

GHF-S.C. CPMC

icf

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1 Introduction

GHF-S.C.CPMC:

Starting with GHF and then applying the results of GHF to S.C.CPMC.

Since the results of GHF is "coupled Slater determinate" (noted as DET state) and the normal form of pseudo-BCS is decoupled, the coupled pseudo-BCS is needed and the related modification of overlap with DET state, Green Function with DET state, Back propagation is needed.

2 Results

Figure 1: This is the results of 4 by 4 2-D Hubbard model in PBS, "GHF" is the Energy of GHF and "first step" is the results of one step CPMC by applying the results of GHF as trial wave function.

t' model	t'	CPMC	S.C. CPMC	GHF	first-step	GHF-S.C.CPMC	ED
44 u=4 6u6nPBC	0.2	-19.189(5)	-19.223(7)	-17.1591	-19.212(6)	-19.226(8)	-19.1814036
	-0.2	-17.624(5)	-17.716(4)	-15.5591	-17.742(5)	-17.699(6)	-17.76140003
44 u=4 7u7nPBC	0.2	-16.773(8)	-17.092(7)	-15.485	-17.127(6)	-17.103(8)	-17.182938
	-0.2	-16.400(5)	-16.414(5)	-13.885	-15.904(5)	-16.393(4)	-16.4105626
44 u=4 8u8nPBC	0.2	-13.237(1)	-13.50(1)	-12.5665	-13.486(6)	-13.499(6)	-13.627869
	-0.2	-13.245(8)	-13.496(8)	-12.5665	-13.473(5)	-13.495(7)	-13.627869

Figure 2: This is the results of 4 by 4 2-D Hubbard model in PBS, $u = -4$ $t' = 0$ half-filling, "FE/UHF/GHF" is the Energy of Free Electrons/UHF/GHF, "FE/UHF/GHF CPMC" are the results of one step CPMC by applying the results of Free Electrons/UHF/GHF as trial wave function and "FE/UHF/GHF S.C.CPMC" are the results of 20 step S.C.CPMC by applying the results of Free Electrons/UHF/GHF as trial wave function at the first step. (The UHF results are from decoupled system and GHF, FE results are from coupled system.)

t' model	t'	FE	FE CPMC	FE S.C. CPMC	UHF	UHF CPMC	UHF S.C. CPMC	GHF	GHF CPMC	GHF S.C. CPMC
44 u=-4 8u8nPBC	0	-40.8203	-45.20(3)	-45.51(1)	-34.1875	-44.366(9)	-45.61(1)	-37.7613	-44.348(9)	-45.52(1)

Figure 3: This is GHF results of $Sz(i) = (N(i)_{up} - N(i)_{dn})/2$ for 4 by 4 2-D Hubbard model in PBS $u = -4$ $t' = 0$ half-filling. ($Sz(i) = 0$ for 4 by 16 2-D Hubbard model in PBS, $u = -4$ $t' = 0$ half-filling)

Density Wave (Sz)			
44 u=4 8u8nPBC			
9.17E-04	3.39E-03	3.14E-03	-1.41E-02
-3.65E-03	9.16E-03	-1.08E-02	1.23E-03
3.14E-03	-1.41E-02	9.17E-04	3.39E-03
-1.08E-02	1.23E-03	-3.65E-03	9.16E-03

3 Conclusion

GHF gives a very good approximation to Ground state of t' model in some cases, but they still won't improve the results of S.C CPMC too much.

References