Naive SWAP estimator in PIGS

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We'll use the notation $|\alpha\rangle = |a, b\rangle$ for the Fock states of bosons on a lattice, partitioned into two sets of sites (the A and B subregions). In one configuration PIGS Monte Carlo, our worldline configurations have weights proportional to

$$\Psi_T^*(\alpha)\big\langle\alpha\big|e^{-\beta H}\big|\alpha'\big\rangle\Psi_T(\alpha') \tag{1}$$

where α and α' are the Fock states at $\tau = 0$ and $\tau = \beta$ respectively. For large β, we have:

$$\sum_{\alpha} \Psi_T^*(\alpha)\big\langle\alpha\big|e^{-\beta H}\big|\alpha'\big\rangle \simeq \big\langle\Psi_0\big|\alpha'\big\rangle = \Psi_0^*(\alpha') \tag{2}$$

So focusing on the $\tau = \beta$ end of our worldlines,

$$\sum_{\alpha} \Psi_T^*(\alpha)\big\langle\alpha\big|e^{-\beta H}\big|\alpha'\big\rangle\Psi_T(\alpha') \simeq \Psi_0^*(\alpha')\Psi_T(\alpha') \tag{3}$$

If we use a non-trivial trial wave function Ψ_T, then the end of the path provides was is call a "mixed estimator" in the Green's function QMC literature. But if we take $\Psi_T(\alpha) = 1$, then the probability of α' at $\tau = \beta$ is proportional to $\Psi_0^*(\alpha')$. So α' at $\tau = \beta$ provides a sample of $\Psi_0^*(\alpha')$, not $|\Psi_0^*(\alpha')|^2$.

In comparison, consider the fock state α'' at the center of the path:

$$\sum_{\alpha,\alpha'} \Psi_T^*(\alpha)\big\langle\alpha\big|e^{-\beta H/2}\big|\alpha''\big\rangle\big\langle\alpha''\big|e^{-\beta H/2}\big|\alpha'\big\rangle\Psi_T(\alpha') \simeq \Psi_0^*(\alpha'')\Psi_0(\alpha'') = |\Psi_0(\alpha'')|^2 \tag{4}$$

So the center of the path samples $|\Psi_0|^2$, while the ends of the path sample Ψ_0.

Now consider the density matrix elements:

$$\rho(\alpha, \alpha') = \Psi_0^*(\alpha)\Psi_0(\alpha') \tag{5}$$

To compute the reduced density matrix ρ_A, we'll trace over B:

$$\rho_A(a, a') = \sum_{b,b'} \Psi_0^*(a, b)\Psi_0(a', b)\delta_{b,b'} \tag{6}$$

And then squaring ρ_A gives:

$$\rho_A^2 = \sum_{a',a''} \left(\sum_{b,b'} \Psi_0^*(a,b)\Psi_0(a',b')\delta_{b,b'} \right) \delta_{a',a''} \left(\sum_{b'',b'''} \Psi_0^*(a'',b'')\Psi_0(a'''',b''')\delta_{b'',b'''} \right) \tag{7}$$

$$= \sum_{a',a'',b,b',b'',b'''} \Psi_0^*(a,b)\Psi_0^*(a'',b'')\Psi_0(a',b')\Psi_0(a'''',b''')\delta_{b,b'}\delta_{a',a''}\delta_{b'',b'''} \tag{8}$$

Finally taking the trace gives us:

$$\mathrm{Tr}\rho_A^2 = \sum_{a,a'''} \left(\sum_{a',a'',b,b',b'',b'''} \Psi_0^*(a,b)\Psi_0^*(a'',b'')\Psi_0(a',b')\Psi_0(a'''',b''')\delta_{b,b'}\delta_{a',a''}\delta_{b'',b'''} \right) \delta_{a,a'''} \tag{9}$$

$$= \sum_{a,a',a'',a''',b,b',b'',b'''} \Psi_0^*(a,b)\Psi_0^*(a'',b'')\Psi_0(a',b')\Psi_0(a'''',b''')\delta_{a,a'''}\delta_{b,b'}\delta_{a',a''}\delta_{b'',b'''} \tag{10}$$

As discussed above, our ensemble of 4 disconnected paths has a weight proportional to:

$$W\Big(\{a,b\},\{a',b'\},\{a'',b''\},\{a''',b'''\}\Big) = \Psi_0^*(a,b)\Psi_0^*(a'',b'')\Psi_0(a',b')\Psi_0(a'''',b''') \tag{11}$$

where $\{a,b\},\{a',b'\},\{a'',b''\},\{a''',b'''\}$ are the Fock states at one end of each of the four disconnected paths. So in this ensemble, the estimator for $(\{a,b\},\{a',b'\},\{a'',b''\},\{a''',b'''\}$ is:

$$\mathrm{Tr}\rho_A^2 = \frac{1}{Z} \sum_{(a,a',a'',a''',b,b',b'',b''')_W} \delta_{a,a'''}\delta_{b,b'}\delta_{a',a''}\delta_{b'',b'''} \tag{12}$$

with the normalization factor

$$Z = \frac{1}{Z} \sum_{(a,a',a'',a''',b,b',b'',b''')_W} \delta_{a,a'}\delta_{b,b'}\delta_{a'',a'''}\delta_{b'',b'''} \tag{13}$$