

Zero temperature calculations for quatum liquids

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Quantum Monte Carlo (T=0)

- general N-body Hamiltonian

$$H = \sum_{i=1}^N \left[-\frac{\hbar^2 \nabla_i^2}{2m} \right] + \sum_{i < j} V(\mathbf{r}_i - \mathbf{r}_j)$$

⇒ **Variational principle** for ground state energy E_0 :

$$E_0 \leq E_T \equiv \frac{\langle \psi_T | H | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle} \quad \text{for any trial wavefunction } |\Psi_T\rangle$$

- How to find good functional forms for trial wavefunctions?
→ Fermi liquids (^3He , electron gas)
- How to extrapolate to the thermodynamic limit?
 $E_T(N) \rightarrow E_T(\infty)$?

Homogeneous trial wavefunctions

- general split in antisymmetric part A plus symmetric correlations U

$$\psi_T(R) = A(R) \exp[-U(R)], \quad R \equiv \{r_1, r_2, \dots, r_N\}$$

- Jastrow part $U(R) = \sum_{i,j} u(r_{ij}), \quad r_{ij} = |r_i - r_j|$

- Antisymmetric part $A(R) = \text{Pf}_{ij} \varphi(r_{ij})$, Pfaffian with antisymmetric φ

unpolarized system: $\text{Pf}_{ij} \varphi(r_i^\uparrow - r_j^\downarrow) = \det_{ij} \varphi(r_i^\uparrow - r_j^\downarrow)$ for spin-singlett pairing

plane wave expansion $\varphi(r) = \sum_k \alpha_k e^{ikr}$

- Fermi liquid trial wavefunction: $\alpha_k \equiv 0$ for $k > k_F$ (step function)

$$\det_{ij} \varphi(r_i^\uparrow - r_j^\downarrow) = \left(\prod_k \alpha_k^2 \right) \left(\det_{ki} e^{ikr_i^\uparrow} \right) \left(\det_{ki} e^{ikr_i^\downarrow} \right)$$

- superfluid pairing: $\varphi(r) \rightarrow 0$ (exponentially) for $r \rightarrow \infty$

level spacing Δk crucial, finite-size effects!

Constructing many-body correlations

- basic elements: many-body vectors and tensors of form

vector $d_i^\alpha = \sum_j r_{ij}^\alpha d(r_{ij}), \quad \alpha = 1, \dots, D, i = 1, \dots, N$

tensor $q_i^{\alpha\beta} = \sum_j r_{ij}^\alpha r_{ij}^\beta q(r_{ij})$

- symmetric correlations:

3-body: $U_3(R) = \sum_{i\alpha} d_i^\alpha d_i^\alpha$

4-body: $U_4(R) = \sum_{i\alpha\beta} d_i^\alpha q_i^{\alpha\beta} d_i^\beta$

- backflow coordinates inside determinants: $A(R) = \det_{ki} \varphi_k(q_i)$ with

backflow: $q_i^\alpha = r_i^\alpha + d_i^\alpha$

3-body backflow: $q_i^\alpha = r_i^\alpha + \sum_\beta q_i^{\alpha\beta} d_i^\beta$

- evaluation of 3 and 4 body correlations/backflow does not cost much

Results using 4-body potential and 3-body backflow: Helium

- unpolarized liquid ${}^3\text{He}$ at Γ point for $N = 66$

ρ	wavefunction	E_v	σ^2	E_{DMC} [K]
16.06	BF-3	-2.201(6)	23	-2.417(1)
16.06	BF-3+3BF-4	-2.284(3)	14	-2.438(1)
16.06	exp			-2.481
19.46	BF-3	-1.775(5)	26	-2.155(5)
19.46	BF-3+3BF-4	-1.905(4)	20	-2.174(3)
19.46	exp			-2.216
23.08	BF-3	-0.055(1)		-0.77 (2)
23.08	BF-3+3BF-4	-0.272(7)	53	-0.834(2)
23.08	exp			-0.885

- polarized liquid much less affected
- pairing of order gap $\sim 1mK$ not important

Results using 4-body potential and 3-body backflow: electron gas, hydrogen

- unpolarized electron gas 3D, $N = 54$

r_s	wavefunction	E_v	σ^2	E_{DMC}
10	BF-A	-0.10843 (2)	0.00017 (1)	-0.10888 (1)
	3BF4	-0.10868 (1)	0.000074 (1)	-0.10892 (1)
20	BF-A	-0.06372 (2)	0.000045 (2)	-0.06408 (1)
	3BF4	-0.063930 (4)	0.000016 (1)	-0.064104 (4)

- high density region ($r_s < 10$) not much changed
- liquid hydrogen:
orbital effects (DFT, bandstructure) dominate,
many-body correlations do not seem to lift degeneracies

Fermi liquid renormalization

- consider particle-hole excitations using backflow-Jastrow wavefunctions

$$\psi_i^{(0)}(R) = \det e^{ik_i q^{(0)}} e^{-U^{(0)}}$$

where k_i is set of \mathbf{k} -vectors, $q^{(0)} = q^{(0)}(R)$, $U^{(0)} = U^{(0)}(R)$

- diagonalize

$$\langle \psi_i^{(0)} | H | \psi_j^{(0)} \rangle$$

- what is the form of the new ground state?
- Fermi liquid theory \rightarrow new ground state is of form

$$\psi_i^{(1)}(R) = \det e^{ik(q^{(0)} + q^{(1)})} e^{-U^{(0)} - U^{(1)}}$$

where $q^{(1)} = q^{(1)}(q^{(0)})$, $U^{(1)} = U^{(1)}(q^{(0)})$

-ITERATE.....

Results: electron gas, ${}^3\text{He}$

- unpolarized electron gas 3D, $N = 54$

r_s	iteration	E_v	σ^2/N	E_{DMC}
10	0	-0.10868 (1)	0.000074 (1)	-0.10892 (1)
	1	-0.10877 (1)	0.000061 (1)	
20	0	-0.063930 (4)	0.000016 (1)	-0.064104 (4)
	1	-0.064025 (4)	0.000011 (1)	

- ${}^3\text{He}$

ρ	iteration	E_v	σ^2	E_{DMC} [K]
16.06	0	-2.284(3)	14	-2.438(1)
16.06	1	much better	14	slightly better
16.06	exp			-2.481

Thermodynamic limit extrapolation

$$E(L), E(2L), E(4L), \dots, E(\infty)$$

or

$$E(L) = \sum_k \frac{k^2}{2m} n_k^L + \sum_k v(k) [S^L(k) - 1]$$

...

$$\longrightarrow \frac{E(\infty)}{V} = \int \frac{d^D k}{(2\pi)^D} \frac{k^2}{2m} n_k^\infty + \int \frac{d^D k}{(2\pi)^D} v(k) [S^\infty(k) - 1]$$

n_k : momentum distribution, $S(k)$: structure factor

finite size errors

- $n_k^L \rightarrow n_k^\infty, S^L(k) \rightarrow S^\infty(k)$ in general rapidly converging

- integration errors

– kinetic energy $T_k^L = \sum_k \frac{k^2}{2m} n_k^\infty \rightarrow V \int \frac{d^D k}{(2\pi)^D} \frac{k^2}{2m} n_k^\infty$

nonanalytic behaviour of n_k from Slater determinant

step function at k_F leads to oscillations, and very slow convergences

\Rightarrow twist-averaging

- potential energy

$$V^L = \sum_{k \neq 0} v(k) [S^\infty(k) - 1] \rightarrow \int \frac{d^D k}{(2\pi)^D} v(k) [S^\infty(k) - 1]$$

integrand can be analytically continued to $k = 0$ (using RPA assumptions),
corrections of order $1/N$

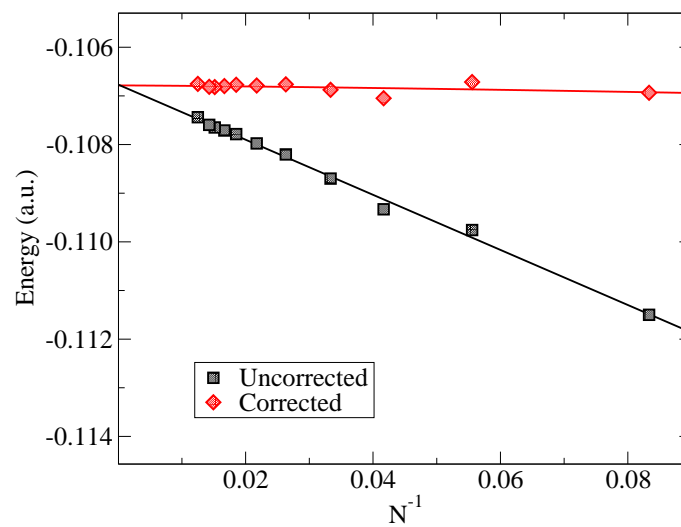
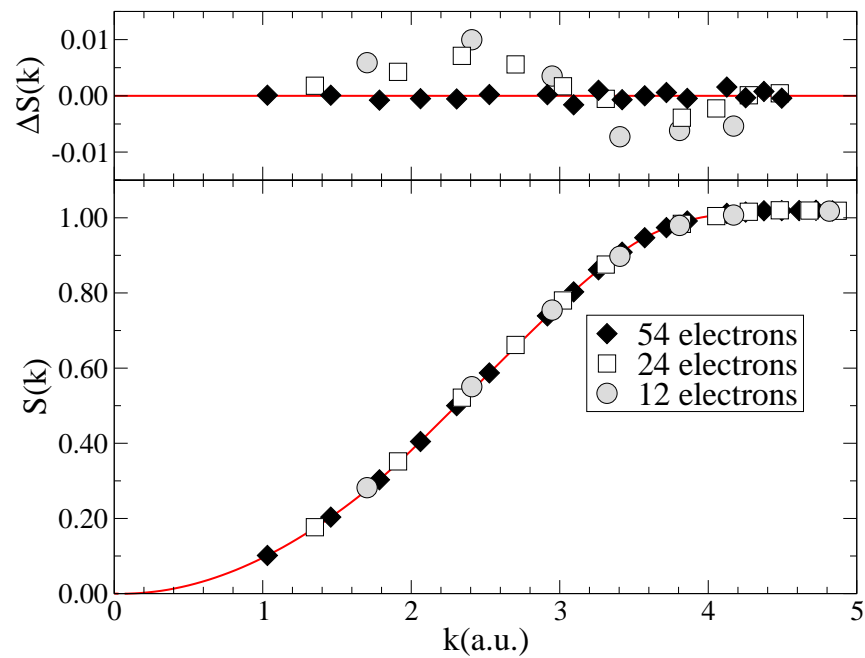
- kinetic energy from bosonic part $\sum_k \frac{k^2}{2m} n_k \rightarrow V \int \frac{d^D k}{(2\pi)^D} \frac{k^2}{2m} u_k^\infty$

where long range part of Jastrow is given by $\log \psi \sim u_k \rho_k \rho_{-k}$ for $k \rightarrow 0$

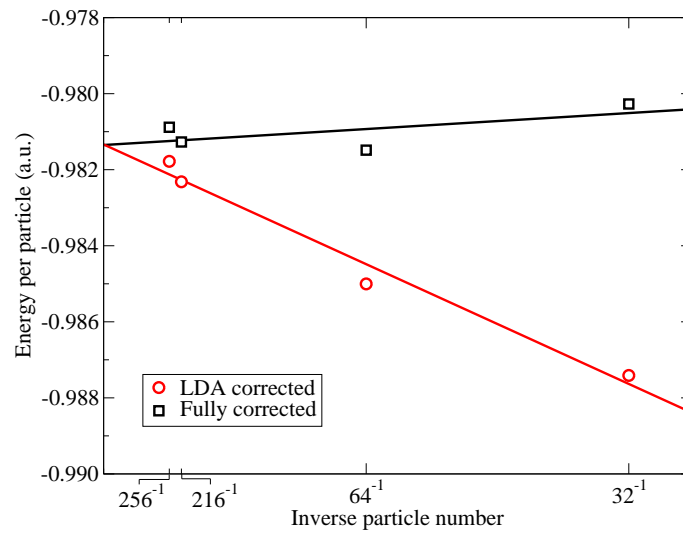
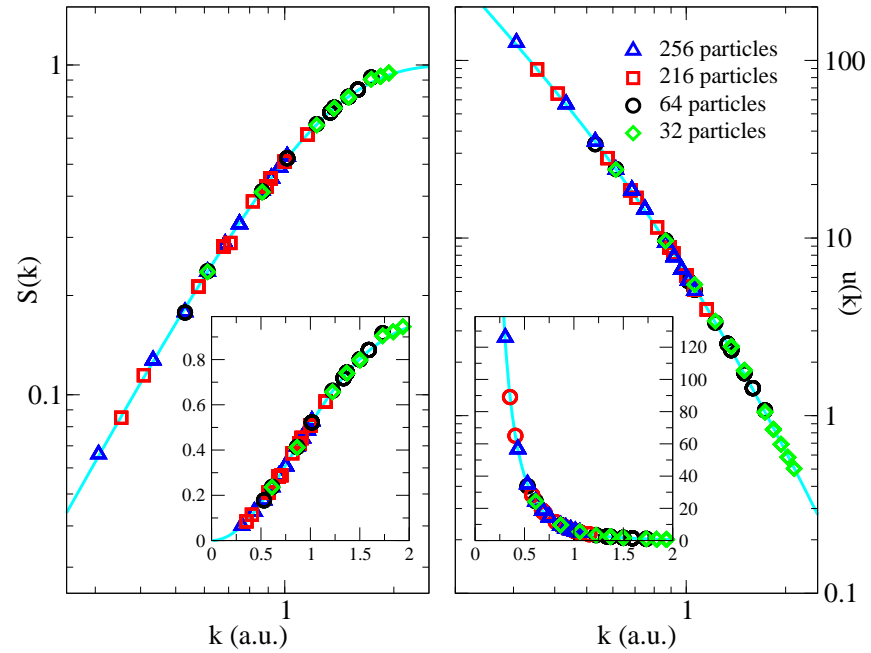
leads to $1/N$ corrections similar to potential energy

- electron gas: $1/N$ corrections corresponds to plasmon zero point motion

Finite size errors: electron gas at $r_s = 10$



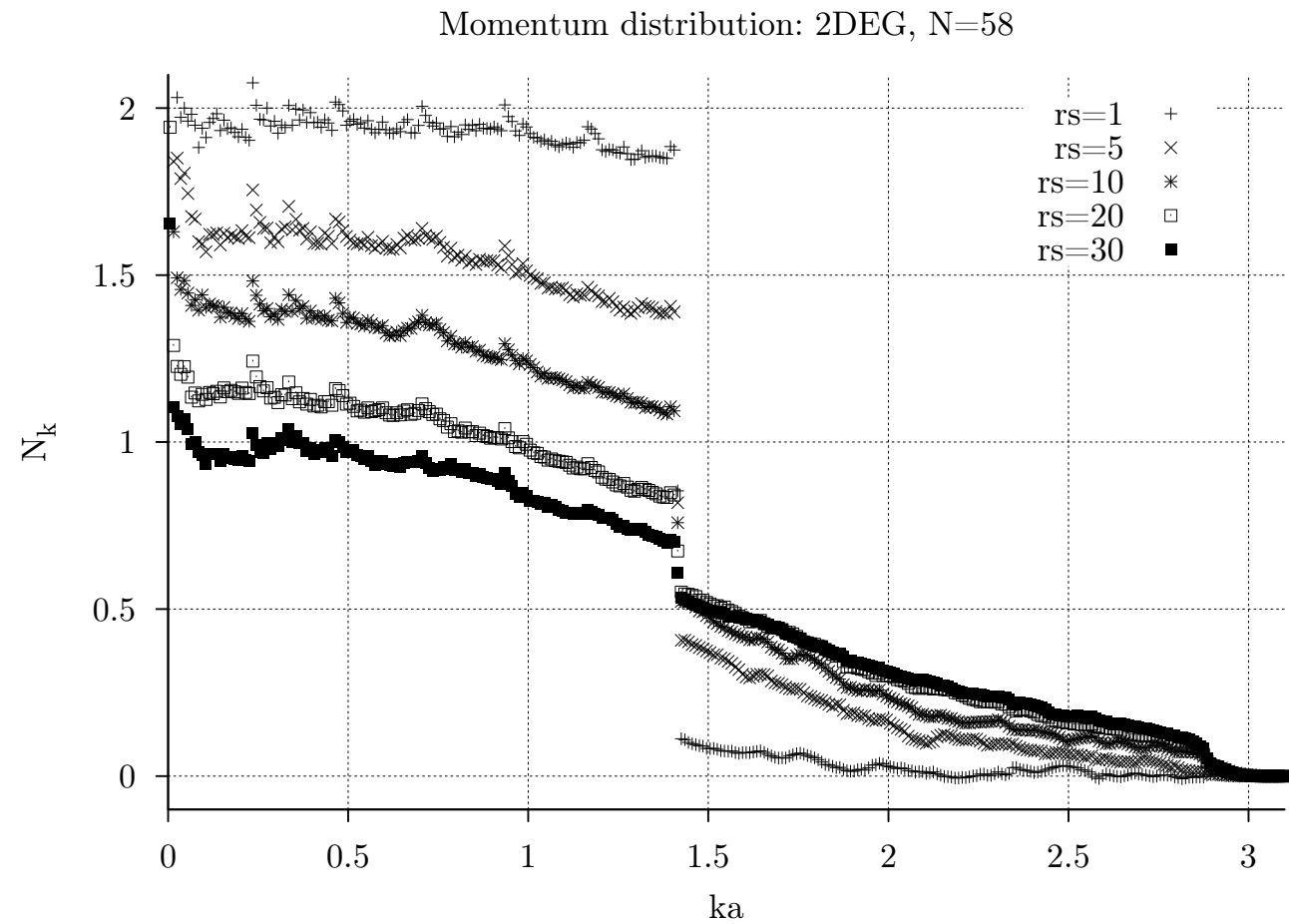
Finite size errors: diamond silicon at $r_s = 2$



Twist averaging: pockets

- Fermi liquid wavefunction with determinant $\det e^{ikr}$ occupies wavevectors $k_i = \frac{2\pi}{L}(i + \theta)$ with integers i for twist $-0.5 \leq \theta < 0.5$
 - choose occupations $n_k = 0, 1$ such that $\sum_i k_i^2 n_{k_i}$ minimal for canonical ensemble or
 - choose all $n_{k_i} = 1$ for $k_i^2 \leq k_F^2$ otherwise $n_k = 0$ (grandcanonical $V^{-1}\langle N \rangle = n$)
- variation in $\theta \longrightarrow \theta + \delta\theta$
inside the same pocket we have
 - $\psi(\theta) \longrightarrow e^{i2\pi\delta\theta \sum_i r_i/L} \psi(\theta)$ (center of mass motion)
 - $P(\theta) = \sum_i n_{k_i}(i + \theta) \longrightarrow P(\theta) + \delta\theta$ (exact momentum eigenstate)
 - $E(\theta) = \sum_i n_{k_i}(i + \theta)^2 \longrightarrow E(\theta) + 2P(\theta)\delta\theta + \delta\theta^2$
- simple transformation rules inside each pockets \Rightarrow inside each pocket only one explicit calculation is necessary \Rightarrow exact twist sampling possible
- for $N \lesssim 100$ less than 200 pockets

Momentum distribution: 2D electron gas with grand-canonic twist



Open questions

- liquid ^3He : what is still missing for energies?
- how to reduce finite size effects to obtain superfluid transition?
- electron gas: do many-body correlations affect polarization transition close to Wigner cristallization?
- disorder: how to treat accurately, how to extrapolate size?