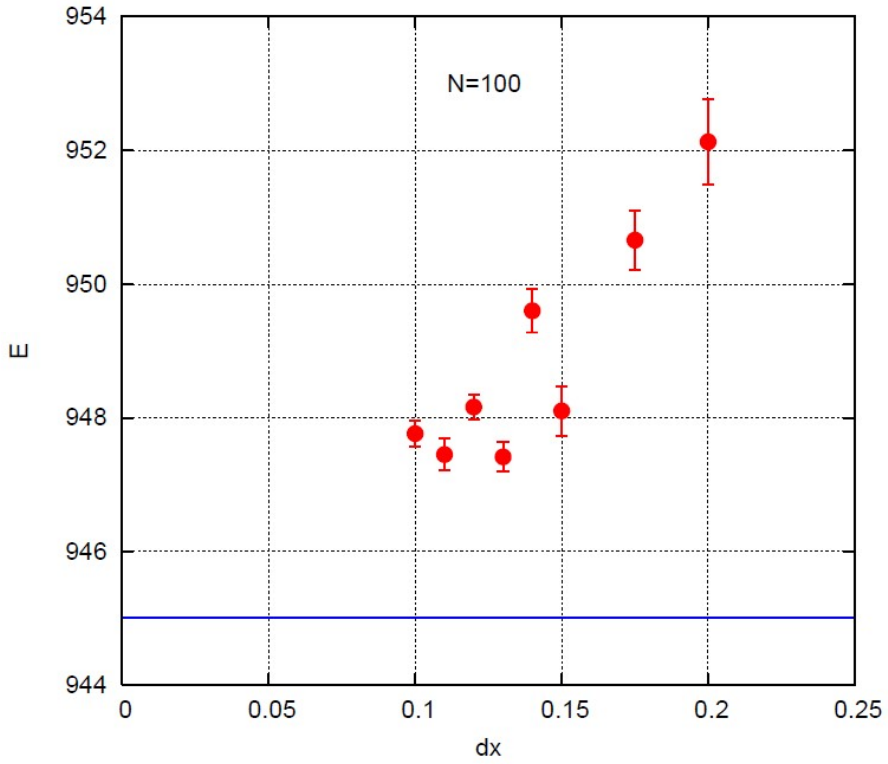
GS energy of N free fermions in HO

For N=80 and 100





Exact energy: 676 and 945

Calculation: 677.2(1), 947.4(2)

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With Coulomb interaction

For the Hamiltonian

$$H = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 + \frac{1}{2}\sum_{i=1}^{N}\mathbf{x}_i^2 + \sum_{i>j}\frac{\lambda}{x_{ij}}$$

the transformed propagator will still give (τ, variational)

$$\Psi_D(\mathbf{x}_1, \mathbf{x}_2 \ldots \mathbf{x}_N) = \det\left|\exp[-\frac{1}{2\tau}(\mathbf{x}_i - \mathbf{s}_j)^2]\right|$$

with $\mathbf{s}_i = \mathbf{x}_i(\tau \to \infty)$ which are stationary points of

$$\frac{d\mathbf{x}_i}{d\tau} = -\nabla_i S(\mathbf{x}_1, \mathbf{x}_2 \ldots, \mathbf{x}_N) \qquad \Psi_B(\mathbf{x}_1, \mathbf{x}_2 \ldots \mathbf{x}_N) = \mathrm{e}^{-S(\mathbf{x}_1, \mathbf{x}_2 \ldots, \mathbf{x}_N)}$$

which are particle positions maximizing the bosonic G.S. wave function, not minimizing the potential energy.

Symmetry-breaking wave functions (I)

The approximate bosonic state wave function

$$S(\mathbf{x}_1, \mathbf{x}_2 \ldots, \mathbf{x}_N) = \frac{1}{2}\sum_{i=1}^{N} \mathbf{x}_i^2 - \sum_{i>j} \frac{\lambda x_{ij}}{1 + b x_{ij}}$$

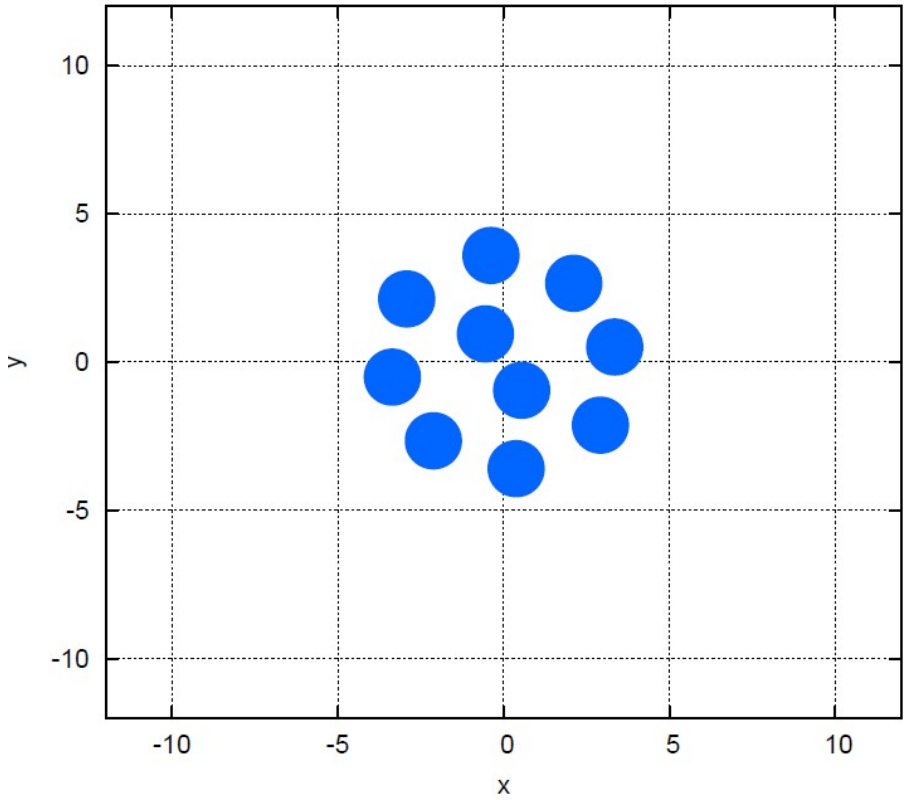
yields trajectory equations

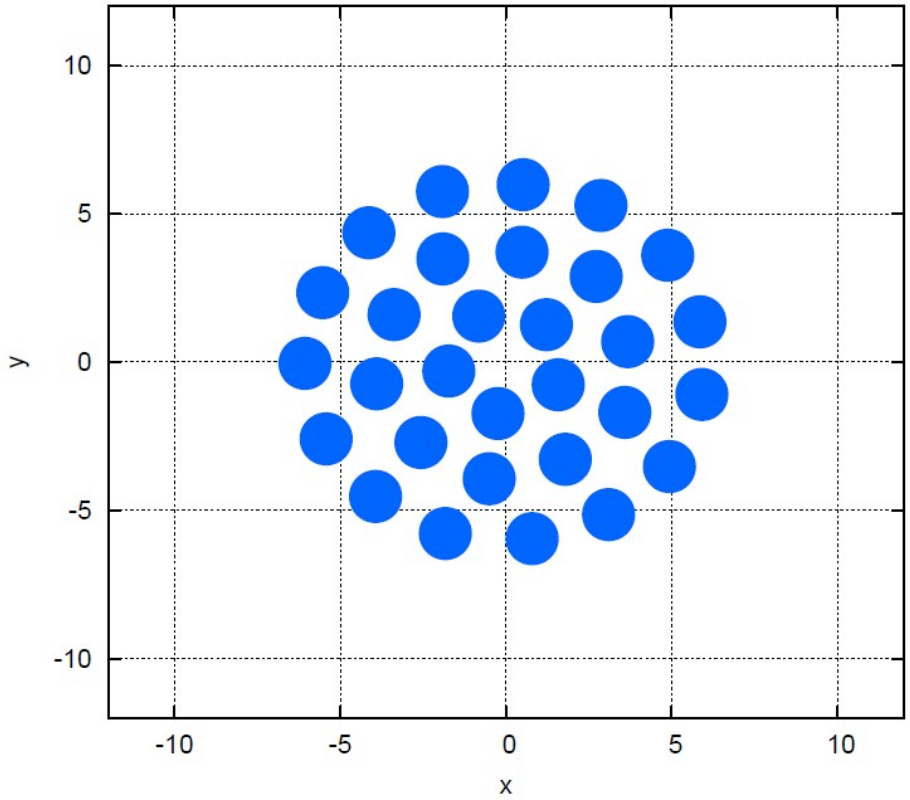
$$\frac{d\mathbf{x}_i}{d\tau} = -\nabla_i S(\mathbf{x}_1, \mathbf{x}_2 \ldots, \mathbf{x}_N) = -\mathbf{x}_i + \sum_{j \neq i} \frac{\lambda \hat{\mathbf{x}}_{ij}}{(1 + b x_{ij})^2}$$

with discrete, distinct, stationary points. The resulting wave function then breaks the rotational symmetry of the original Hamiltonian. (Yannouleas and Landman, 02)

Symmetry-breaking wave functions (II)

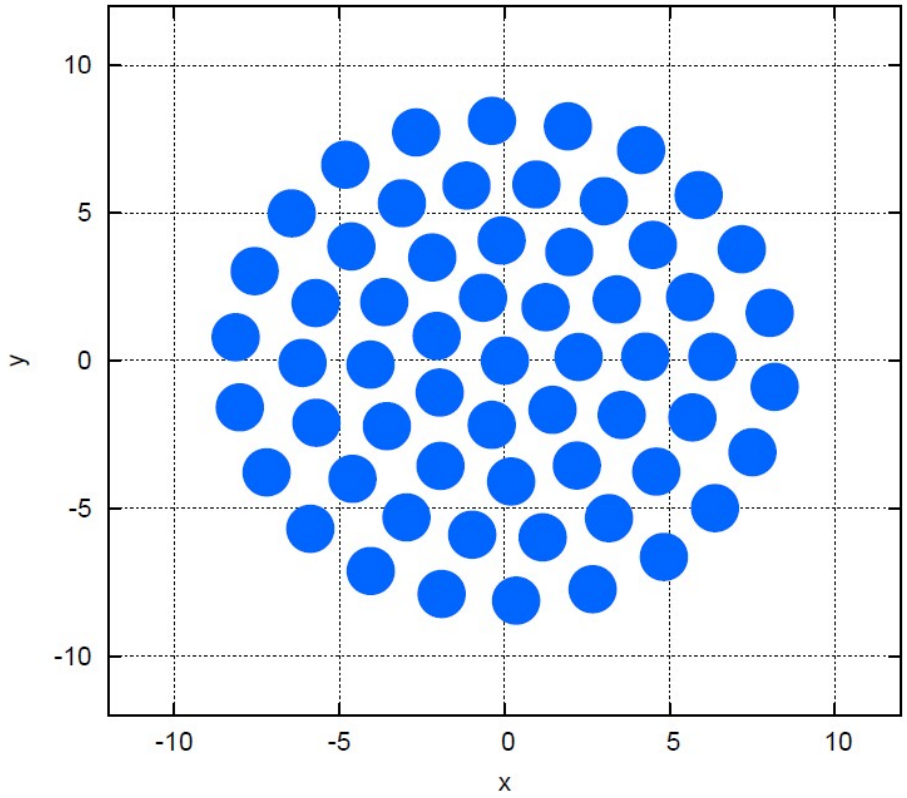
N=10, 30 stationary points for coupling λ =8, Wigner limit, with dot radius = $\sqrt{\tau}$, approximate one-body wave function. Well separated and localize.

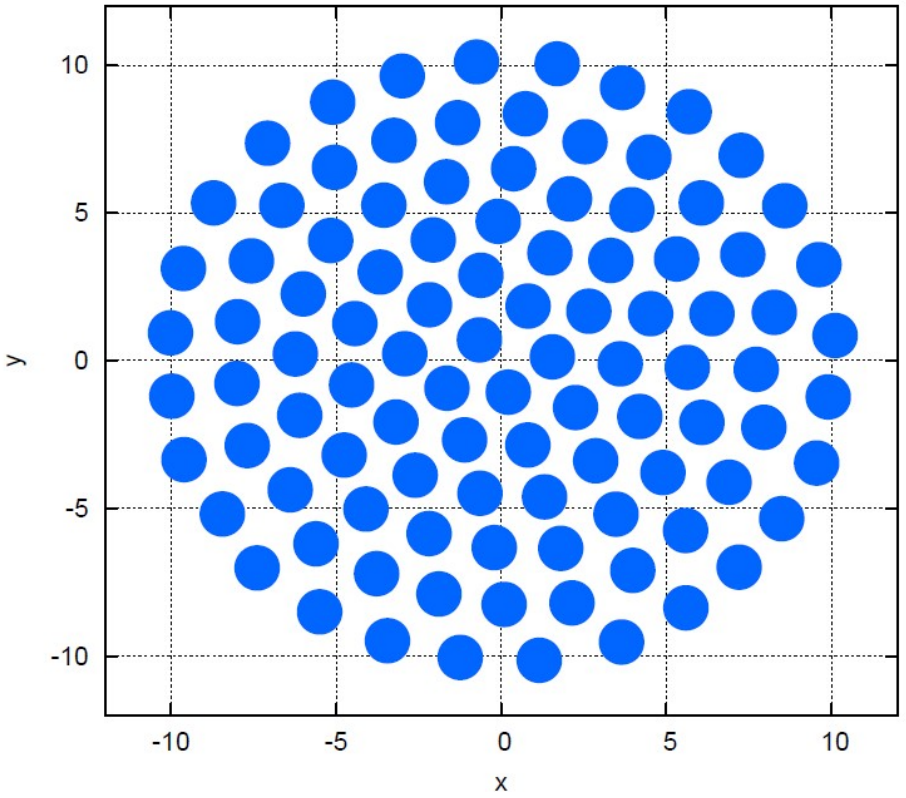




Symmetry-breaking wave functions (III)

N=60, 100 stationary points for coupling λ =8, Wigner limit, with dot radius =$\sqrt{\tau}$, approximate one-body wave function.





Spin-polarized quantum dot energies

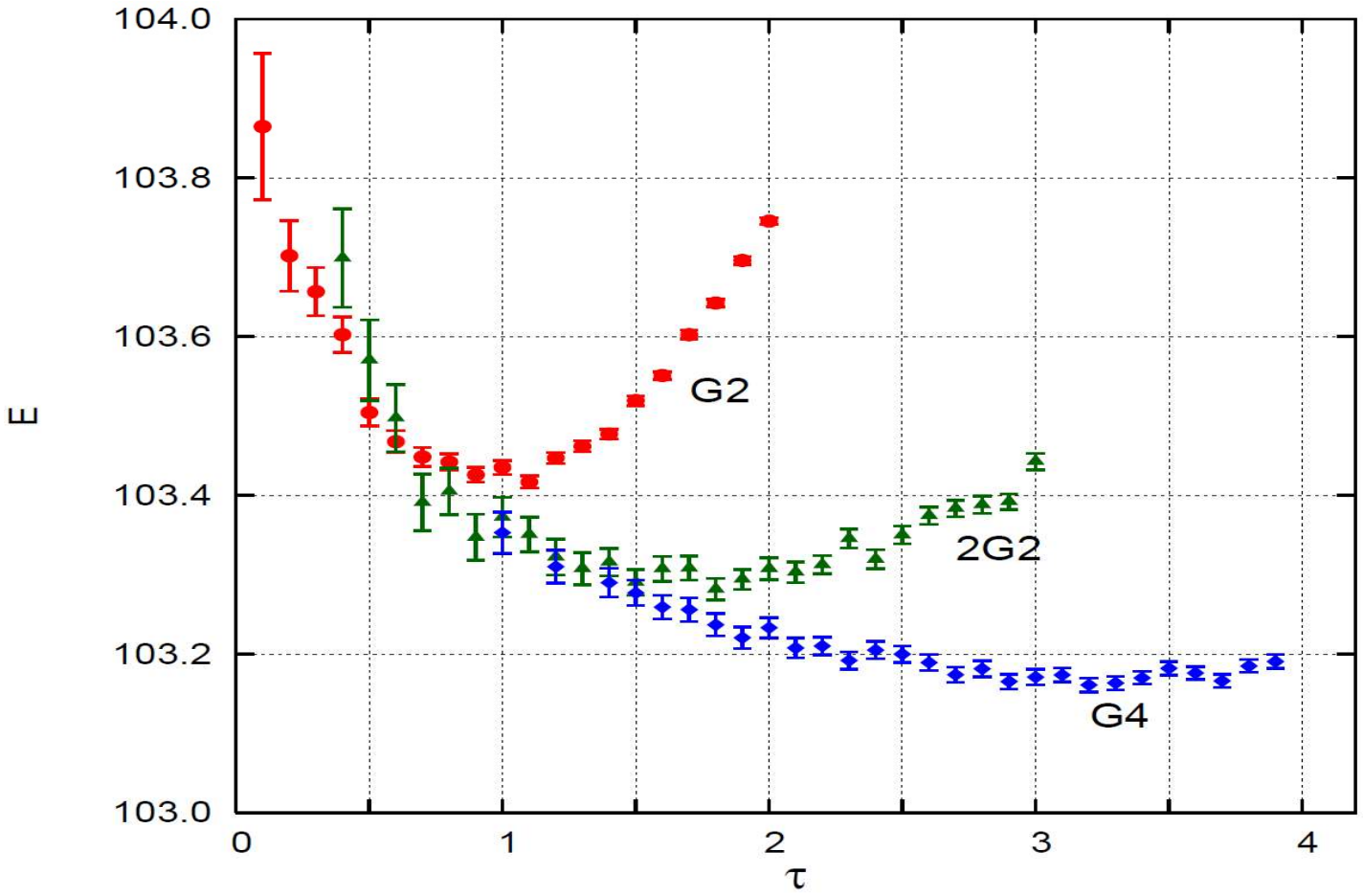
Ground state energy at coupling $\lambda = 8$

N	τ	b	SBWF	B2*	GSPI2	GSPI4	PIMC[4]	CI[16]	DMC[23, 24]
4	0.80	0.60	28.217(3)	28.266(5)	27.927(3)	27.818(5)	27.823(11)	27.828	
6	0.80	0.65	61.257(5)	61.403(7)	60.686(4)	60.475(6)	60.42(2)	60.80	60.3924(2)
8	0.70	0.67	104.21(1)	104.45(1)	103.425(8)	103.161(9)	103.26(5)		103.0464(4)
10	0.70	0.68	156.75(1)	156.77(1)	155.57(1)	155.23(1)			
20	0.65	0.70	537.56(2)	538.07(3)	534.71(5)	534.1(1)			
30	0.60	0.75	1091.60(4)	1091.7(1)	1086.5(1)	1085(1)			
40	0.60	0.74	1795.74(9)	1795.9(1)	1787.9(5)				
50	0.55	0.76	2636.73(6)		2627.0(3)				
60	0.50	0.78	3604.45(7)		3593(1)				
80	0.50	0.78	5893.2(3)						
100	0.45	0.80	8618.1(3)						

Ground state PIMC

Starting from SBWF, can evolve closer to the exact ground state via

$$E_0 = \lim_{\tau\to\infty} \frac{\int d\mathbf{X}' d\mathbf{X}_1 d\mathbf{X} \Psi_D(\mathbf{X}') G(\mathbf{X}', \mathbf{X}_1; \tau) HG(\mathbf{X}_1, \mathbf{X}; \tau) \Psi_D(\mathbf{X})}{\int d\mathbf{X}' d\mathbf{X}_1 d\mathbf{X} \Psi_D(\mathbf{X}') G(\mathbf{X}', \mathbf{X}_1; \tau) G(\mathbf{X}_1, \mathbf{X}; \tau) \Psi_D(\mathbf{X})}$$



Upper bound property only with the use of the Hamiltonian estimator at the center of the path integral.

Complications with spin-balanced quantum dots I: frustrations

For N=6, two stationary configurations (0,6) or (1,5),

Generally, (1,5) is lower in energy.

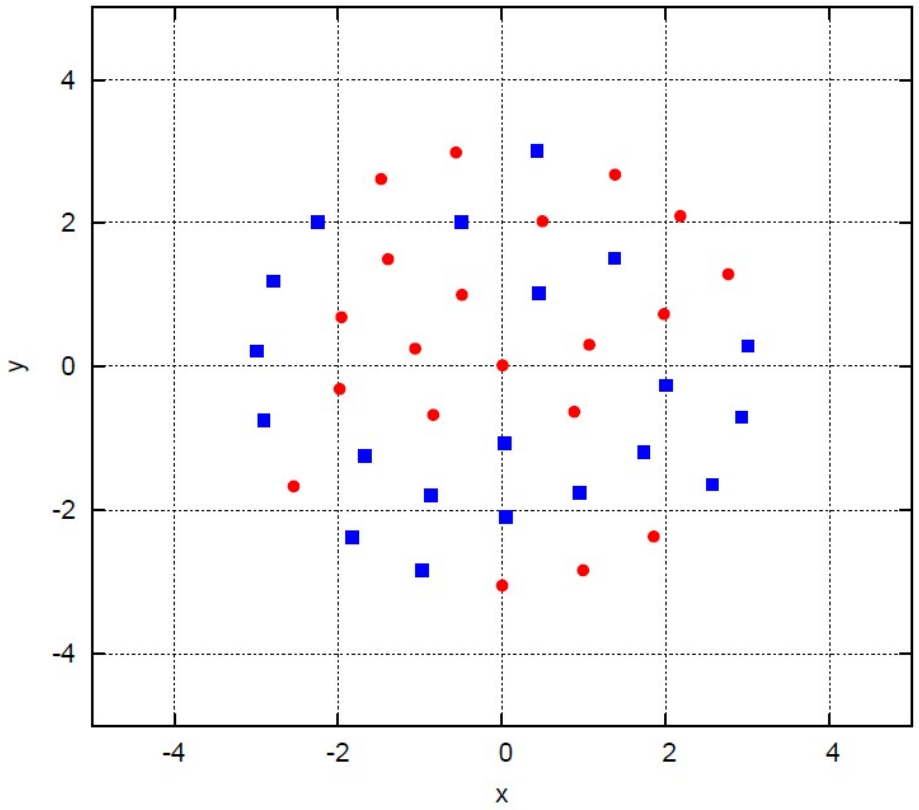
For polarized spin, using (1,5) is fine.

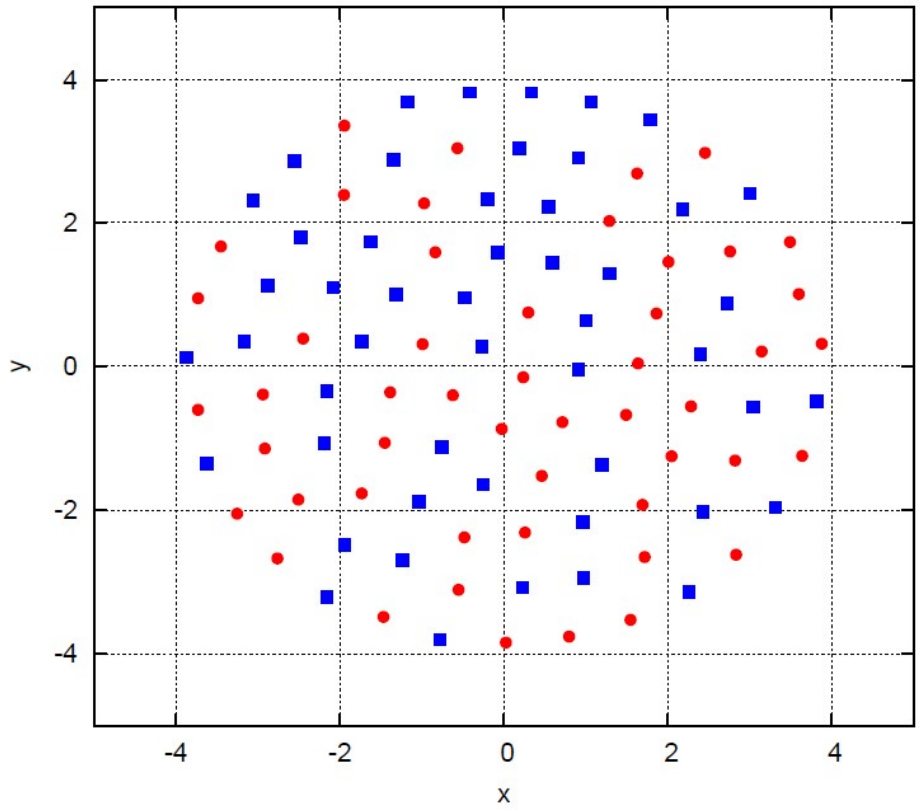
For balanced spin, (1,5) causes frustration, and breaks the symmetry between spin up and spin down electrons.

All PIMC calculations for spin-balanced quantum dots converge slowly with τ, probably due to frustration.

Complications with spin-balanced quantum dots II: spin discontinuity

For N=40 and 100 stationary points, how should one chose which 20 or 50 are to be spin up, or down? Below, randomly assigned.





Spin-balanced quantum dot energies

The symmetry-breaking wave function still gives reasonable energy, but ground state path integral results are poor due to large τ.

PIMC= Kylanpaa and Rasanen;

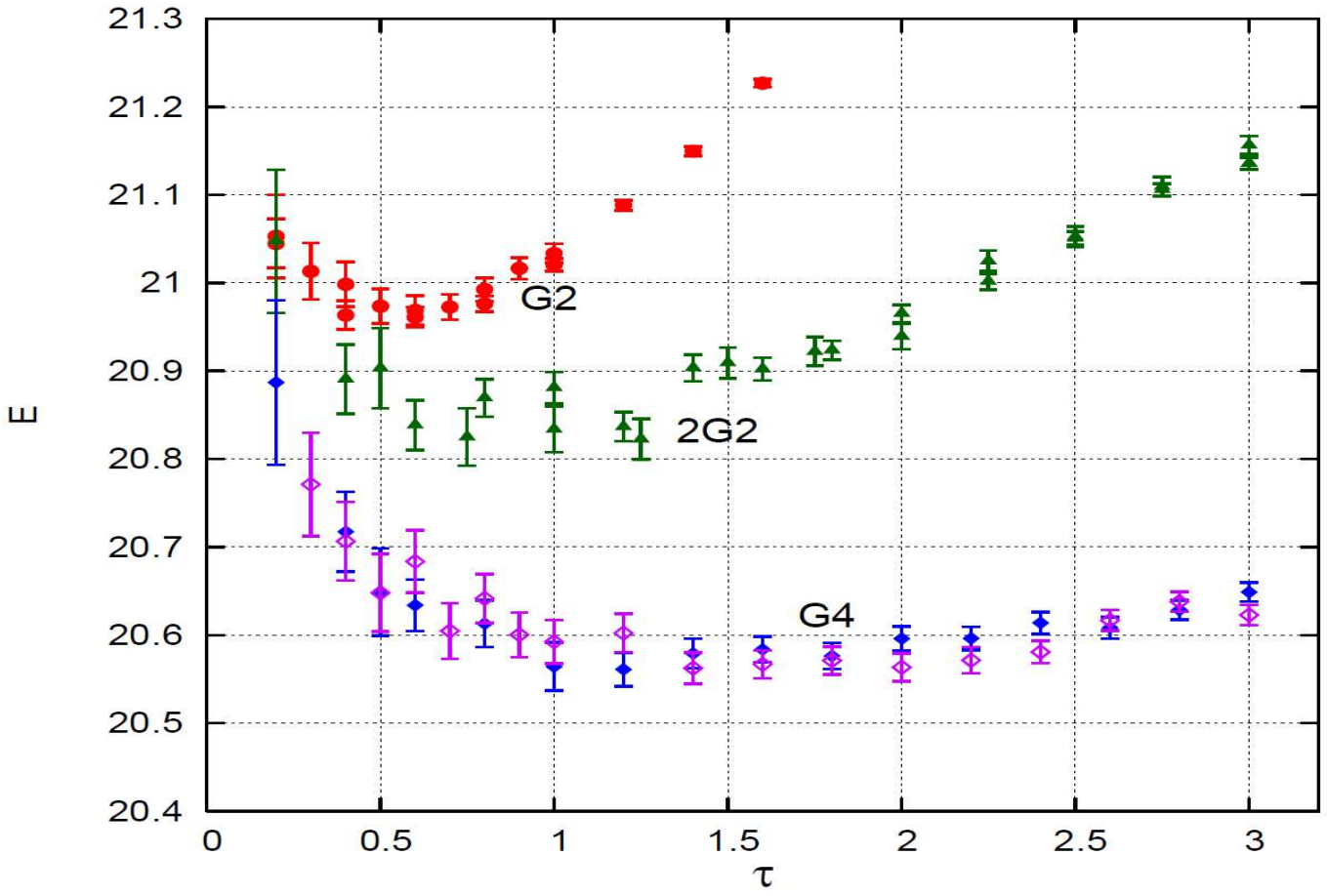
DMC=Lohne, Hagen, Hjorth-Jensen, Kvaal, and Pederiva,

TABLE II. Ground state energies $E_0/\hbar\omega$ of N *spin-balanced* electrons at coupling at $\lambda = 1$.

N	τ	b	SBWF	GSPI2	GSPI4	PIMC[26]	CCSD(T)[27]	DMC[27]
6	1.3	0.70	20.815(5)	20.96(1)	20.56(1)	20.1063(8)	20.1570	20.1597(2)
12	1.2	0.70	67.856(7)		67.2(1)	65.488(5)	65.6886	65.700(1)
20	1.3	0.70	159.62(3)			155.41(2)	155.8571	155.868(6)
40	1.3	0.70	509.34(3)			498.8(4)		
60	1.4	0.80	998.33(6)			987.9(5)		
80	1.6	0.90	1612.8(2)					
100	1.7	1.00	2338.0(3)					

Ground state PIMC for spin-balanced quantum dots

Cannot produce the trial energy with (0,6) configuration at small τ, because (0,6) is unstable. G4 still lowers the energy, but not close enough to the exact ground state energy.



Upper bound property only with the use of the Hamiltonian estimator at the center of the path integral.

Conclusions

1) The use of similarity transformed propagators naturally give rises to symmetry-breaking wave functions (but only for harmonic confinement).
2) The stationary points are positions that maximize the bosonic ground state wave function rather than just minimize the potential energy.
3) The use of SBWF enables one to compute the ground state energy of the largest spin-polarized 2D quantum dot to date.
4) The use of SBWF gives insight into the frustration problem in spin-balanced quantum dots.