

Phase of the Many-Body Wavefunction

UNDER CONSTRUCTION!

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Real vs complex

Why is QMC done with real trial functions?

- For non-degenerate states, they can be made real
- Real arithmetic is faster
- Real wfs map into probabilities easier.

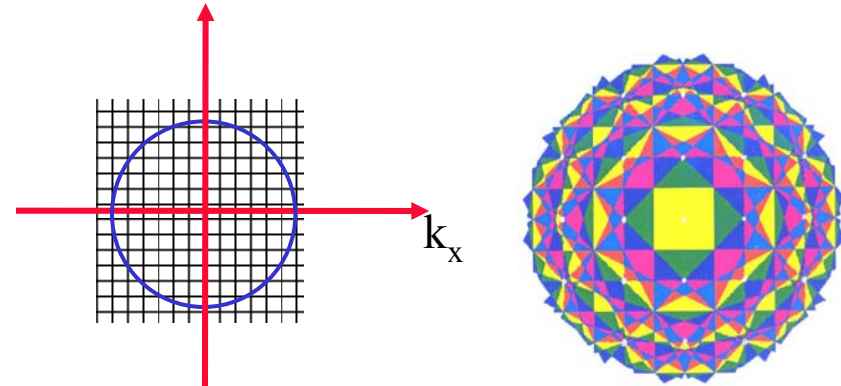
- But QM is usually done with complex wavefunctions!
- Especially if you want pure states: i.e. momentum, spin
- Magnetic fields (i.e. quantum hall effect), vortices require complex wf.
- Twisted boundary conditions.

Twist averaged boundary conditions

- In periodic boundary conditions (Γ point), the wavefunction is periodic \Rightarrow Large finite size effects for metals because of shell effects.
- In twist averaged BC we use an arbitrary phase θ as $r \rightarrow r+L$
- If one integrates over all phases the momentum distribution changes from a lattice of k-vectors to a fermi sea.
- Much smaller finite size effects
- States are non-degenerate
- BUT COMPLEX

$$\varphi = e^{ikr}$$

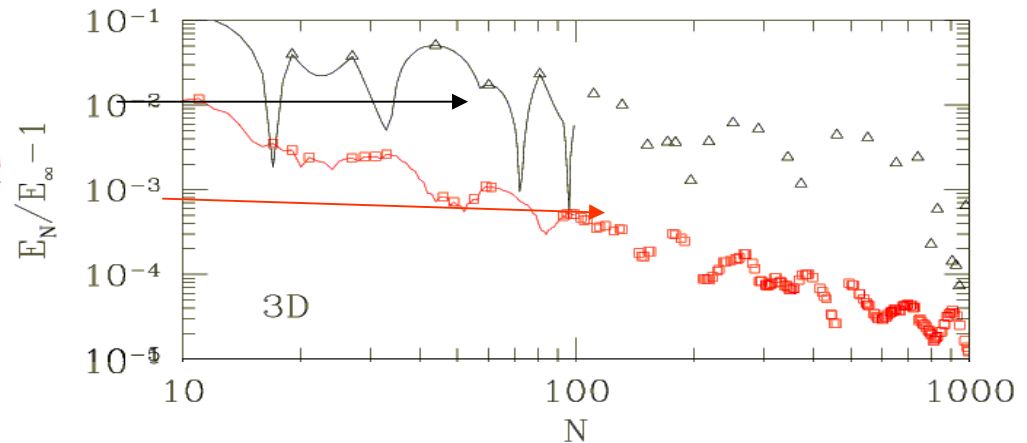
$$kL = 2\pi n + \theta$$



$$\Psi(x + L) = e^{i\theta} \Psi(x)$$

$$\bar{A} = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} d^3\theta \langle \Psi_{\theta} A \Psi_{\theta} \rangle$$

Error with PBC
Error with TABC



Nodal Properties

If we know the sign of the exact wavefunction (the nodes), we can solve the fermion problem with the fixed-node method.

- If $\phi(\mathbf{R})$ is real, nodes are $\phi(\mathbf{R})=0$ where \mathbf{R} is the $3N$ dimensional vector.
- Nodes are a $3N-1$ dimensional surface. (Do not confuse with single particle orbital nodes!)
- Coincidence points $\mathbf{r}_i = \mathbf{r}_j$ are $3N-3$ dimensional hyper-planes
- In 1 spatial dimension these “points” exhaust the nodes: *fermion problem is easy to solve in 1D* with the “no crossing rule.”
- Coincidence points (and other symmetries) only constrain nodes in higher dimensions, they do not determine them.
- The nodal surfaces define nodal volumes. **How many nodal volumes are there? Conjecture:** there are typically only 2 different volumes (+ and -) except in 1D. (but only demonstrated for free particles.)

Nodal Picture: 2d slice thru 322d space

Free electron
Other electrons

- Nodes pass thru their positions
- Divides space into 2 regions
- Wavelength given by interparticle spacing

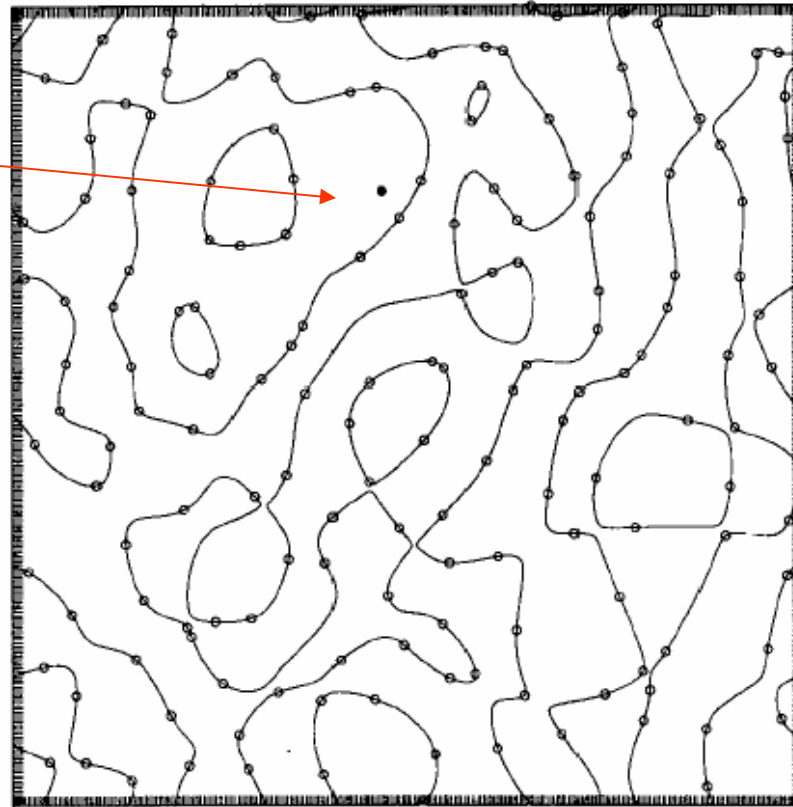
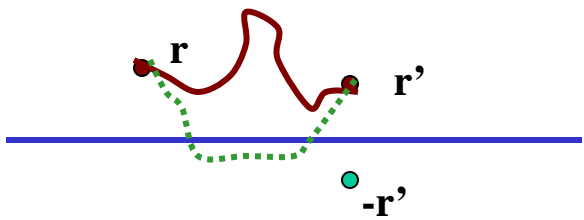


Fig. 3. A 2D cross section of the ground-state wave function of 161 free (polarized) fermions in a periodic square. All 161 particle positions were sampled using variational Monte Carlo from $\phi(R)^2$. The filled circle indicates the original position of the first particle. The other 160 particles are fixed at positions indicated by the open circles, and nodes of the wave function as a function of the position of the first particle are plotted. The resolution of the contouring program is approximately half of the fine scale shown around the border of the plot.

Nodal action (cross-recross)

J. B. Anderson 1977

- “Primitive Rule:” simply reject paths if they cross a node.
- Will lead to an error proportional to $\sqrt{\lambda\tau} / r_{nn}$
- Improved nodal action: solve for a particle next to a planar node. Use method familiar from electrostatics, the method of images:

$$\rho(r', r; t) = e^{-\frac{(r-r')^2}{4\lambda\tau}} - e^{-\frac{(r-r^*)^2}{4\lambda\tau}} \quad r^* = -r'$$


$$\delta S(r', r; t) = -\ln\left(1 - e^{-\frac{dd'}{\lambda\tau}}\right) \quad d = \text{distance to node} \approx \left|\nabla \ln(\rho(R, R'; \tau))\right|^{-1}$$

- Determine nodal distance using “Newton estimate.”
- As paths approach within a thermal wavelength of the node, we get a repulsion, to account for the probability that a path could have crossed and recrossed within τ .
- How do we change this in going to complex trial functions?

Generalization of Nodes

How does the the real machinery generalize to complex wfs?

Can we generalize the concept of nodal surfaces?

For insulators we expect that electrons are localized (quantum mechanics is “nearsighted”) so boundary conditions should not matter.

How about metals?

Fixed-Phase method

Ortiz, Martin, DMC 1993

- Generalize the FN method to complex trial functions: $\Psi(R) = e^{-U(R)}$
- Since the Hamiltonian is Hermitian, the variational energy is real:

$$E_V = \frac{\int dR e^{-2\Re U(R)} \left[V(R) + \lambda \nabla^2 U(R) - \lambda [\Re \nabla U(R)]^2 + \lambda [\Im \nabla U(R)]^2 \right]}{\int dR e^{-2\Re U(R)}}$$

- Only one term in the energy depends on the phase of the wavefunction.
- If we **fix the phase**, then we add this \sum term to the potential energy.
- In a magnetic field we get also the vector potential.

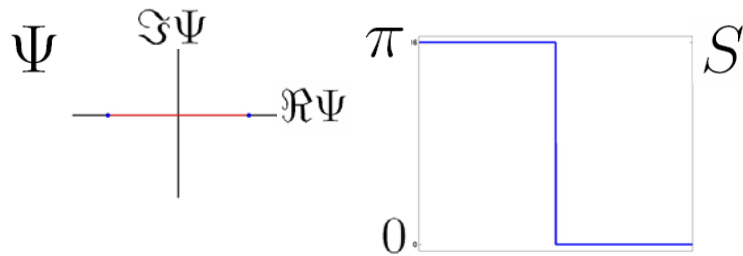
$$\text{effective potential} = V(R) + \sum \lambda_i \left[A(r_i) + \Im \nabla_i U(R) \right]^2$$

- We can now do VMC or DMC and get upper bounds as before.
- The imaginary part of the local energy will not be zero unless the right phase is used: continuity equation.

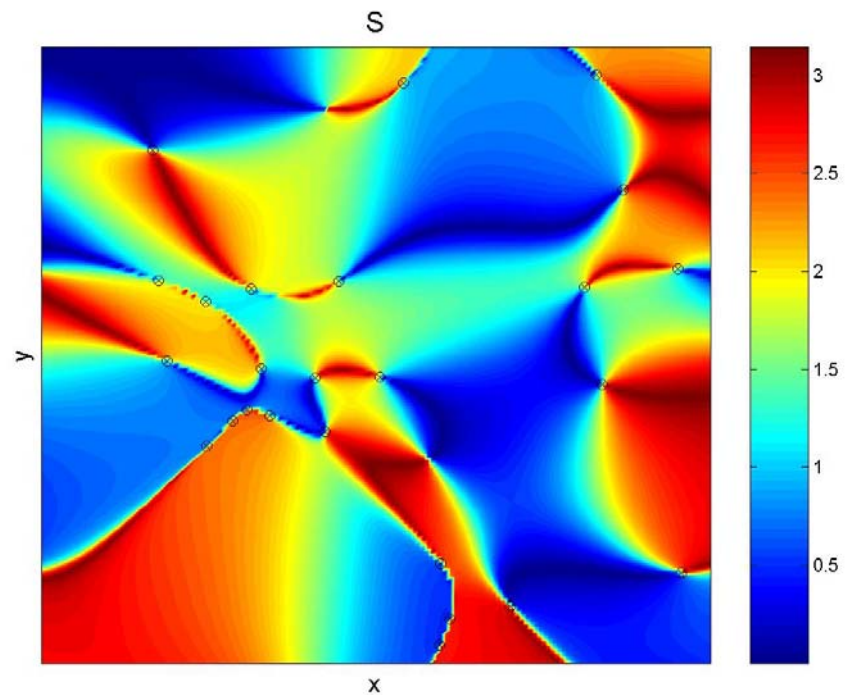
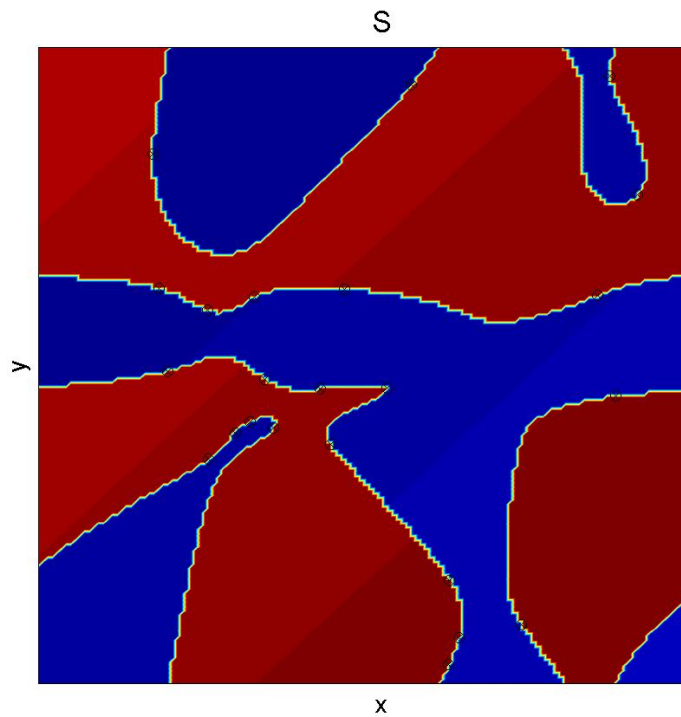
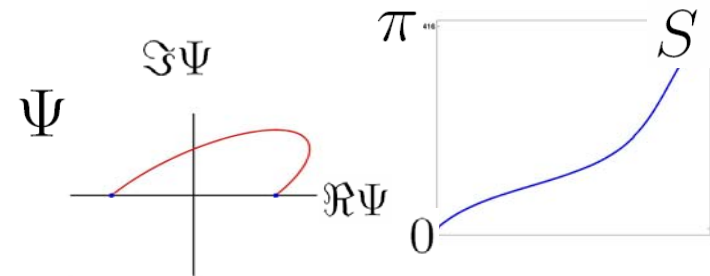
$$\sum_i \nabla_i \left[|\Psi|^2 \{ \nabla_i S + A \} \right] = 0$$

The nodes and phases under interchange

Real or Real-like Wavefunction



Complex Wavefunction



Phase of density matrix

- Lin thesis (2001)
- Step structure reappears!

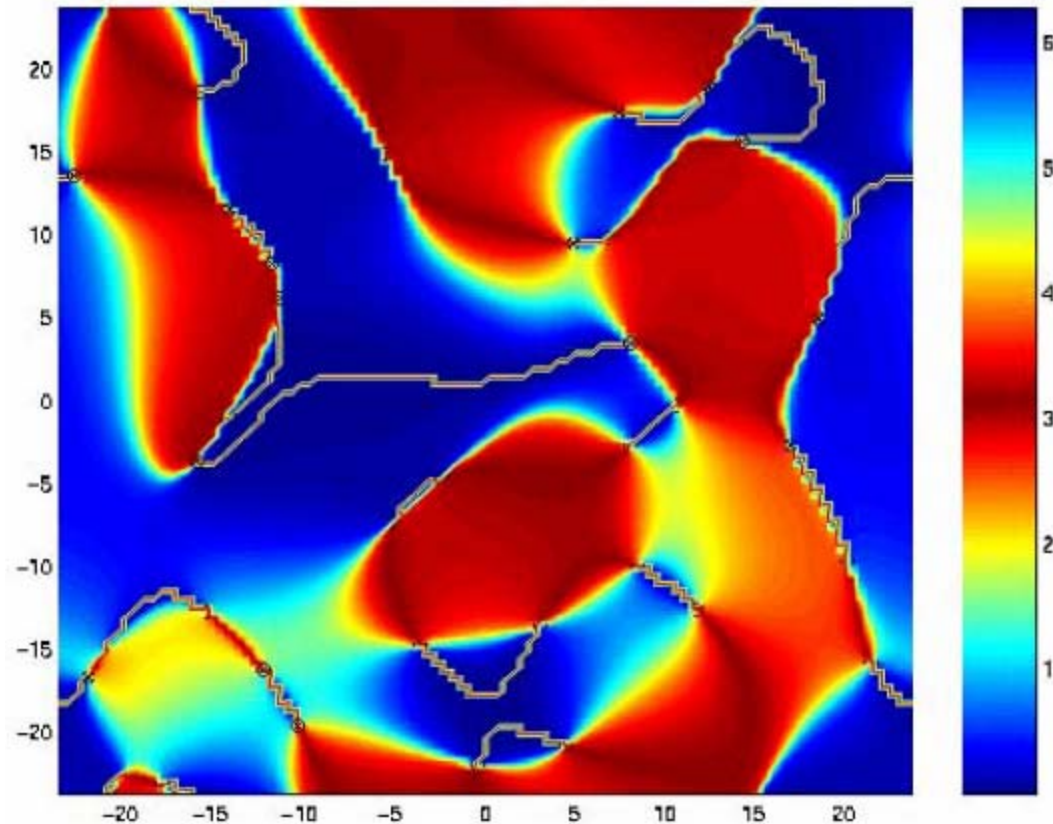
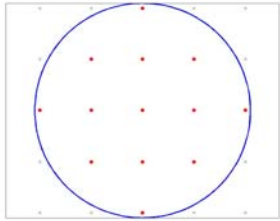


Figure 2.3: 2D phase contour of the density matrix of 21 free spinless fermion in a periodic box. The phase here is represented by colors, with blue corresponding to 0 or 2π and red corresponding to π , respectively. The plot is generated by moving one of the particles while keeping the other 20 fixed. The open circles are the fixed positions of 20 fermions; The contour lines are places where \mathcal{S} changes by 2π , and have no significance. The temperature is $T = 0.2K$ (the Fermi temperature for this system is $T_\kappa \simeq 7K$).

Two Model Systems

Free Electrons: Metal



$$V = 0$$

$$\phi_i(\mathbf{r}_j) \propto e^{i\mathbf{k}_i \cdot \mathbf{r}_j}$$

Model Insulator

$$V = V_0 \left(\cos \frac{2\pi}{a} x + \cos \frac{2\pi}{a} y \right)$$

$$\phi_i(\mathbf{r}_j) \propto \sum_{\ell} c_{i\ell} e^{i\mathbf{k}_{\ell} \cdot \mathbf{r}_j}$$

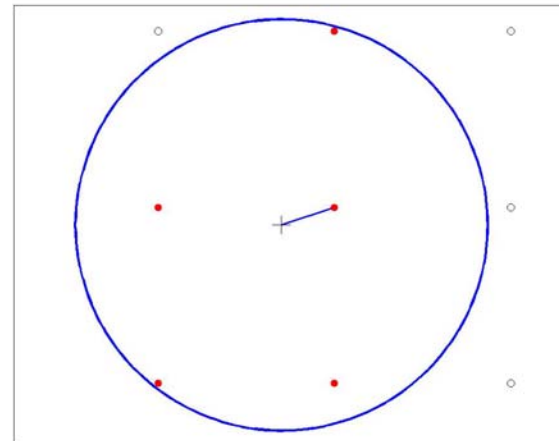
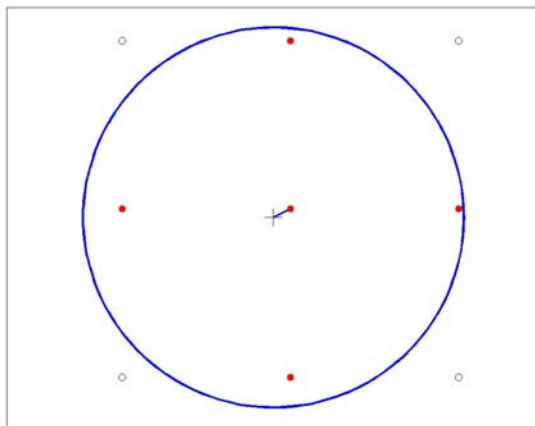
$$\Psi = \text{Det} (\phi_i(\mathbf{r}_j))$$

Is the phase of the wf different in these cases?

Band insulator vs. metal?

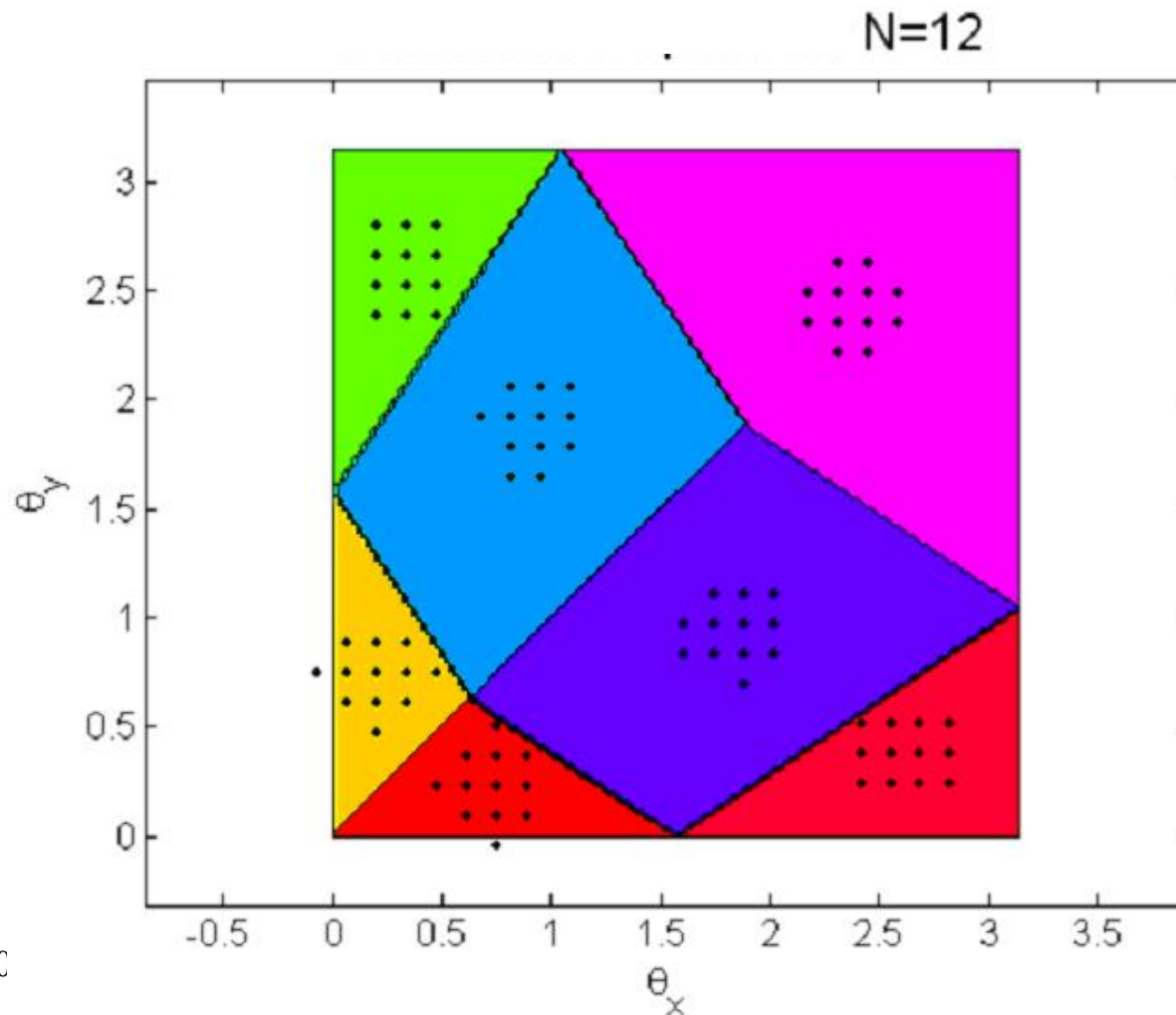
Pockets for free electrons

- Set of occupied k-points changes with θ $\mathbf{k} = (2\pi\mathbf{n} + \theta)/L$
- A pocket is the set θ with the same integers
- Boundaries of pockets are lines (2d) or planes(3d) for free particles
- Boundaries could change with interacting trial functions
- We only need one point in each pocket (Holtzmann) to do twist averaging



Real-Like Ψ : Free Electrons

If the k-points have inversion symmetry, then the wf can be made real-like inside the pocket.



Find average momentum and subtract out:

$$\vec{P} = \frac{1}{N} \sum_i k_i \quad \tilde{k}_i \equiv k_i - \vec{P}$$

A state is paired if both \tilde{k}_i and $-\tilde{k}_i$ are occupied (or if $\tilde{k}_i=0$).

Multiply the Slater matrix by

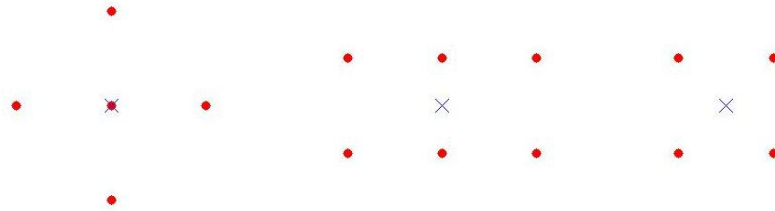
$$\begin{pmatrix} 1 & 1 & 0 & 0 \\ -i & i & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The new matrix is $\exp\left[iP\left(\sum_i r_i\right)\right] M_{real}$

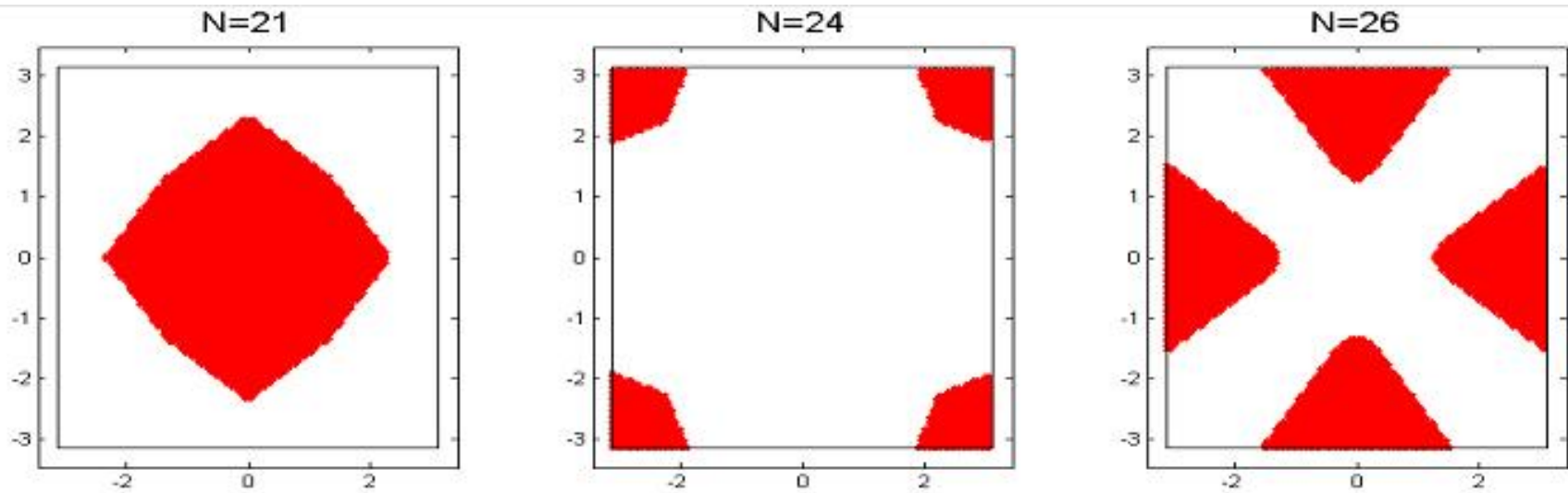
$$\nabla S(R) = P$$

3 classes of real-like Ψ in 2d

- Phase will jump by π within real-like pockets
- Centers must be around $\theta_i = \pi m_i$, $m_i = -1, 0, 1$

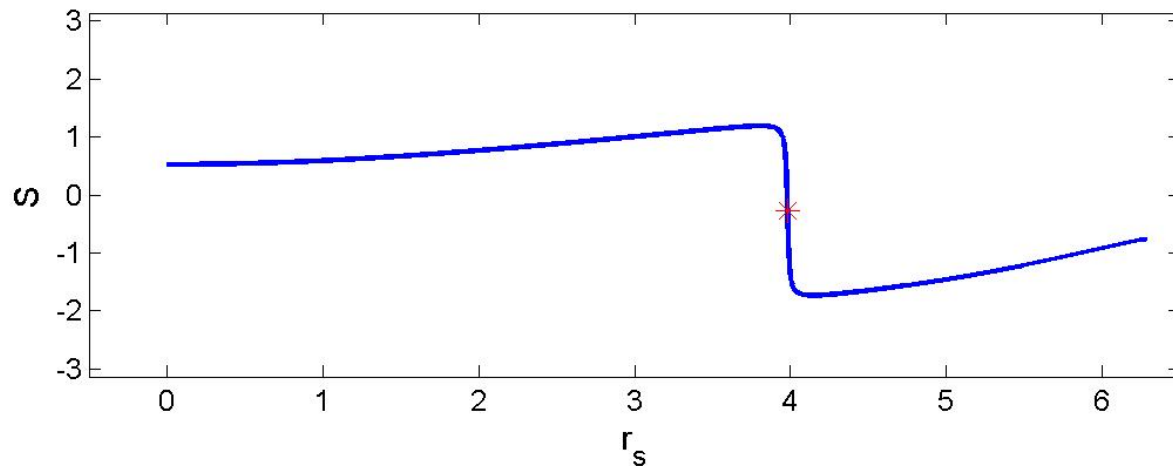
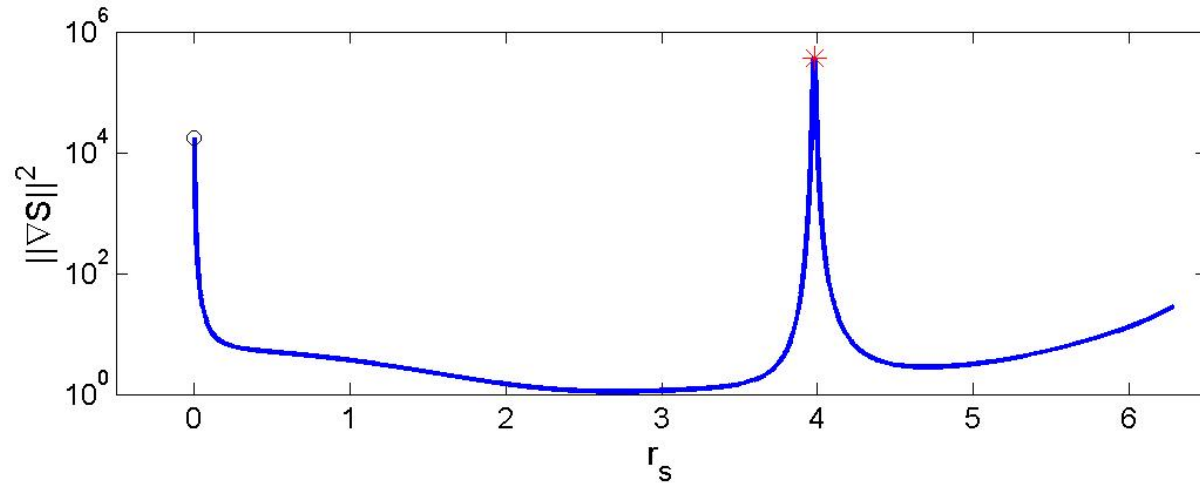


- Real pockets become less frequent as N gets large.



Back to general case. How does the wavefunction change when an electron wraps around the box?

Coincident point has jump in phase but also other points.



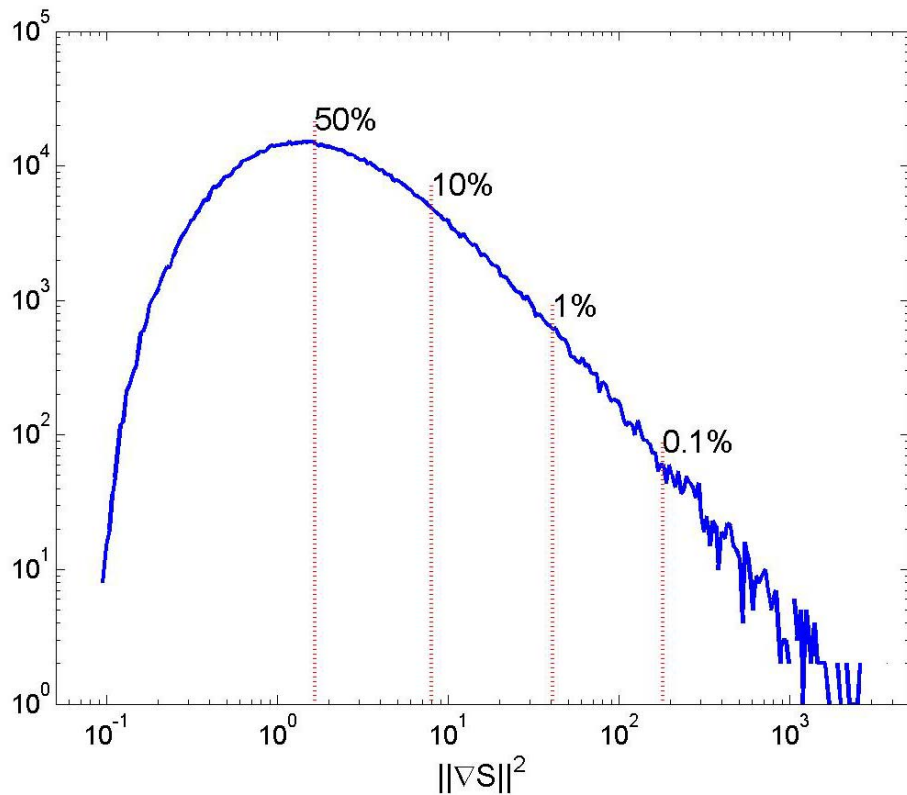
We measure of the 'steepness' of S with $G \equiv |\nabla S|^2$

Distribution of G from VMC simulation:

Free Electrons

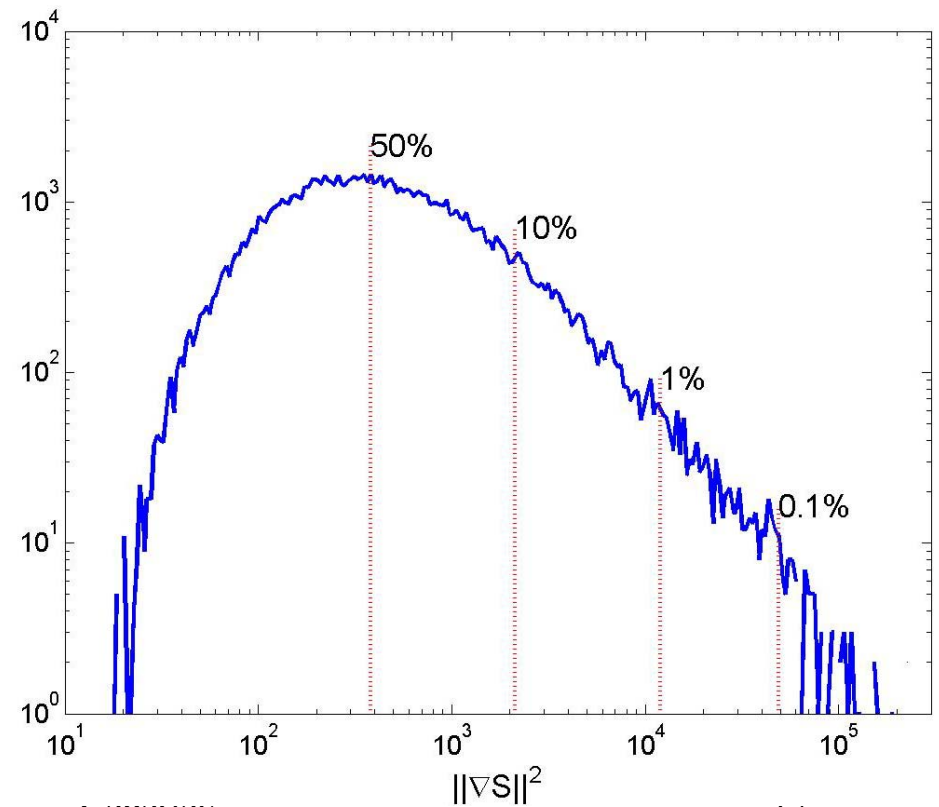
$P(G)$

Model Insulator



9/11/2007

CECAM07



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$$\mathcal{P}(G) \xrightarrow{G \rightarrow \infty} \alpha G^{-\nu} \quad G \equiv \|\nabla S\|^2$$

Free Electrons

$$\nu \approx 1.45 - 1.66$$

Model Insulator

$$\nu \approx .9 - 1.1$$

$$\langle G^n \rangle = \int dG \mathcal{P}(G) G^n = \infty \quad , \quad n \geq 1$$

Power law tail determines analytical convergence of moments.

First moment should exist, but higher moments do not:
possible variance problem.

What is the cause of the divergence?

Look at co-incident points (in 2d)

$$\nabla S = \Im \Psi^{-1} \nabla \Psi \quad r_s \text{ is inter-electron distance}$$

$$\Psi \propto r_s \Rightarrow \|\nabla S\|^2 \propto r_s^{-2}$$

$$\mathcal{P}(G) = \int d\mathbf{R} |\psi|^2 \delta(G - \|\nabla_{\mathbf{R}} S\|^2)$$

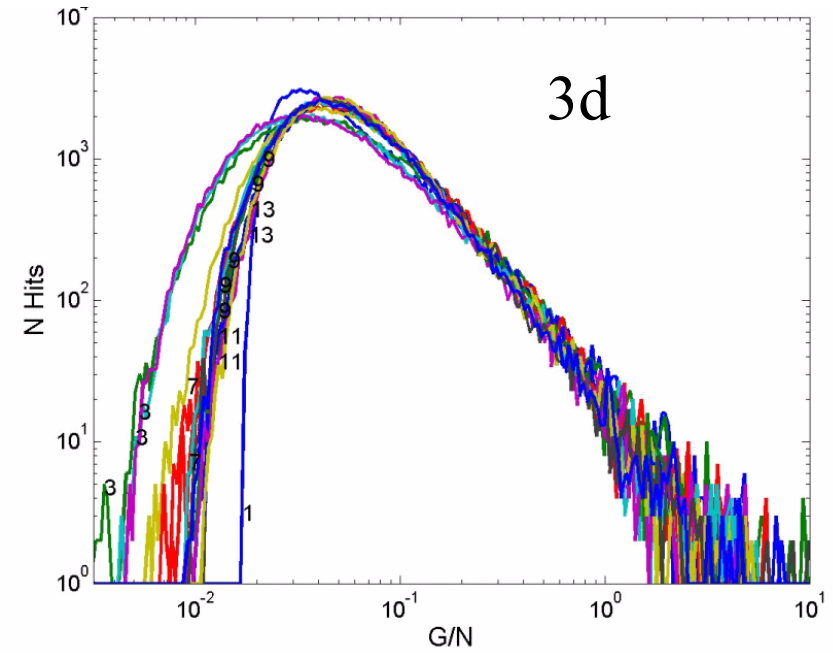
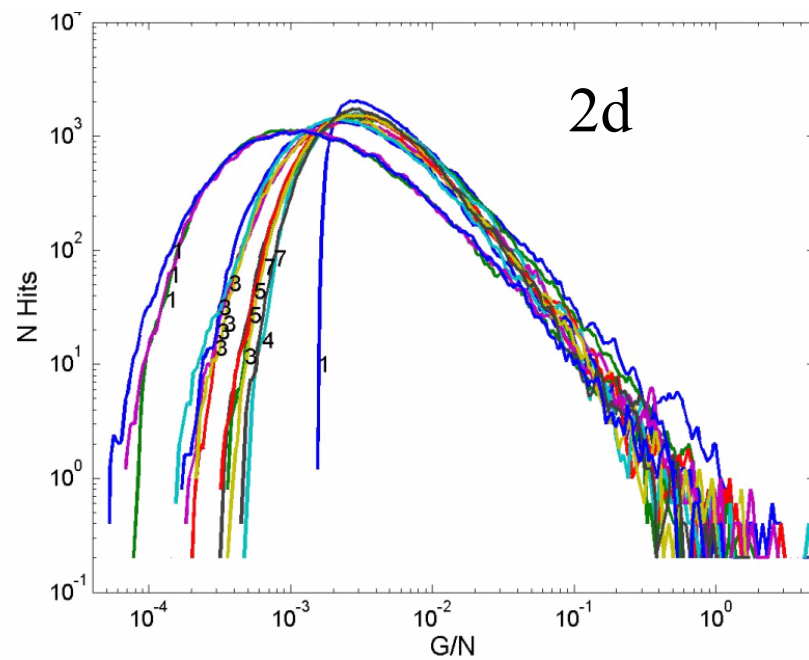
$$\approx \int dr_s d\phi r_s |\psi|^2 \delta(G - \|\nabla_{\mathbf{r}} S\|^2)$$

$$\propto \int dr_s d\phi a(\phi) r_s^3 G^{-\frac{3}{2}} \delta\left(r_s - b(\phi) G^{-\frac{1}{2}}\right)$$

$$\propto G^{-3}$$

Wrong exponent \rightarrow Must be quasi-nodes not points

Distribution of G values for free electrons



- Shows strong dependence on number of unpaired states for small G. (flatness depends on twist angles)
- Large values of G show an invariant distribution as N changes.

Implications for action

- Real like pockets: there we can use actions developed for real wavefunctions.
- Perhaps for large N everywhere.
- Small N patches: still need to consider interpolation in complex plane
- What about for intermediate actions.
- Important to use both phase and gradient information

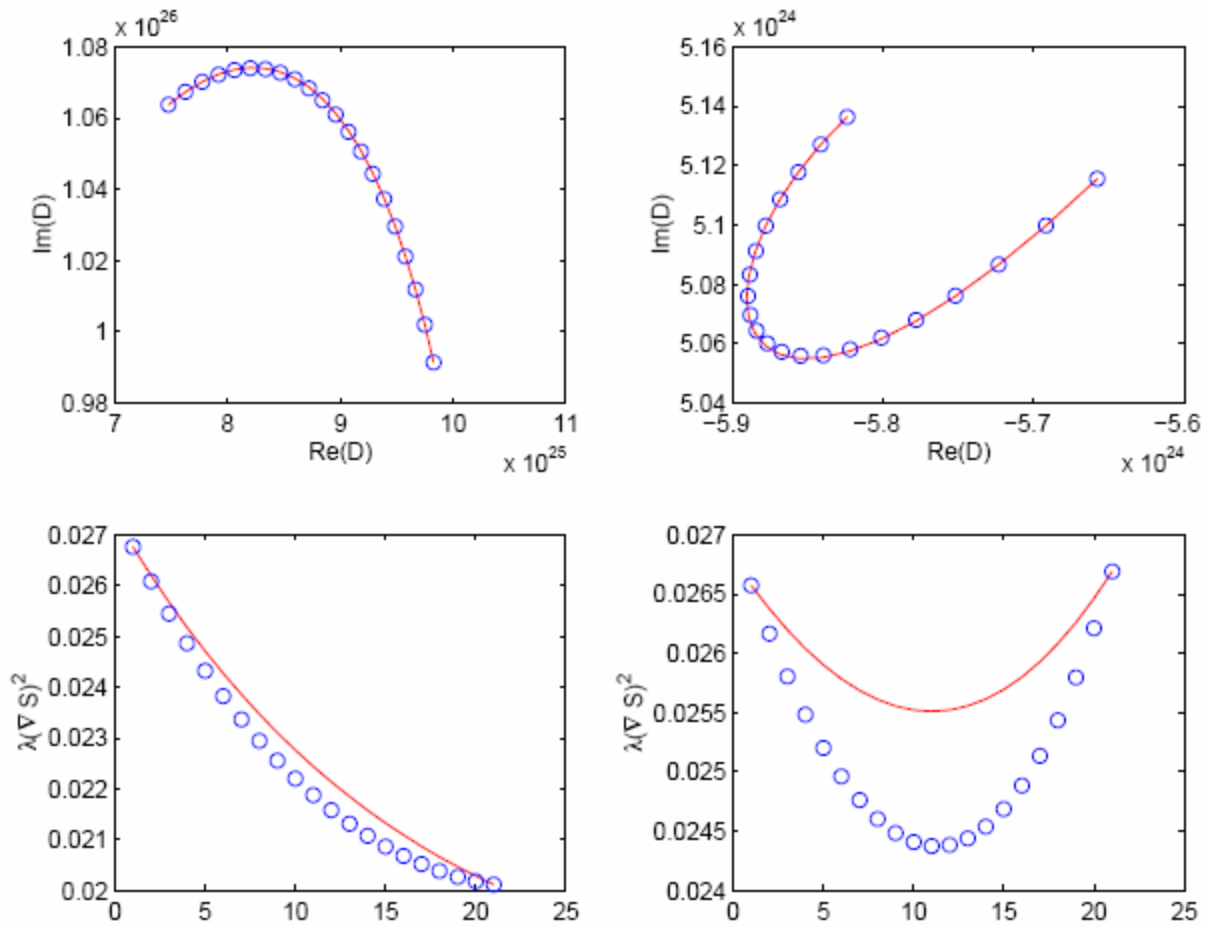
Lin-Ceperley complex action

Lin thesis, UIUC (2001).

- Consider a move from R to R' $\left\langle \exp \left[-\int_0^\tau dt |\nabla S(R_t)|^2 \right] \right\rangle$
- Average is over brownian bridges
- Consider the straight line path: $R_t = R + (t/\tau)(R' - R)$
- To evaluate $S(R)$ make cubic spline interpolation of $\psi(R_t)$ using $\psi(R), \psi(R'), \nabla\psi(R) \cdot [R - R'], \nabla\psi(R') \cdot [R - R']$
- Finally, perform the integral numerically.
- Test for electron gas $N=54$:

	I	II
δ_{end}	-0.084 ± 2.22	0.0066 ± 0.065
δ_{cubic}	0.0012 ± 0.65	0.0003 ± 0.028

Lin-Ceperley action



Conclusions

- Free electrons exhibit real-like wavefunctions in θ space patches centered at $\theta = (0, 0), (0, \pm\pi), (\pm\pi, 0), (\pm\pi, \pm\pi)$
- Ψ becomes real-like in the thermodynamic limit \rightarrow boundary conditions don't matter.
- Why and how does this happen?
 - Perturbation argument?
 - Bands fold into the Γ point.
 - Only points at fermi surface are unpaired. The number scale to zero.
- $\mathcal{P}(\|\nabla S\|^2)$ has divergent moments
 - Likely due to quasi-nodal surface
 - Need to use care with quantities related to $\|\nabla S\|^2$
- Connection to nodal topology?
- How to construct accurate actions?

Chiesa, S., D. M. Ceperley, R. M. Martin and M. Holzmann,
[Finite Size Error in Many-body Simulations with Long-Ranged Interactions](#),

Phys. Rev. Letts. **97**, 076404 (2006); cond-mat/0605004.

- What is the finite size error in the potential energy?
- Easiest to understand in fourier space:

$$V_N = \sum_k \frac{4\pi}{k^2} (S_k^N - 1) \quad V_\infty = \int dk \frac{4\pi}{k^2} (S_k^\infty - 1)$$

assume $S_k^N = S_k^\infty$

$$T_N = \sum_k k^2 u_k (S_k^N - 1) + \text{single particle term (TABC)}$$

- FSE effects come from changing sum to integral
- Key region is at $k=0$. Other important points are for $k=k_F, 2k_F$
- Make an interpolation formula to go between computed values
E.g. $S(k)=ak^2+bk^3+\dots$ Based on analytic and QMC

Further Improvements for e gas (Markus)

- Go beyond $S(k)=k^2$
- As $r_s \rightarrow 0$ $S(k) \rightarrow k$

action energy per particle is given by

$$\delta V = \frac{e^2}{4\pi^2} \int_{-\pi/L}^{\pi/L} d^3k \frac{S(k)}{k^2}$$

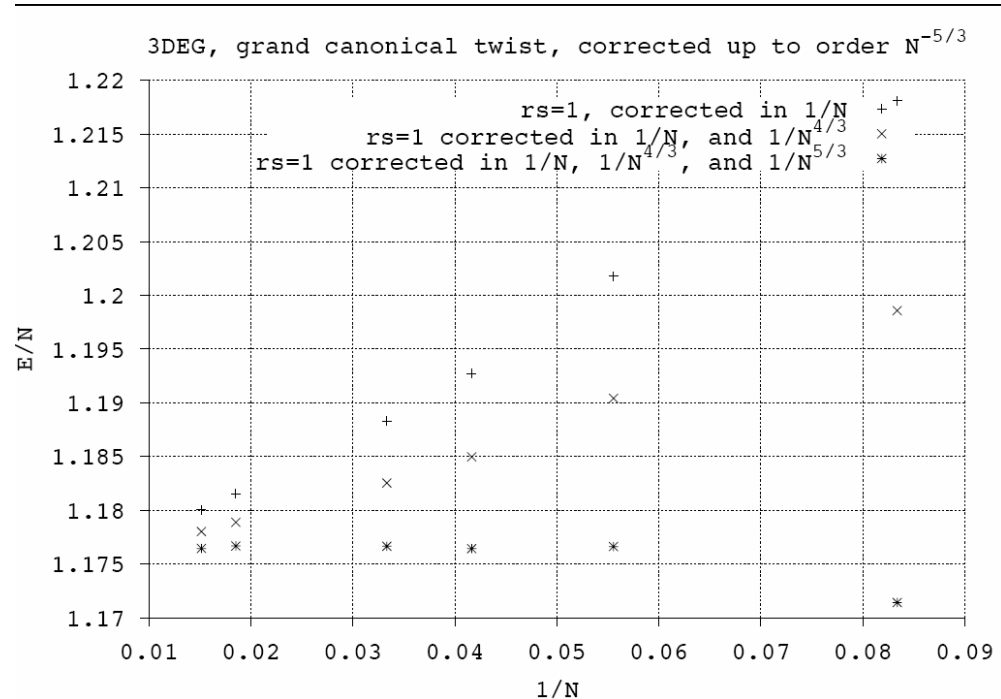
kinetic energy is

$$\delta T = -\frac{\hbar^2}{4m} \int_{-\pi/L}^{\pi/L} \frac{d^3k}{(2\pi)^3} k^2 u_k [S(k) - 1]$$

$$2nu_k = -1 + (1 + 2nv_k/e_k)^{1/2}$$

$\epsilon_k = k^2/2m$ and the corresponding structure factor

$$S(k) = (2nu_k + 1/S_0(k))^{-1}$$



Advantages of correlation function method for FSE

- Based on simple physical observables that are already computed: $S(k)$ + twist averaging and fundamental principles.
- No DFT calculations needed!
- Should work for any quantum or classical system: e.g. helium, electrons, positrons,
- Other methods can also work, but this approach seems the most general.