Supplementary Information of Topological phases of extended Su-Schrieffer-Heeger-Hubbard model

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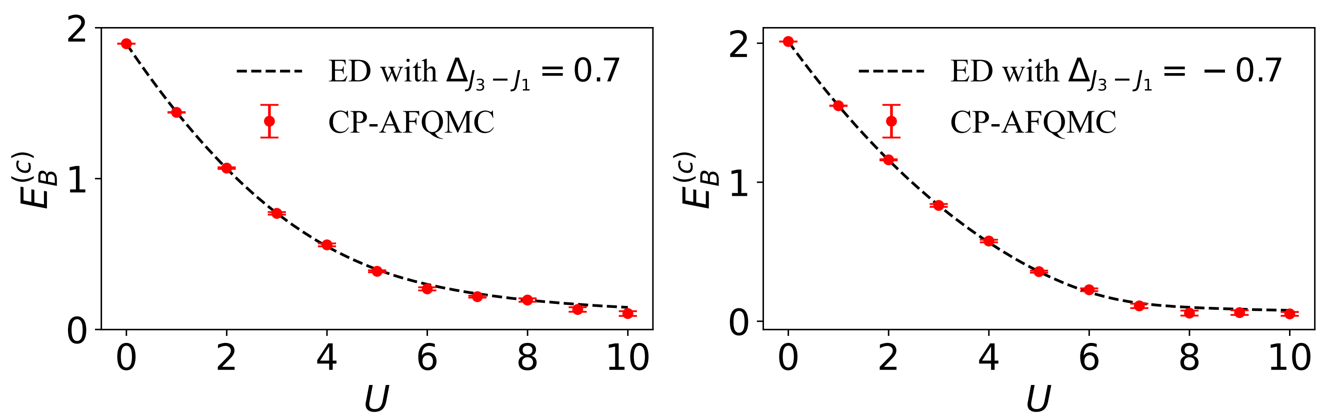
ABSTRACT

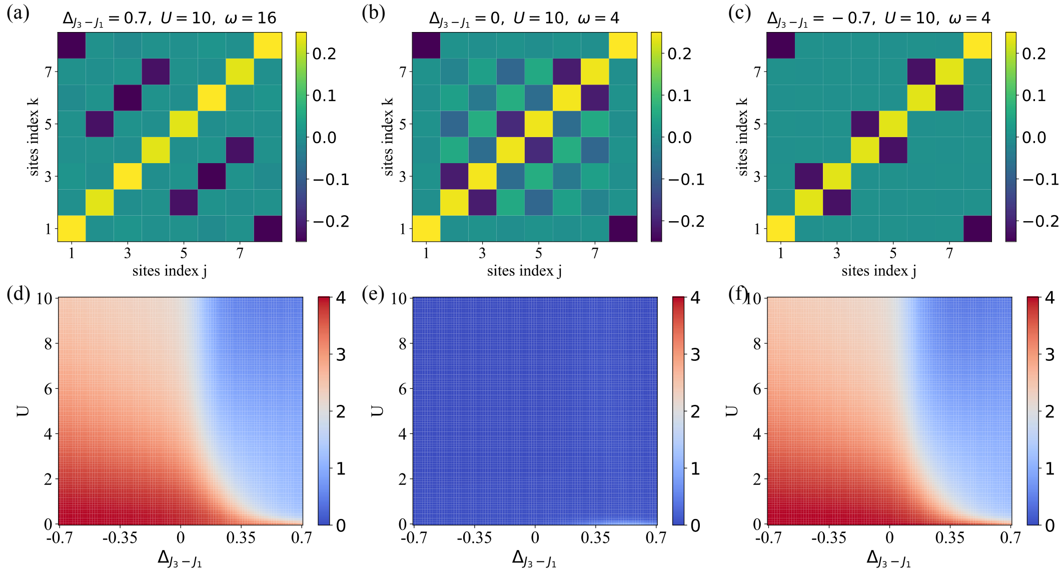
This section serves as a supplementary part of the main text and is primarily composed of the following four components: 1) A comparison of the CP-AFQMC results with those obtained from exact diagonalization calculations for small-sized systems; 2) An explanation of how to compute spin correlations within the CP-AFQMC framework; 3) The determination of spin correlations via exact diagonalization calculations; 4) The calculation of critical magnetic fields under different parameters using CP-AFQMC.

Comparison of ED and CP-AFQMC results with 1D $N = 8$ chain

To demonstrate the precision of CP-AFQMC results especially when there is a sign problem, we calculate the magnitude of the critical field for a quarter-filling 1D chain with $N = 8$ sites as a function of Hubbard U, selecting $\Delta_{J_3-J_1} = -0.7$ and $\Delta_{J_3-J_1} = 0.7$, which correspond to the leftmost and rightmost parameters in Fig. 6(e) of the main text. Due to the reduced system size, the imaginary time evolution length for the CP-AFQMC calculations was appropriately shortened. This optimization improves computational efficiency without compromising accuracy for small systems, such as the chain with $N = 8$ sites and the number of electrons $n = 4$. The parameters we choose here are: $\tau = 0.01$, $N_{walker} = 200$, $\beta = 40 \times 16 \times \tau = 6.4$. Under the above parameters, we can calculate a relatively accurate value of the critical magnetic field, as shown in Supplementary figure 1. Compared with the exact diagonalization results, CP-AFQMC gives consistent calculation results.



Supplementary figure 1. The magnitude of the critical field for a quarter-filling 1D chain with $N = 8$ sites and electron numbers $n = 4$ as a function of Hubbard U.



Supplementary figure 2. ED results same as Fig. 4 of the main text Spin correlation $\langle S_{z,j}S_{z,k}\rangle$ with $\Delta_{J_3-J_1}=0.7$, topological edge states appear at 1_{st} site, 3_{rd} site, 6_{th} site and 8_{th} site. (b) Spin correlation with $\Delta_{J_3-J_1}=0$ and there is a long-range anti-ferromagnetic order. (c) Spin correlation with $\Delta_{J_3-J_1}=-0.7$, and topological edge states appear at 1_{st} site and 8_{th} site. And ω is the degeneracy of ground state. (d) The entanglement Rényi entropy between subsystem $A=[3_{rd},6_{th}]$ sites and the remaining sites $\overline{A}$. (e) Rényi entropy (d) but subsystem $A=[1_{st},8_{th}]$ sites and (f) with subsystem $A=[1_{st},3_{rd},6_{th},8_{th}]$ sites. In (d)-(f), the position where the transition occurs is far from $\Delta_{J_3-J_1}=0$, which is result of finite-size effects.

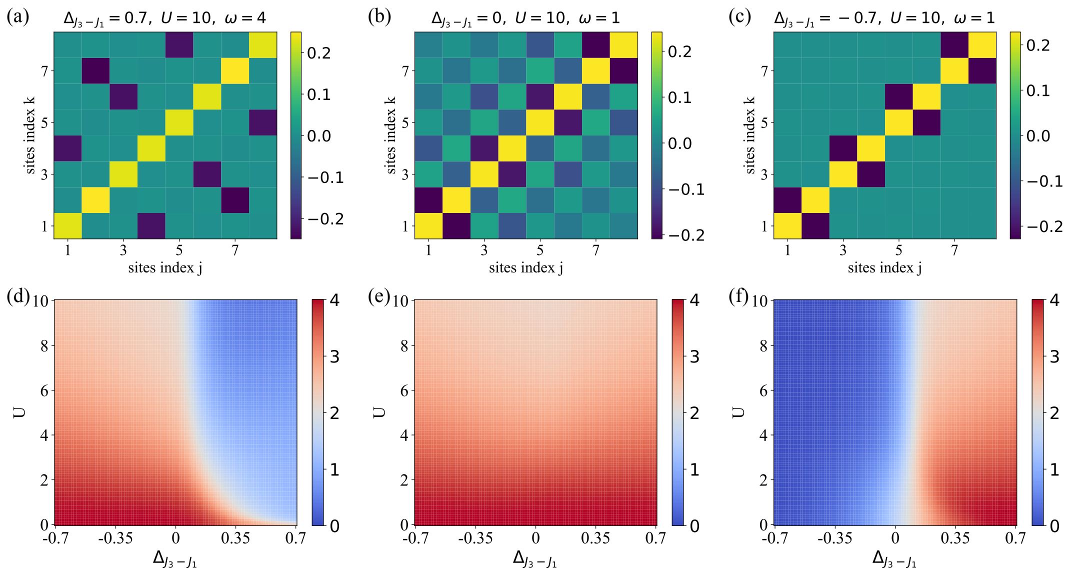
Calculation of spin correlation in CP-AFQMC

As before, we define the spin correlation as $C_{j,k}=\langle S_{z,j}S_{z,k}\rangle$ with $S_{z,j}=\frac{1}{2}(\hat{n}_{j,\uparrow}-\hat{n}_{j,\downarrow})$. In CP-AFQMC we can calculate the spin correlation through the Green function.

$$C_{j,k}=\frac{1}{4}\langle(\hat{n}_{j,\uparrow}-\hat{n}_{j,\downarrow})(\hat{n}_{k,\uparrow}-\hat{n}_{k,\downarrow})\rangle=\frac{1}{4}(G_{up}^{jj}G_{up}^{kk}-G_{up}^{kj}G_{up}^{jk}+G_{up}^{jk}\delta_{j,k}+G_{dn}^{jj}G_{dn}^{kk}-G_{dn}^{kj}G_{dn}^{jk}+G_{dn}^{jk}\delta_{j,k}-G_{dn}^{jj}G_{up}^{kk}-G_{up}^{jj}G_{dn}^{kk}). \tag{1}$$

Spin correlation and entropy base on Exact Diagonalization

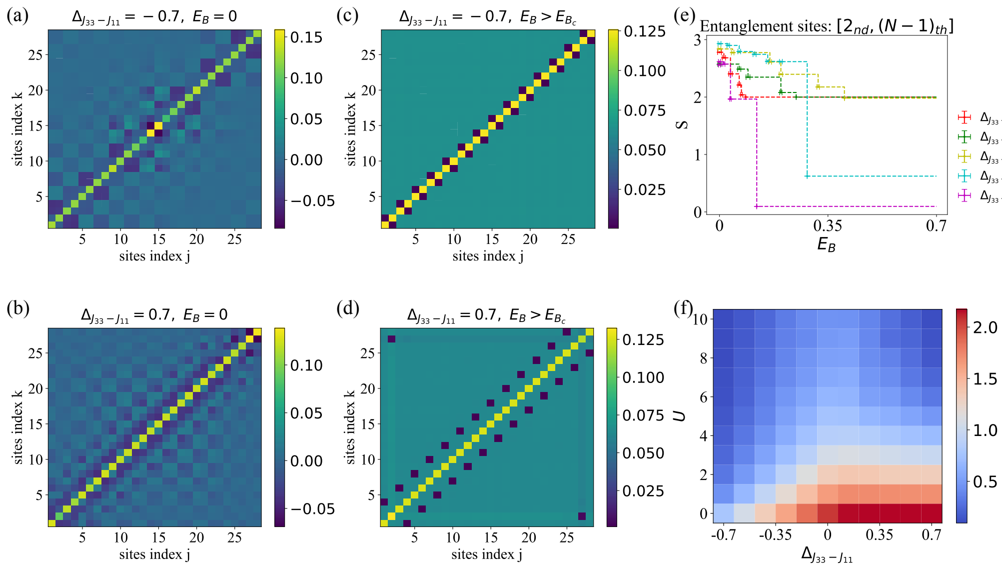
In this study, we employ the CP-AFQMC method to compute the spin correlation and second-order Rényi entropy at half-filling. To validate the precision of the CP-AFQMC results, we perform additional calculations using exact diagonalization on a small system to obtain the long-range spin correlation and second-order Rényi entanglement entropy, as shown in Supplementary figure 2 and Supplementary figure 3. The second-order Rényi entanglement entropy values obtained via ED exhibit a larger deviation from zero compared to the CP-AFQMC results. This discrepancy suggests more pronounced finite-size effects in the calculations using ED, probably attributable to the inherent limitations of exact diagonalization when applied to small systems.



Supplementary figure 3. ED results same as Fig. 5 of the main text. (a) Spin correlation $\langle S_{z,j} S_{z,k} \rangle$ with $\Delta_{J_{33}-J_{11}} = 0.7$, topological edge states appear at 2_{nd} site and 7_{th} site. (b) Spin correlation with $\Delta_{J_{33}-J_{11}} = 0$ and there is a long-range anti-ferromagnetic order. (c) Spin correlation with $\Delta_{J_{33}-J_{11}} = -0.7$, and there are bulk dimers without topological edge states. (d) The entanglement Rényi entropy between subsystem $A = [2_{nd}, 7_{th}]$ sites and the remaining sites $\overline{A}$. (e) Rényi entropy with subsystem $A = [1_{st}, 8_{th}]$ sites and (f) with subsystem $A = [1_{st}, 2_{nd}, 7_{th}, 8_{th}]$ sites. And due to the formation of dimers, there will be a drop in Rényi entanglement entropy.

Quarter-filling with changing $\Delta_{J_{33}-J_{11}}$

To further substantiate our conclusions, we employ the CP-AFQMC method to investigate the behavior of the system at varying values of $\Delta_{J_{33}-J_{11}}$ as shown in Supplementary figure 4. The results obtained corroborate the findings presented in Fig. 7 of the main text, demonstrating the restoration of long-range spin correlation and the disappearance of Rényi entanglement entropy above the critical magnetic field. Furthermore, the critical field strength exhibits a gradual decrease with increasing Hubbard U.



Supplementary figure 4. Same as Fig. 7 of the main text but for $J_1 = J_3 = 0.1$, and $U = 10$ for (a)-(e). (a) Spin correlation $\langle S_{z,j} S_{z,k} \rangle$ with $\Delta_{J_{33}-J_{11}} = -0.7$. (b) Spin correlation with $\Delta_{J_{33}-J_{11}} = 0.7$ and topological edge states appear at 2_{nd} site and $(N-1)_{th}$ site. (c) Spin correlation $\langle S_{z,j} S_{z,k} \rangle$ with $\Delta_{J_{33}-J_{11}} = -0.7$ above the critical magnetic field. (d) Spin correlation with $\Delta_{J_{33}-J_{11}} = 0.7$ above the critical magnetic field. (e) Rényi entanglement entropy with changing external magnetic field and hopping amplitude difference $\Delta_{J_{33}-J_{11}}$. (f) Critical field strength at various of the on-site interaction and hopping amplitude difference and it can be seen that for a certain $\Delta_{J_{33}-J_{11}}$, the value of the critical magnetic field will decrease as U increases.