Recent advances in understanding the sign problem in path integral Monte Carlo simulation of harmonic fermions

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What are the advances?

I) Discovery of operator contraction identity for any number of non-interacting harmonic fermions in any dimension:

[SAC, J. Chem. Phys. 159, 134109 (2023)]

$$\mathrm{e}^{-a\hat{T}}\mathrm{e}^{-b\hat{V}}\mathrm{e}^{-c\hat{T}} = \mathrm{e}^{-\nu\hat{V}}\mathrm{e}^{-\kappa\hat{T}}\mathrm{e}^{-\mu\hat{V}}$$

$$\hat{V} = \frac{1}{2}\mathbf{x}^2 = \sum_{i=1}^{N}\frac{1}{2}\mathbf{r}_i^2 \qquad \langle\mathbf{x}'|\mathrm{e}^{-\tau\hat{T}}|\mathbf{x}\rangle = \frac{1}{N!}\det\left(\frac{1}{(2\pi\tau)^{d/2}}\exp\left[-\frac{1}{2\tau}(\mathbf{r}_i' - \mathbf{r}_j)^2\right]\right)$$

$$\kappa = a + abc + c \qquad \nu = \frac{bc}{\kappa} \qquad \mu = \frac{ab}{\kappa}$$

Any symmetric short time propagator can be contracted to the standard form : $\mathrm{e}^{-\mu_1\hat{V}}\mathrm{e}^{-\kappa_1\hat{T}}\mathrm{e}^{-\mu_1\hat{V}}$

Any PIMC can then be further contacted also into a single $\hat{T}$ form.

II) A completely analytical PIMC model (results at any number of beads, for any short time propagator) for the study of non-interacting harmonic fermions with analytical thermodynamic and Hamiltonian energies.

[SAC, J. Chem. Phys. 159, 244104 (2023)]

III) The exact harmonic oscillator propagator has exactly the same nodal structure as the free fermion propagator.

IV) Closed-shell states have no sign problem in the low temperature limit! (Same reason why there is no sign problem in 1d. [SAC, PRE 109, 065312(2024)]

V) Can solve many 2d quantum dots, with Coulomb interaction, with only 3-5 beads (3-5 anti-symmetric free fermion propagators).

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What is the fermion sign problem?

Fermion path integral, where $\mathbf{x} = (\mathbf{r}_1, \mathbf{r}_2 \cdots \mathbf{r}_N)$

$$\tau = k\epsilon = \hbar\omega / k_B T$$

$$\begin{aligned} G_k(\mathbf{x}, \mathbf{x}; \tau) &= \langle \mathbf{x} | (\mathrm{e}^{-\epsilon(\hat{T}+\hat{V})})^k | \mathbf{x} \rangle \\ &= \int_{-\infty}^{\infty} d\mathbf{x}_1 \cdots d\mathbf{x}_{k-1}\, G_1(\mathbf{x}, \mathbf{x}_1; \epsilon) G_1(\mathbf{x}_1, \mathbf{x}_2; \epsilon) \cdots G_1(\mathbf{x}_{k-1}, \mathbf{x}; \epsilon) \end{aligned}$$

Short time propagator

$$\begin{aligned} G_1(\mathbf{x}', \mathbf{x}; \epsilon) &= \langle \mathbf{x}' | \mathrm{e}^{-\epsilon(\hat{T}+\hat{V})} | \mathbf{x} \rangle \\ &\approx \mathrm{e}^{-(\epsilon/2)V(\mathbf{x}')} G_0(\mathbf{x}', \mathbf{x}; \epsilon) \mathrm{e}^{-(\epsilon/2)V(\mathbf{x})} \qquad \text{PA} \end{aligned}$$

Free fermion propagator

$$G_0(\mathbf{x}', \mathbf{x}; \epsilon) = \frac{1}{N!} \det \left(\frac{1}{(2\pi\epsilon)^{d/2}} \exp \left[-\frac{1}{2\epsilon} (\mathbf{r}'_i - \mathbf{r}_j)^2 \right] \right)$$

The product $G_1(\mathbf{x}, \mathbf{x}_1; \epsilon) G_1(\mathbf{x}_1, \mathbf{x}_2; \epsilon) \cdots G_1(\mathbf{x}_{k-1}, \mathbf{x}; \epsilon)$ is not always positive and therefore cannot be sampled by Monte Carlo methods.

The integrand can be sampled with respect to

$$P \propto |G_1(\mathbf{x}, \mathbf{x}_1; \epsilon) \cdots G_1(\mathbf{x}_{k-1}, \mathbf{x}; \epsilon)|$$

with observable *A* evaluated via

$$\langle A \rangle = \frac{\langle As \rangle_P}{\langle s \rangle_P}$$

where $s = sgn(G_1(\mathbf{x}, \mathbf{x}_1; \epsilon) \cdots G_1(\mathbf{x}_{k-1}, \mathbf{x}; \epsilon))$

One has a sign problem when $\langle s \rangle_P \rightarrow 0$,

but a manageable problem if $\langle s \rangle_P > \approx 0.1$.

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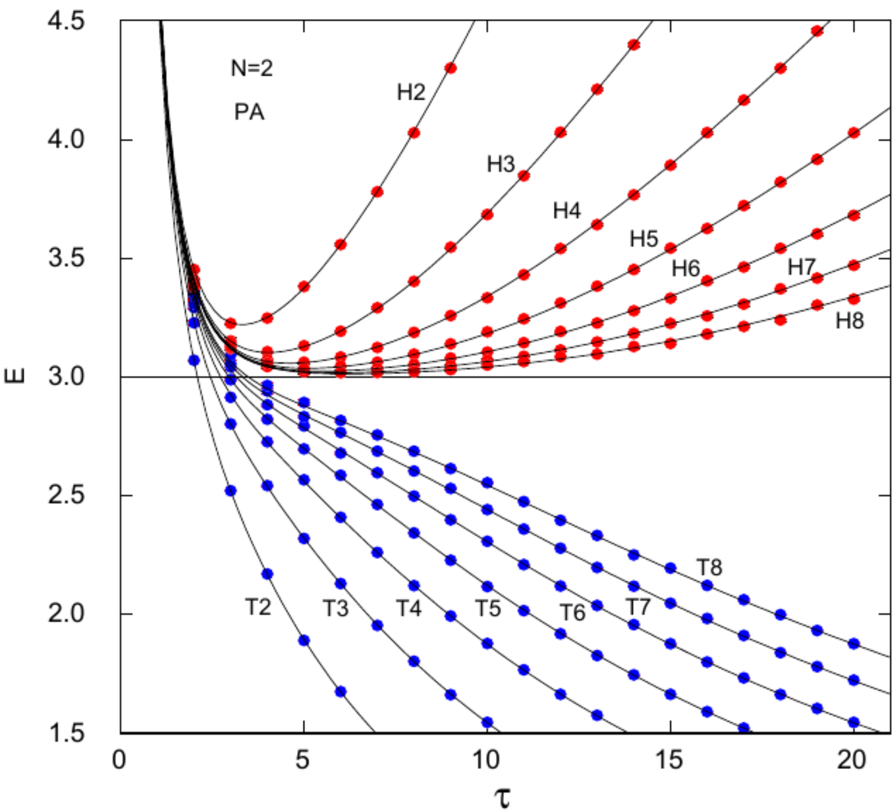
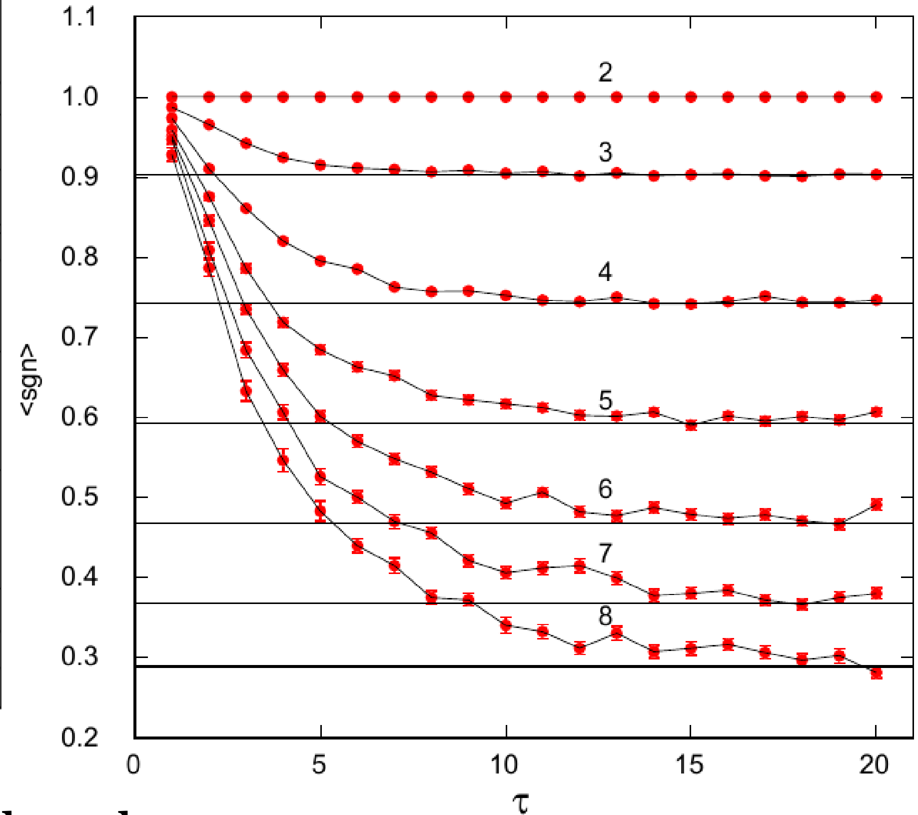
Two 2d free harmonic fermions





Analytical energies for 2 to 8 beads.

Asymptotic <sgn> at large τ for 3 to 8 beads:

$$\frac{2\pi^2}{12+\pi^2} = 0.9026,\ 0.7426,\ 0.5927,$$

$$0.4680,\ 0.3687,\ 0.2890$$

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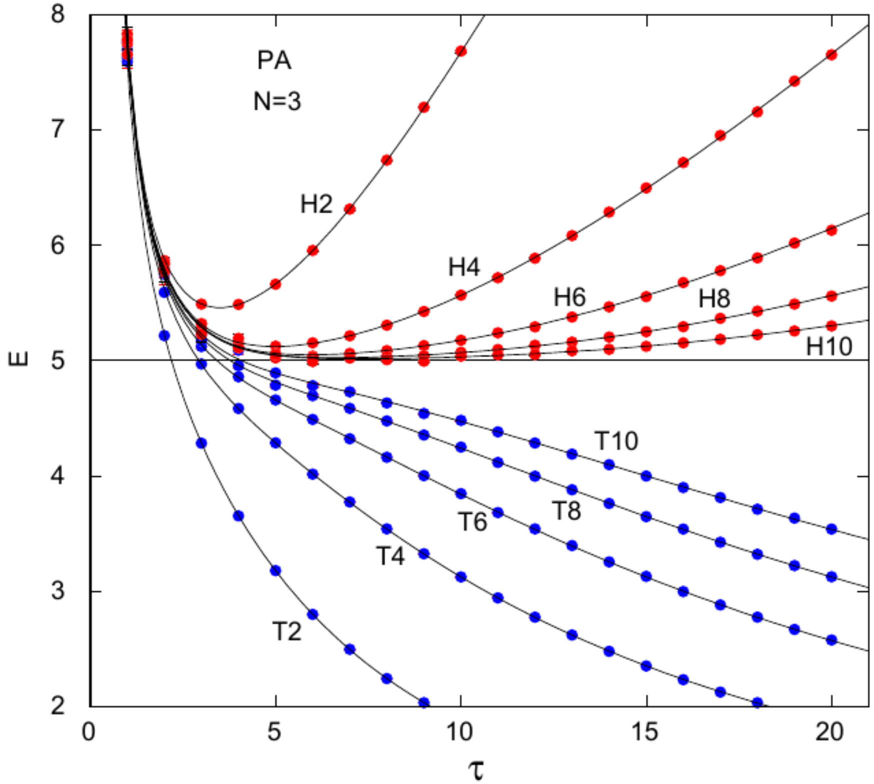
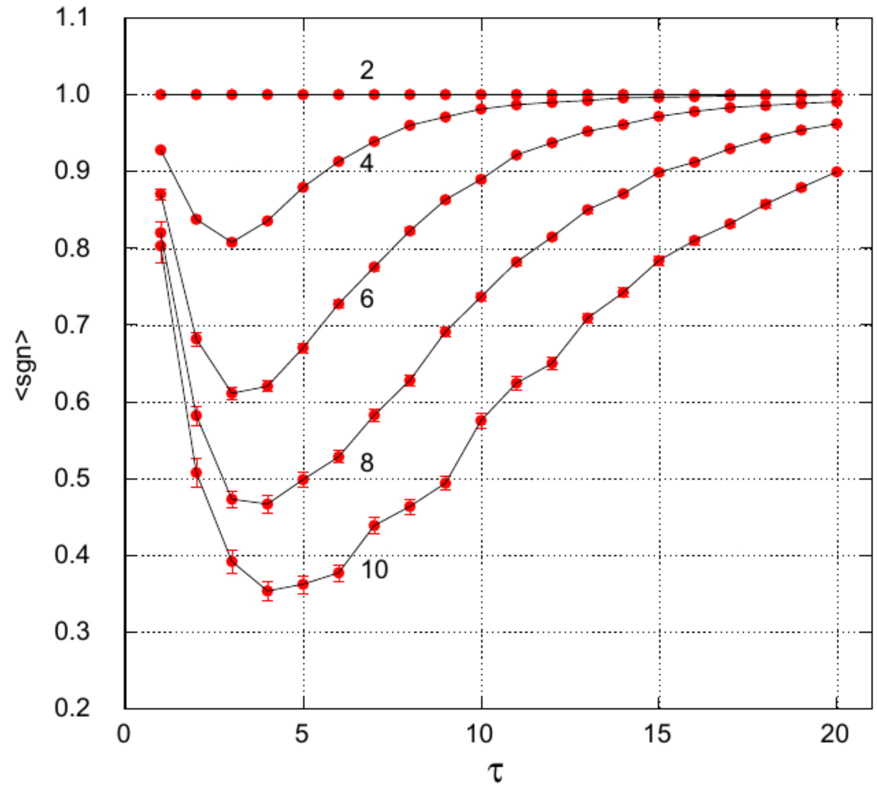
Three 2d free harmonic fermions





Again, analytical energies.

The average <sgn> → 1 at the large τ ,

low temperature limit!

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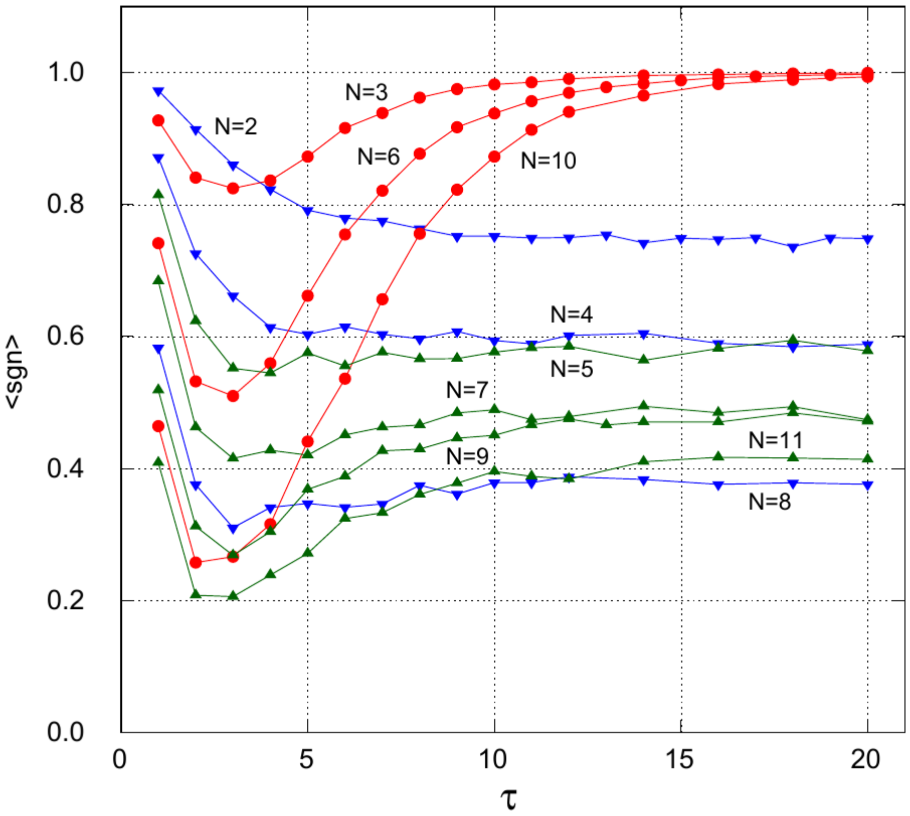
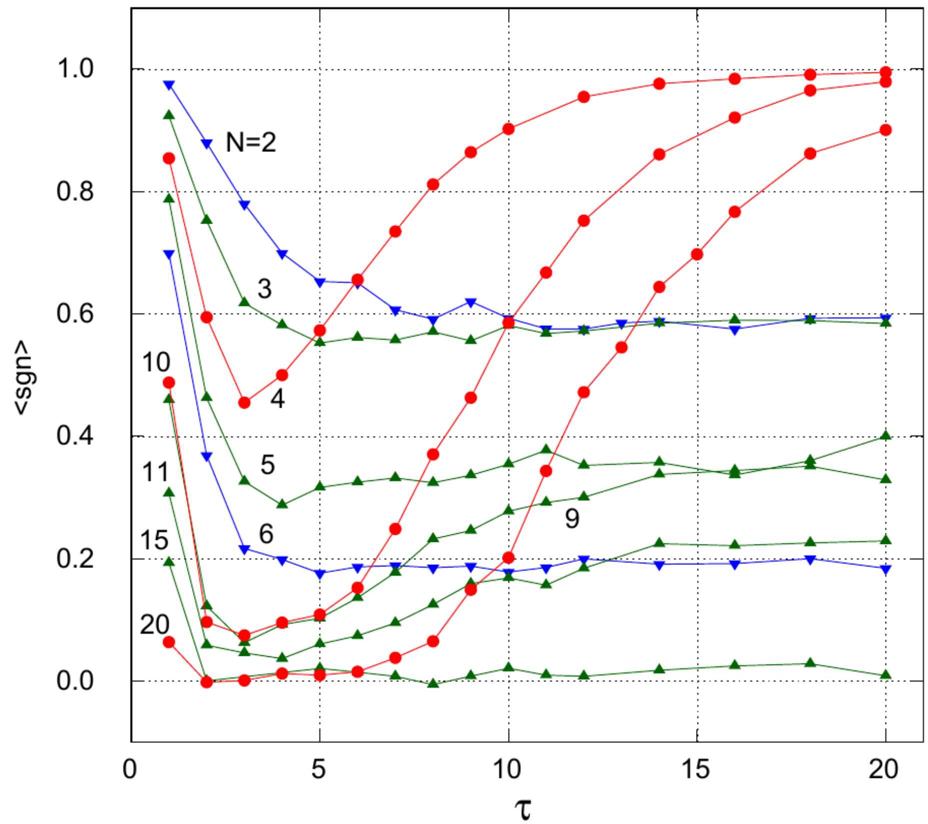
No sign problem for closed shell states



2d



3d

<sgn> in the 4-bead case as a function of the number of fermions. Will explain why there is no sign problem for closed-shell states later.

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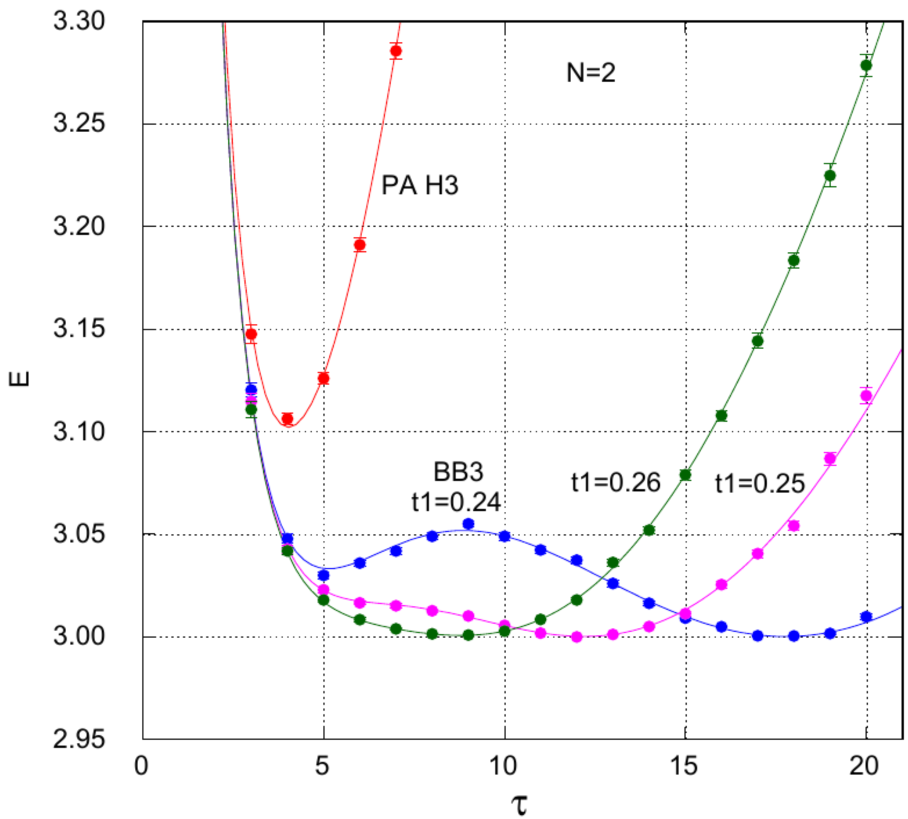
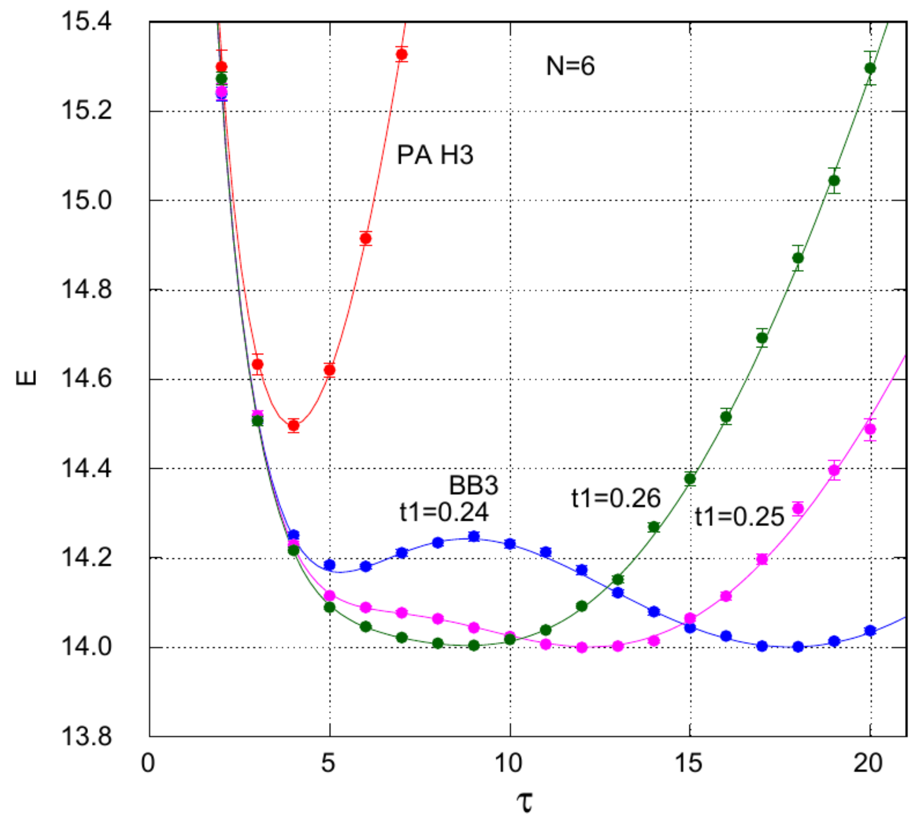
Using high-order propagators I





Optimize t_1, Best Bead (BB), with 3 $\widehat{T}$: BB3

$$\mathcal{T}^{(4)}_{BB3} = e^{v_0\epsilon\hat{V}} e^{t_1\epsilon\hat{T}} e^{v_1\epsilon\hat{V}^*} e^{t_2\epsilon\hat{T}} e^{v_1\epsilon\hat{V}^*} e^{t_1\epsilon\hat{T}} e^{v_0\epsilon\hat{V}}$$

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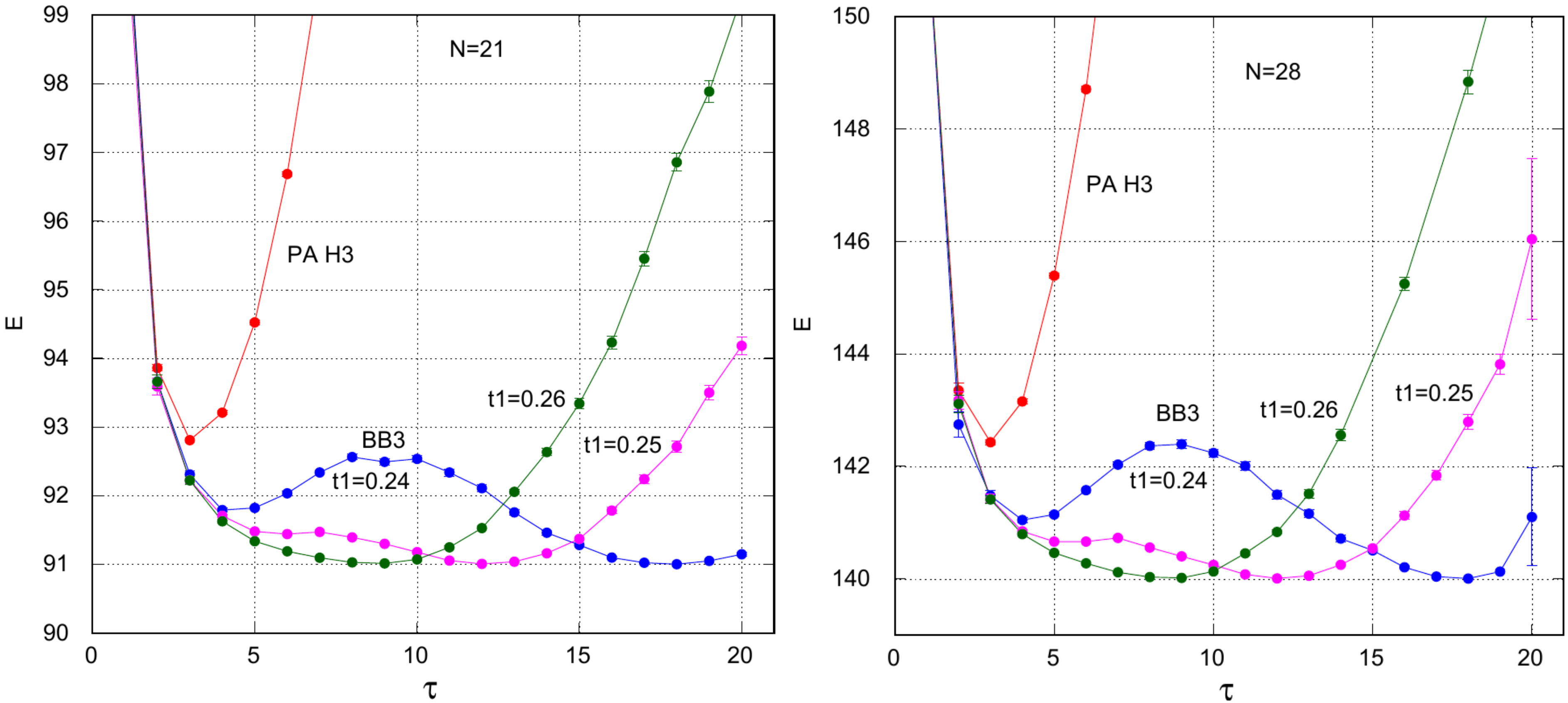
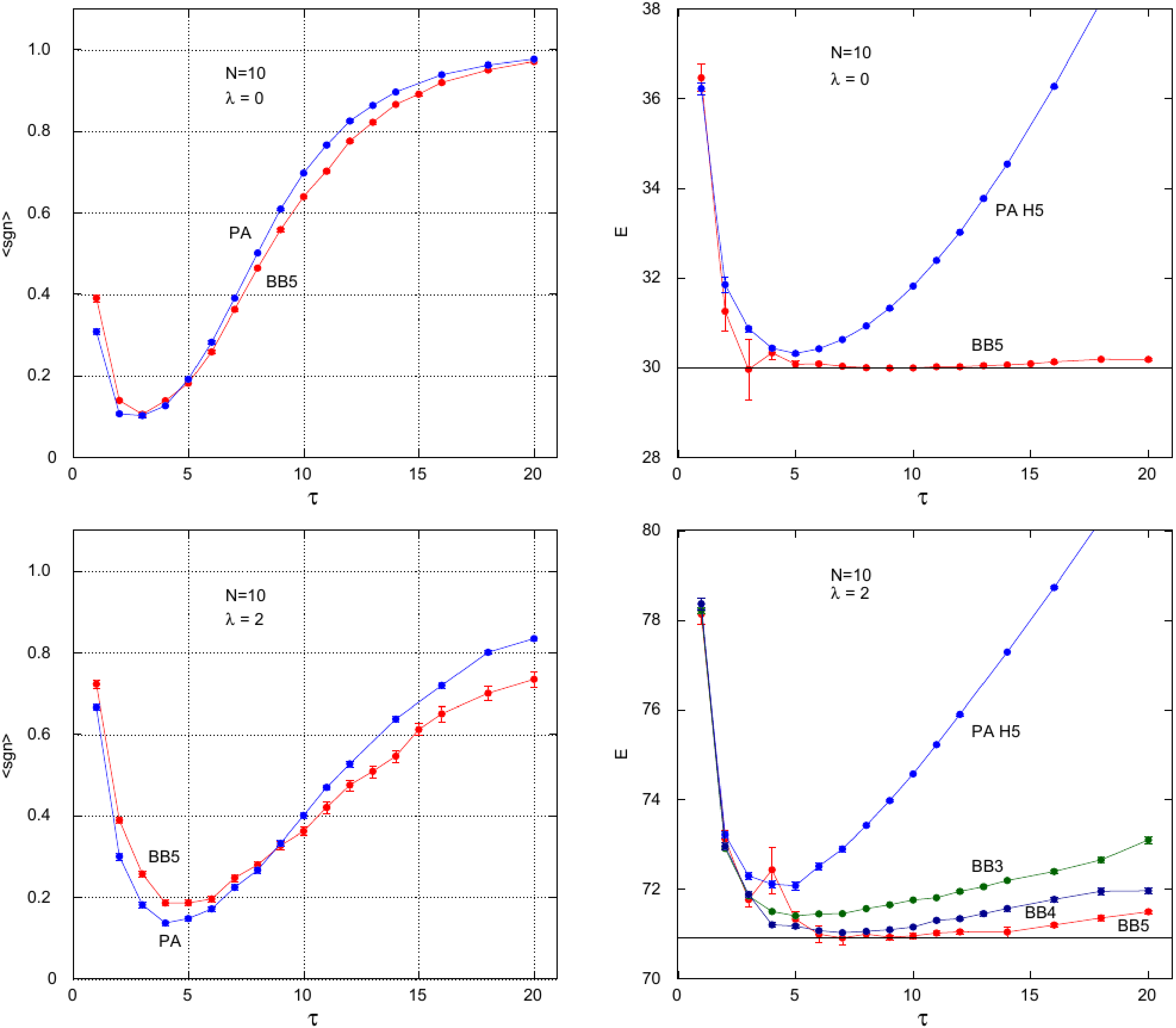
Using high-order propagators II



Work just as well on larger systems. Analytical expression too lengthy, not computed. Three beads sufficient for non-interacting fermions.

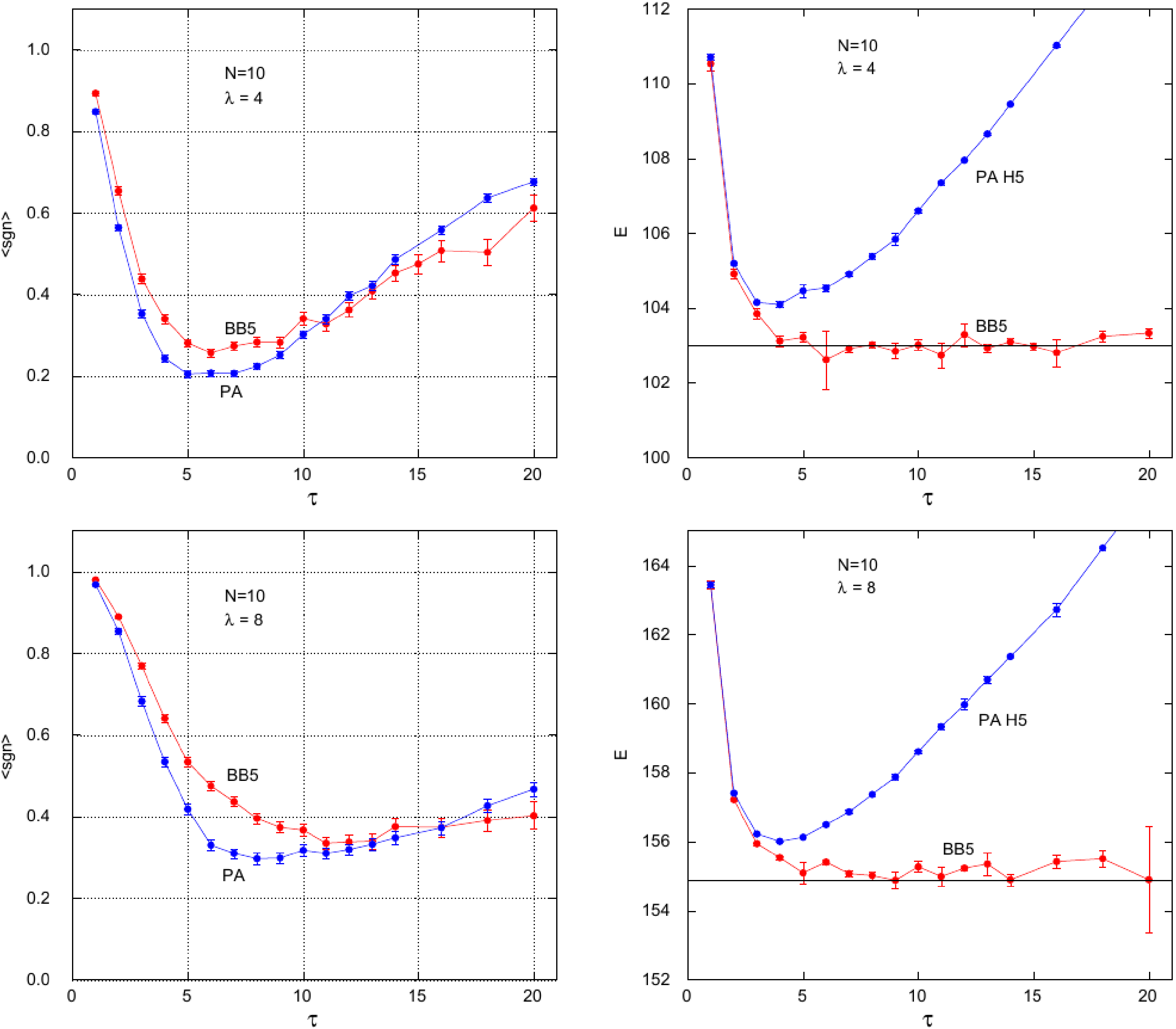
Harmonic fermions with Coulomb forces



Use a 5-bead propagator for accuracy.

Coulomb Interactions $v = \lambda / r_{ij}$ lessen the sign problem at small τ, but enhance it at large τ.

Harmonic fermions with Coulomb forces

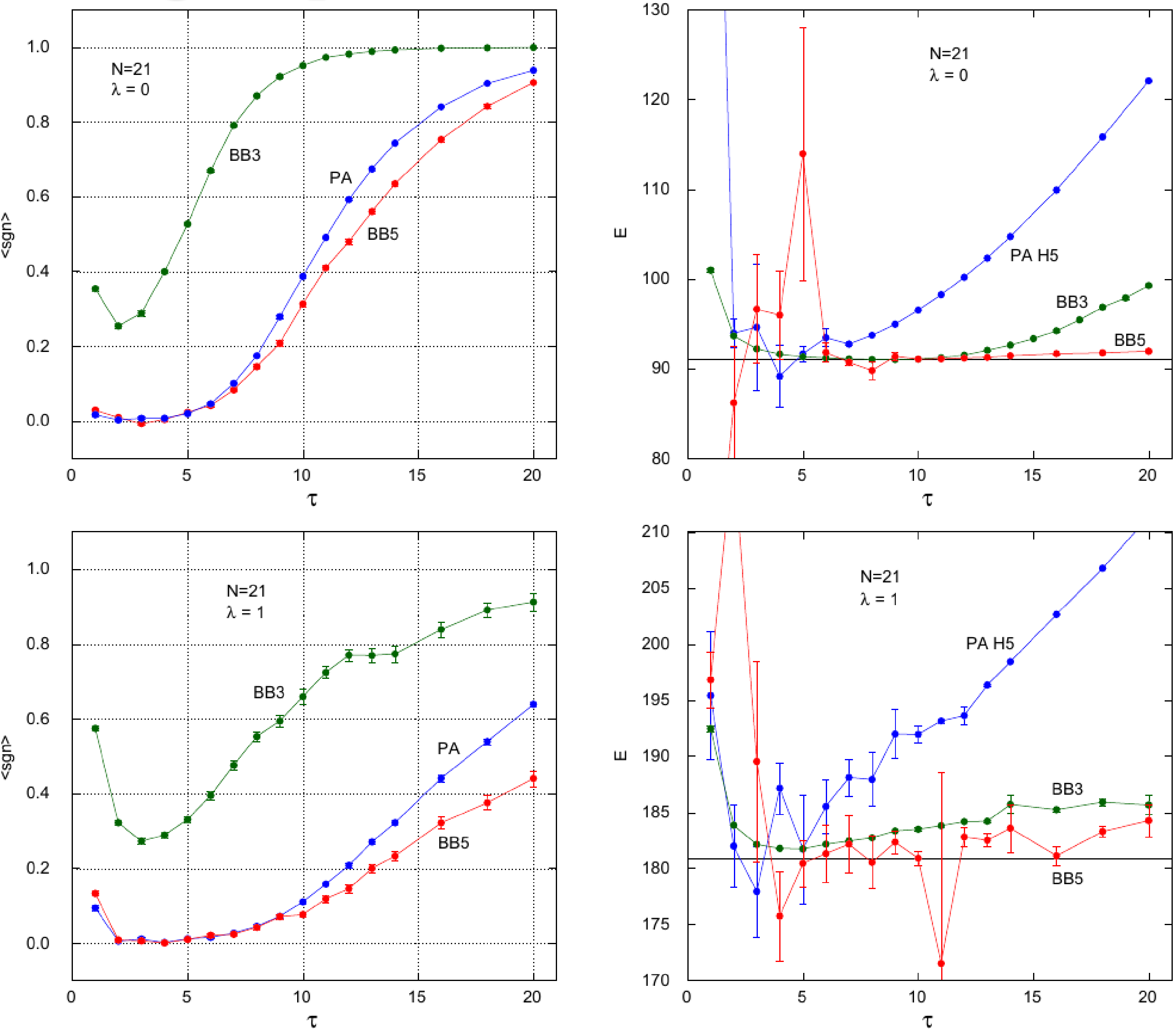


Strategy:

Strong Interaction, start at small τ.

Weak interaction, Start at large τ.

Larger quantum dots



Work reasonably well on larger systems, but must run longer to reduce the error bars.

Why no sign problem in 1d?

The 2-fermion free propagator is given by

[SAC, PRE 109, 065312 (2024)]

$$G_0(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_1, \mathbf{r}_2; \epsilon) = \frac{1}{2}\frac{1}{(2\pi\epsilon)^d} \det \begin{pmatrix} e^{-(\mathbf{r}_1'-\mathbf{r}_1)^2/(2\epsilon)} & e^{-(\mathbf{r}_1'-\mathbf{r}_2)^2/(2\epsilon)} \\ e^{-(\mathbf{r}_2'-\mathbf{r}_1)^2/(2\epsilon)} & e^{-(\mathbf{r}_2'-\mathbf{r}_2)^2/(2\epsilon)} \end{pmatrix}$$

$$= \frac{1}{2}\frac{1}{(2\pi\epsilon)^d} e^{-\frac{1}{2\epsilon}\left[(\mathbf{r}_1'-\mathbf{r}_1)^2+(\mathbf{r}_2'-\mathbf{r}_2)^2\right]} \left(1 - e^{-\frac{1}{\epsilon}(\mathbf{r}_2'-\mathbf{r}_1')\cdot(\mathbf{r}_2-\mathbf{r}_1)}\right)$$

Its sign is given by

$$\mathrm{sgn}(G_0) = \mathrm{sgn}\Big(1 - \exp(-\frac{1}{\epsilon}\mathbf{r}_{21}' \cdot \mathbf{r}_{21})\Big) = \mathrm{sgn}(\mathbf{r}_{21}' \cdot \mathbf{r}_{21})$$

For three beads, sign problem

$$\mathrm{sgn}\Big(G_0(\mathbf{r}_{21}, \mathbf{r}_{21}')G_0(\mathbf{r}_{21}', \mathbf{r}_{21}'')G_0(\mathbf{r}_{21}'', \mathbf{r}_{21})\Big) = \mathrm{sgn}\Big((\mathbf{r}_{21} \cdot \mathbf{r}_{21}')(\mathbf{r}_{21}' \cdot \mathbf{r}_{21}'')(\mathbf{r}_{21}'' \cdot \mathbf{r}_{21})\Big),$$

$$= |\mathbf{r}_{21}|^2|\mathbf{r}_{21}'|^2|\mathbf{r}_{21}''|^2\mathrm{sgn}\Big(\cos\theta\cos\theta'\cos\theta''\Big).$$

However, in 1d, no cosines, no sign problem.

$$\mathrm{sgn}\Big(G_0(x_{21}, x_{21}')G_0(x_{21}', x_{21}'')G_0(x_{21}'', x_{21})\Big) = \mathrm{sgn}\Big((x_{21}x_{21}')(x_{21}'x_{21}'')(x_{21}''x_{21})\Big)$$

$$= \mathrm{sgn}\Big((x_{21})^2(x_{21}')^2(x_{21}'')^2\Big) \geq 0$$

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Why no sign problem for closed shells?

The sign of the 3-fermion free propagator can be shown, in the large τ limit, to be given by

$$\mathrm{sgn}(G_0) = \mathrm{sgn}[(\mathbf{r}'_{21} \times \mathbf{r}'_{31}) \cdot (\mathbf{r}_{21} \times \mathbf{r}_{31})]$$

In 3d, this spells the sign problem because of the cosine function of the dot product.

However, in 2d, there is only the z-component of the cross-product,

$$\mathrm{sgn}(G_0) = (x'_{21}y'_{31} - x'_{31}y'_{21})(x_{21}y_{31} - x_{31}y_{21})$$

Again with no cosine function and therefore no sign problem. It is just the signed area, which pairs up to perfect squares in a closed loop.

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Final insight – nonharmonic fermions

For harmonic fermions,

contraction formula $\Rightarrow$ single determinant.

For $\hat{V}$ nonharmonic,

$$\mathrm{e}^{-a\hat{T}}\mathrm{e}^{-b\hat{V}}\mathrm{e}^{-c\hat{T}} = \mathrm{e}^{-a\hat{T}}\left(\sum_i C_i \mathrm{e}^{-b_i \frac{1}{2}\mathbf{x}^2}\right)\mathrm{e}^{-c\hat{T}}$$

$$= \sum_i C_i \left(\mathrm{e}^{-\nu_i \hat{V}}\mathrm{e}^{-\kappa_i \hat{T}}\mathrm{e}^{-\mu_i \hat{V}}\right)$$

contraction spawns multiple determinants.

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Conclusions

1) The sign problem has been exaggerated by the widespread use of the low order PA propagator and the poor convergence of the thermodynamic energy.
2) Many fermion problems can be solved by the use of high order propagators without solving the sign problem. The two are not synonymous.
3) A completely analytical model for harmonic fermions is now available for the analysis of the sign problem.
4) The sign problem goes away at large τ for closed-shell states. This may have similar affects in other fermi systems, such as nuclei or Helium-3 droplets.