Error in pBCS-S.C. CPMC

icf

1/2019

1 Introduction

For the "worried part" we discussed before, I found that due to some mistake it converged to the wrong results in S.C.CPMC with exact input and when I correct, it then converge to the correct results. (Please check the Figure.1)

There are two main "hard to understand" parts in the experiments of Error in pBCS S.C. CPMC

1. With exact density matrix from ED, we can get following pBCS state and with Variational Method the error between the density matrix of pBCS and Ground state can be minimized.

However, we found that in 4*4 u=8 3up 3dn, 4*4 u=8 5up 5dn, 4*4 u=8 7up 7dn the mixed density matrix $\langle FE|C_i^\dagger C_j|pBCS\rangle/\langle FE|pBCS\rangle$ always equal to $\langle FE|C_i^\dagger C_j|FE\rangle/\langle FE|FE\rangle$. ("FE" means "Free electrons")

2. With exact density matrix from ED and extrapolation, statistic error must cover exact error ($ExactDensityMatrix - DensityMatrixfromCPMC$) . However in system 4*4 u=8 3up 3dn and 4*4 u=8 7up 7dn, systemic error always exist. Because of degeneracy?

Also there is one small question: how to get a good results in 4*4 u=8 3up 3dn with CPMC like Hao's "Symmetry" paper?

2 Results

Figure 1: This is the results of 4 by 4 2-D Hubbard model in PBS with 7up 7dn electrons. 20 step S.C. CPMC with "Analytic Decomposed pBCS" trial wave functions.

Error in Density, extrapolate, Exact input pBCS CPMC							
4477u8 t0.01t0.02 Exact Energy:-11.875287631894714			step 20 Energy:-11.86421714		0.01674376	-11.36972425	0.00284917
Exact			Nsample: 20 Nwalker: 500*2*20				
real	imag		real	imag	error	real abs(exact-cpmc)	imag abs(exact-cpmc)
0.4375	0		0.431053	2.08E-05	2.17E-03	0.006447019	2.07513E-05
0.132315	4.47E-03		0.129476	-3.39E-03	2.03E-03	0.002838677	0.007862298
0.4375	0		0.440519	1.04E-04	2.56E-03	0.003019348	0.000104109
					1.06E+00	**1.24E+01**	**2.74E+00**
4477u8 with t0.01t0.02 inpuyt Exact Energy: -11.8688			step 20 Energy:-11.89700886		0.01264702	-11.42273882	0.00347112
Exact			Nsample: 20 Nwalker: 500*2*20				
real	imag		real	imag	error	real abs(exact-cpmc)	imag abs(exact-cpmc)
0.4375	0		0.434426	1.52E-06	1.87E-03	0.003074049	1.52376E-06
0.140854	0		0.129763	6.93E-06	1.88E-03	0.011090724	6.92843E-06
0.4375	0		0.437924	-5.23E-06	1.58E-03	0.000424262	5.23312E-06
					1.08E+00	**8.19E+00**	**5.91E-03**

Figure 2: This is the results of 4 by 4 2-D Hubbard model in PBS with 3up 3dn electrons, "Analytic", "DET" and "FE" are "Analytic Decomposed pBCS", "Determinant Decomposed pBCS" and "Free Electrons" trial wave functions.

Error in Density, extrapolate, Exact input pBCS CPMC												
4433u8 Exact Energy: -14.7235403	Energy: -14.45620188	0.04688154	-14.13803685	0.006	Energy: -14.37520483	0.02654943	-14.14105856	0.0031	Energy: -14.37024105	0.02282915	-14.13816755	0.00143155
Exact	Nsample: 5 Nwalker: 500*4	Error	ABS(Exact-CPMC)		Nsample: 10 Nwalker: 500*4	Error	ABS(Exact-CPMC)		Nsample: 20 Nwalker: 500*4	Error	ABS(Exact-CPMC)	
0.1875	0.194188812	5.78E-03	0.006689		0.195082504	2.90E-03	0.007583		0.197547126	2.08E-03	0.010047	
0.1875	0.201927973	5.30E-03	0.014428		0.200189528	3.19E-03	0.01269		0.201581582	1.82E-03	0.014082	
		2.72E+00	**2.97E+00**			**2.00E+00**	**2.47E+00**			**1.42E+00**	**2.19E+00**	

Figure 3: This is the results of 4 by 4 2-D Hubbard model in PBS with 5up 5dn electrons, "Analytic", "DET" and "FE" are "Analytic Decomposed pBCS", "Determinant Decomposed pBCS" and "Free Electrons" trial wave functions.

Error in Density, extrapolate, Exact input pBCS CPMC										
4455u8 Exact Energy:	Analytic step 1 Energy:-17.46047399	0.05233907	-17.6347	Analytic step 1 Energy:-17.48395020	0.03169573	-17.62970079	Analytic step 1 Energy: -17.43572441	0.02470176	-17.63823991	0.00266869
Exact	Nsample: 5 Nwalker: 500*4	error	abs(exact-cpmc)	Nsample: 10 Nwalker: 500*4	error	abs(exact-cpmc)	Nsample:20 Nwalker: 500*4	error	abs(exact-cpmc)	
0.3125	0.313523057	4.28E-03	0.001023	0.311046278	1.47E-03	0.001454	0.313709897	1.82E-03	0.00121	
0.3125	0.312244648	1.89E-03	0.000255	0.313780409	4.56E-03	0.00128	0.31098138	2.95E-03	0.001519	
		2.54E+00	**2.195605**		**1.93E+00**	**1.7678**		**1.42E+00**	**1.404117**	
	DET step 1 Energy:-17.53840230	0.07492043	-17.4447384	DET step 1 Energy:-17.46658851	0.01599752	-17.44785561 0.	DET step 1 Energy:-17.47044231	0.02621622	-17.44871372	0.00359000
Exact	Nsample: 5 Nwalker: 500*4	error	abs(exact-cpmc)	Nsample: 10 Nwalker: 500*4	error	abs(exact-cpmc)	Nsample:20 Nwalker: 500*4	error	abs(exact-cpmc)	
0.3125	0.31198012	4.46E-03	0.00052	0.313423995	2.91E-03	0.000924	0.313337831	1.90E-03	0.000838	
0.3125	0.307727689	3.18E-03	0.004772	0.313177431	4.85E-03	0.000677	0.311494321	1.86E-03	0.001006	
		2.50E+00	**2.339496**		**1.90E+00**	**1.817722**		**1.51E+00**	**1.413546**	
	FE step 1 Energy:-17.45587549	0.04011663	-17.45087672	FE step 1 Energy:-17.47736162	0.03355420	-17.44830195 0.0	FE step 1 Energy:-17.47667895	0.02275442	-17.45142914	0.00304038
Exact	Nsample: 5 Nwalker: 500*4	error	abs(exact-cpmc)	Nsample: 10 Nwalker: 500*4	error	abs(exact-cpmc)	Nsample:20 Nwalker: 500*4	error	abs(exact-cpmc)	
0.3125	0.316154197	7.07E-03	0.003654	0.314971574	4.03E-03	0.002472	0.315619603	2.18E-03	0.00312	
0.3125	0.308877554	2.41E-03	0.003622	0.310400338	2.21E-03	0.0021	0.311995392	1.69E-03	0.000505	
		2.45E+00	**2.223363**		**1.79E+00**	**1.66393**		**1.28E+00**	**1.259751**	

Figure 4: This is the results of 4 by 4 2-D Hubbard model in PBS with 7up 7dn electrons. CPMC with "Analytic Decomposed pBCS" trial wave functions.

Error in Density, extrapolate, Exa			Extrapolate																	
4477u8 t0.01t0.02 Exact Energy:-			step 1 Energy:-11.94277480			0.11438742	-11.40644238	0.02	step 1 Energy:-11.89983622			0.08053707	-11.39274051	0.02	step 1 Energy: -11.85013709			0.05106370	-11.36726030	0.00897944
Exact			Nsample: 5 Nwalker: 500*4						Nsample: 10 Nwalker: 500*4						Nsample: 20 Nwalker: 500*4					
real	imag		real	imag	error	real abs(ex	imag abs(exact-cpmc		real	imag	error	real abs(ex	imag abs(exact-cpmc		real	imag	error	real abs(ex	imag abs(exact-cpmc)	
0.4375	0		0.440525	-5.48E-04	1.11E-02	0.003025	0.000548		0.42855	2.51E-04	9.73E-03	0.00895	0.000251		0.438845	6.67E-04	6.66E-03	0.001346	0.006659	
0.132315	4.47E-03		0.131414	-2.63E-03	3.57E-03	0.0009	0.007102		0.122207	-2.26E-03	6.00E-03	0.010108	0.00673		0.136054	-1.10E-03	5.32E-03	0.003739	0.000842	
0.4375	0		0.472916	-7.29E-04	1.11E-02	0.035416	0.000729		0.420339	-4.14E-04	9.11E-03	0.017161	0.000414		0.465867	-2.53E-04	7.40E-03	0.028367	0.0074	
					6.09E+00	**1.53E+01**	**3.91E+00**				**5.72E+00**	**1.50E+01**	**3.17E+00**				**3.31E+00**	**1.35E+01**	**3.74E+00**	
4477u8 with t0.01t0.02 inpuyt Exact Energy: -11.8688															step 1 Energy:-11.87210960			0.05635029	-11.42729617	0.00945646
Exact															Nsample: 20 Nwalker: 500*4					
real	imag														real	imag	error	real abs(ex	imag abs(exact-cpmc)	
0.4375	0														0.426261	3.53E-06	5.51E-03	0.011239	3.53E-06	
0.140854	0														0.137516	-1.83E-05	7.40E-03	0.003338	1.83E-05	
0.4375	0														0.440952	-6.24E-05	8.64E-03	0.003452	6.24E-05	
																	3.31E+00	**9.06E+00**	**2.70E-02**	

Figure 5: The error between the Density Matrix of Analytic pBCS, VMpBCS and Exact Denisty Matrix.

pBCS -- traget Green(eigen value)

4455u8

Exact Gree	pBCS Gree	abs(Green-pBCS)	VMpBCS	abs(Green-VMpBCS)
3.02E-02	1.78E-02	0.012380473	1.05E-02	0.01968
3.03E-02	1.79E-02	0.012436473	3.24E-02	0.002136
3.05E-02	1.80E-02	0.012533293	3.26E-02	0.002033
3.06E-02	1.81E-02	0.012573787	3.26E-02	0.002002
3.25E-02	1.92E-02	0.013314797	3.40E-02	0.001471
7.89E-02	4.83E-02	0.030637401	8.01E-02	0.001227
8.06E-02	4.94E-02	0.031248657	8.15E-02	0.000815
8.14E-02	4.99E-02	0.03151538	8.21E-02	0.000678
8.16E-02	5.00E-02	0.031579157	8.22E-02	0.000653
8.24E-02	5.06E-02	0.031866746	8.29E-02	0.000456
8.42E-02	5.17E-02	0.032486097	8.68E-02	0.002621
0.857759	0.912974	0.055214976	0.858804	0.001045
0.858882	0.913737	0.054855138	0.859731	0.000849
0.861026	0.91519	0.054164675	0.861498	0.000472
0.862062	0.915891	0.053829057	0.86235	0.000288
0.916941	0.951449	0.034508413	0.919876	0.002935
		0.505144518		**0.039361**