Understanding and managing the sign problem in path integral Monte Carlo simulation of harmonic fermions

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Abstract

This work found that surprisingly: 1) The Coulomb repulsion reduces the sign problem at small imaginary time, and 2) there is *no* sign problem in the large imaginary time limit for closed-shell non-interacting harmonic fermions. Therefore, the sign problem for closed-shell *interacting* fermions can be managed by working at some intermediate imaginary time using fourth-order short time propagators to compute the Hamiltonian energy.

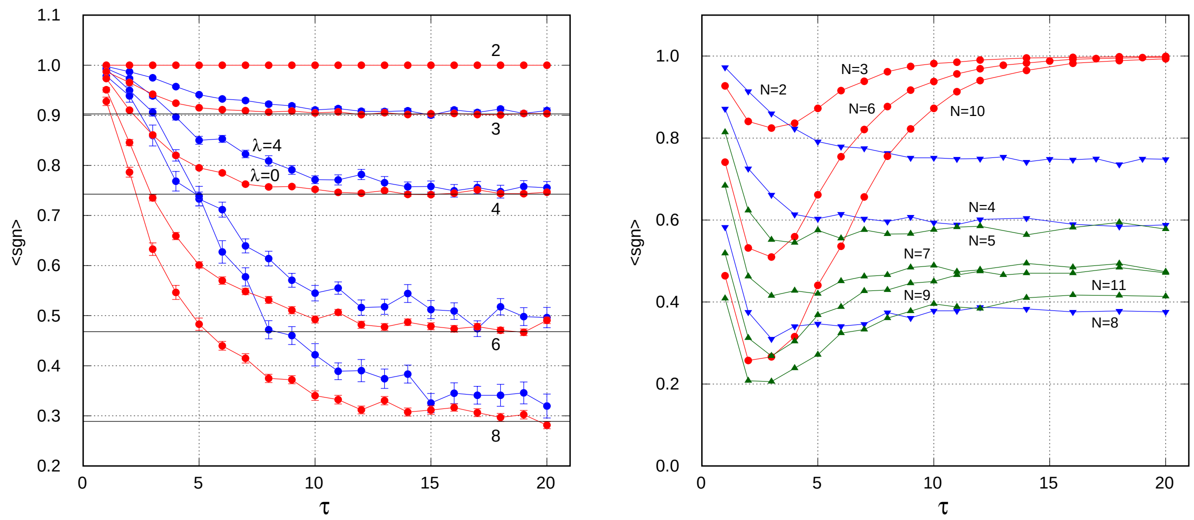

FIG. 1: (color online) **Left: A**. The average sign for two fermions in a 2d harmonic oscillator with Coulomb interaction $V = \lambda/|\mathbf{r}_1 - \mathbf{r}_2|$. The numbers denote the numbers of "bead" (the number of anti-symmetric free fermion propagator) used in the PIMC simulation. **Right: B**. The average sign of a 4-bead calculation for various N non-interacting fermions.

Fig.1A shows that the average sign for two fermions decreases with increasing number of beads. Coulomb repulsion reduces the sign problem at small imaginary time τ. Fig.1B shows the average sign of a four-bead calculation for various number of non-interacting fermions. At closed-shell numbers of $N = 3, 6, 10$, the sign problem disappears at large τ. Similar chosed-shell behaviors are also seen in 3d harmonic fermions. Fig.2A shows that for a 5-bead calculation of 10 non-interacting fermions, both the PA and the fourth-order BB5[1]

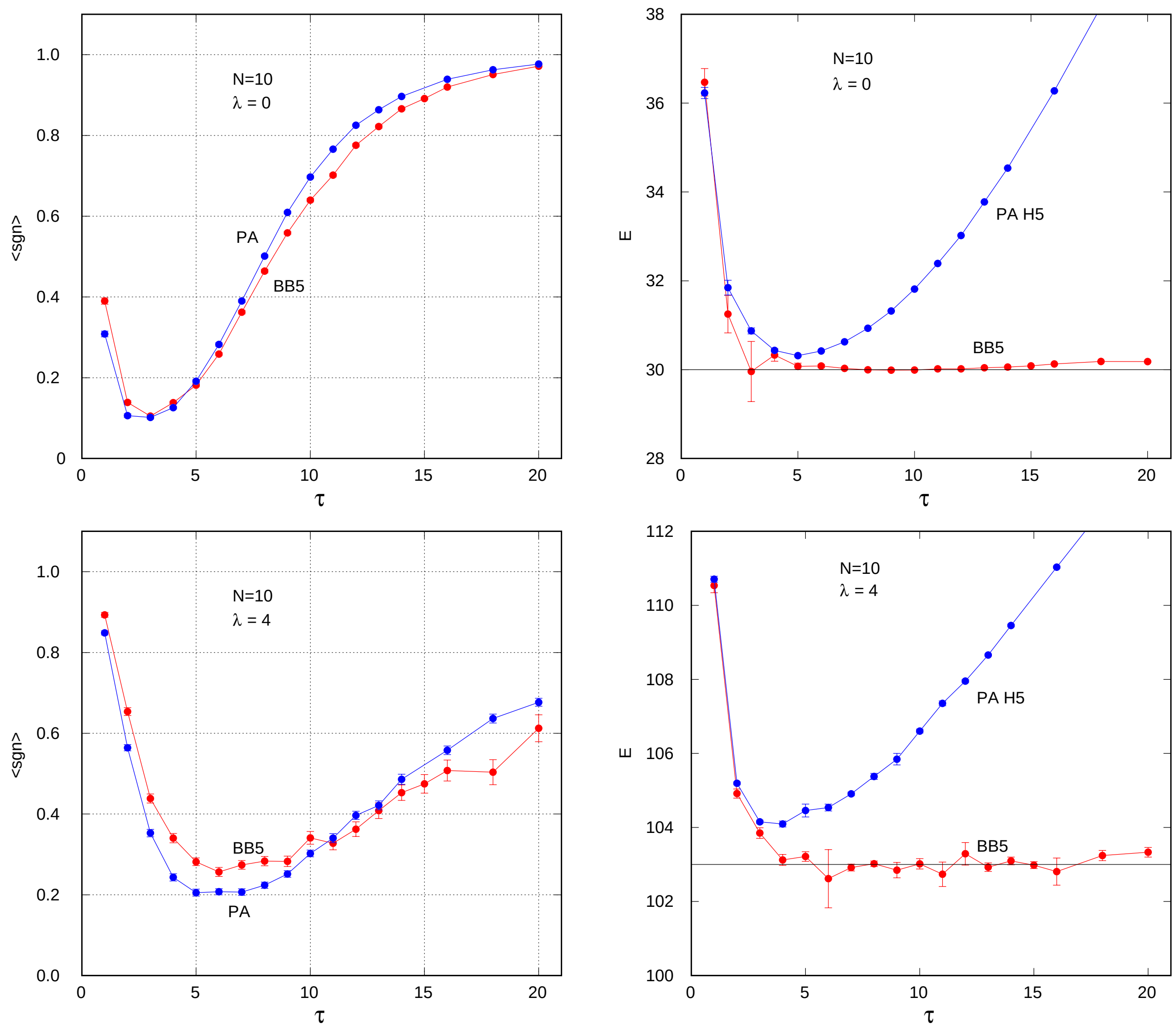

FIG. 2: (color online) **Upper left:A**. The average sign of a 5-bead calculation for 10 free fermions using the second-order PA and the fourth-order BB5[1] propagator. **Lower left:C** The average sign for 10 *interacting* fermions. **Upper right:B**. The Hamiltonian energy for 10 free fermions. **Lower right:D**. The Hamiltonian energy for 10 interacting fermions.

propagator have similar average sign, with low values at small τ. Fig.2B shows the better Hamiltonian energy produced by BB5. Fig.2C shows the average sign for 10 interacting fermions. The Coulomb interaction has raised the average sign, thereby reduced the sign problem at small τ. Fig.2D gives the near exact ground state energy produced by BB5.

References

[1] S. A. Chin, "High-order path-integral Monte Carlo methods for solving quantum dot problems", Phys. Rev. E **91**, 031301(**R**) (2015)