On Floquet-Hubbard model

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Model The Floquet-Hubbard Hamiltonian is written as [1]

$$
\begin{aligned}
H &= -\sum_{n.n.,\sigma} t_x \left[\mathcal{J}_0(K_0)\hat{a}_{ij\bar{\sigma}} + \mathcal{J}_l(K_0)\hat{b}^l_{ij\bar{\sigma}}\right] c^\dagger_{i\sigma}c_{j\sigma} + h.c. + g\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} \\
&= -\sum_{\substack{i\in A, j\in B\\ n.n.,\sigma}} t_x \Big(\mathcal{J}_0(K_0)\left[(1-\hat{n}_{i\bar{\sigma}})(1-\hat{n}_{j\bar{\sigma}}) + \hat{n}_{i\bar{\sigma}}\hat{n}_{j\bar{\sigma}}\right] \\
&\qquad + \mathcal{J}_l(K_0)\left[(-1)^l(1-\hat{n}_{i\bar{\sigma}})\hat{n}_{j\bar{\sigma}} + \hat{n}_{i\bar{\sigma}}(1-\hat{n}_{j\bar{\sigma}})\right]\Big) c^\dagger_{i\sigma}c_{j\sigma} + h.c. \\
&\quad + g\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}
\end{aligned} \tag{1}
$$

Denote $t_0 = t_x\mathcal{J}_0(K_0)$ and $t_1 = t_x\mathcal{J}_l(K_0)$ and set $l = 2$, it is rewriten as

$$
\begin{aligned}
H = -\sum_{\langle i,j\rangle\sigma} &\Big(t_0\left[(1-\hat{n}_{i\bar{\sigma}})(1-\hat{n}_{j\bar{\sigma}}) + \hat{n}_{i\bar{\sigma}}\hat{n}_{j\bar{\sigma}}\right] + t_1\left[(1-\hat{n}_{i\bar{\sigma}})\hat{n}_{j\bar{\sigma}} + \hat{n}_{i\bar{\sigma}}(1-\hat{n}_{j\bar{\sigma}})\right]\Big) c^\dagger_{i\sigma}c_{j\sigma} \\
&+ h.c. + g\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}
\end{aligned} \tag{2}
$$

Here $\langle i,j\rangle$ means $i\in A, j\in B$ sitting on nearest neighbouring sites. In the following we consider this model on a square lattice.

Mean field Introducing charge density wave (CDW) order parameter c and spin density wave (SDW) order parameter s, along with their Lagrangian multipliers η_c and η_s respectively, we write down a mean-field Hamiltonian as

$$
\begin{aligned}
H_{\text{meanF}} = \sum_k &\Big[-P_\uparrow(c,s)Q(k)a^\dagger_{k\uparrow}b_{k\uparrow} - P_\downarrow(c,s)Q(-k)a^\dagger_{k\downarrow}b_{k\downarrow}\Big] + H.c. \\
&+ \frac{gN}{2}(1 + c^2 - s^2) \\
&+ \eta_c\left[c - \frac{(\hat{n}_{A\uparrow} + \hat{n}_{A\downarrow}) - (\hat{n}_{B\uparrow} + \hat{n}_{B\downarrow})}{2}\right]N \\
&+ \eta_s\left[s - \frac{(\hat{n}_{A\uparrow} - \hat{n}_{A\downarrow}) - (\hat{n}_{B\uparrow} - \hat{n}_{B\downarrow})}{2}\right]N
\end{aligned} \tag{3}
$$

where $Q(k) = \sum_i \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_i)$ and

$$
P_\uparrow(c,s) = \frac{t_0}{2}[1-(c-s)^2] + \frac{t_1}{2}[1+(c-s)^2] \tag{4}
$$

$$
P_\downarrow(c,s) = \frac{t_0}{2}[1-(c+s)^2] + \frac{t_1}{2}[1+(c+s)^2] \tag{5}
$$

$a(b)$ is the anniliation operator on A(B) sublattice.

The mean field phase diagram is shown in Fig.1

The free region seems unreasonable in a mean-field framework. To revisit, we modify the mean-field Hamiltonian to accommodate also cases with enlarged unit cell.

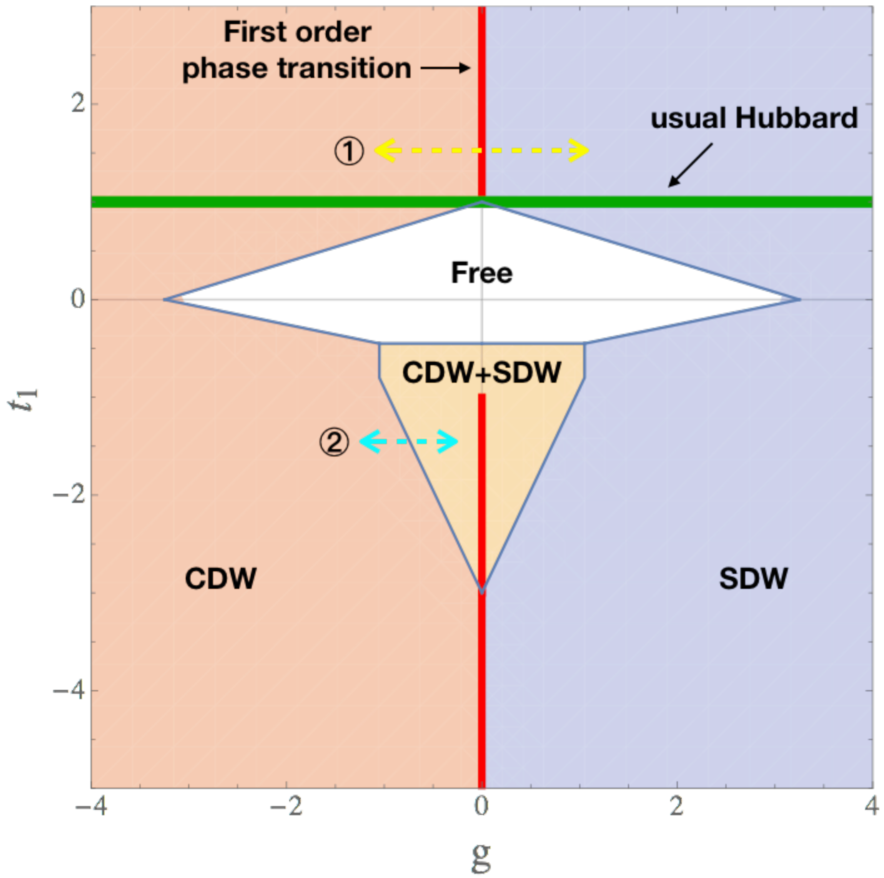

Figure 1: Mean-field phase diagram (I). With $t_0 = 1$ fixed, total particle density $n = 1$ fixed. Red line: phase boundary with first-order phase transition. Green line: usual Fermi-Hubbard model. Other lines: phase boundary with second-order phase transition. ①: typical first-order phase transition. ②: typical second-order phase transition.

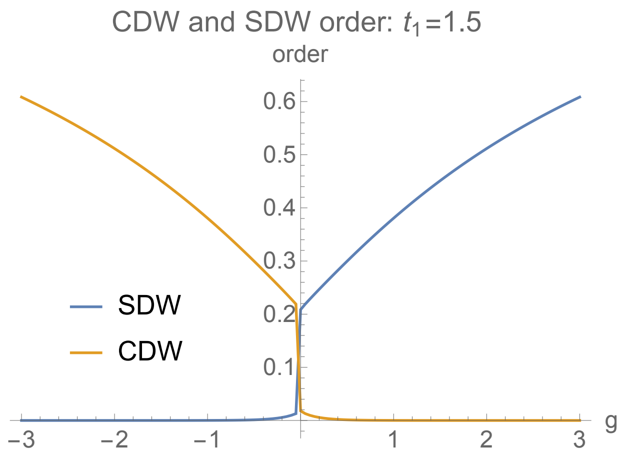

Figure 2: Magnitude of order parameters along ① in Fig.1, a demonstration of the first-order phase transition.

Unit cell enlarged Lattices with enlarged unit cell (eUC) is shown in Fig.3 for 2×2 case and 3×3 case.

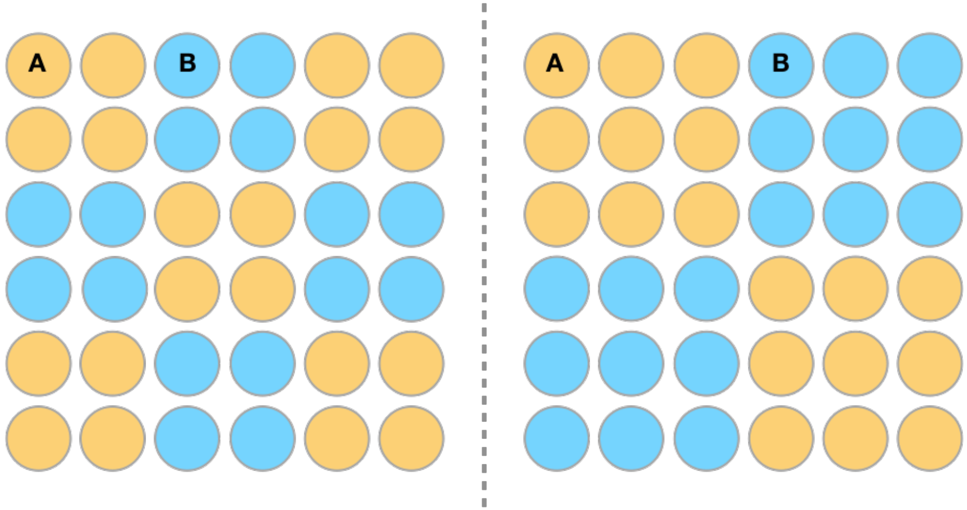

Figure 3: Schematic eUC. Left panel: 2×2. Right panel: 3×3

Under such circumstances, the tunneling part of the Hamiltonian is modified as

$$P_{\uparrow}^{(AA)}(c,s) = \frac{1}{2}[t_0 + t_1 + (t_0 - t_1)(c-s)^2] \tag{6}$$

$$P_{\uparrow}^{(BB)}(c,s) = P_{\uparrow}^{(AA)}(c,s) \tag{7}$$

$$P_{\uparrow}^{(AB)}(c,s) = \frac{1}{2}[t_0 + t_1 - (t_0 - t_1)(c-s)^2] \tag{8}$$

$$P_{\downarrow}^{(AA)}(c,s) = \frac{1}{2}[t_0 + t_1 + (t_0 - t_1)(c+s)^2] \tag{9}$$

$$P_{\downarrow}^{(BB)}(c,s) = P_{\downarrow}^{(AA)}(c,s) \tag{10}$$

$$P_{\downarrow}^{(AB)}(c,s) = \frac{1}{2}[t_0 + t_1 - (t_0 - t_1)(c-s)^2] \tag{11}$$

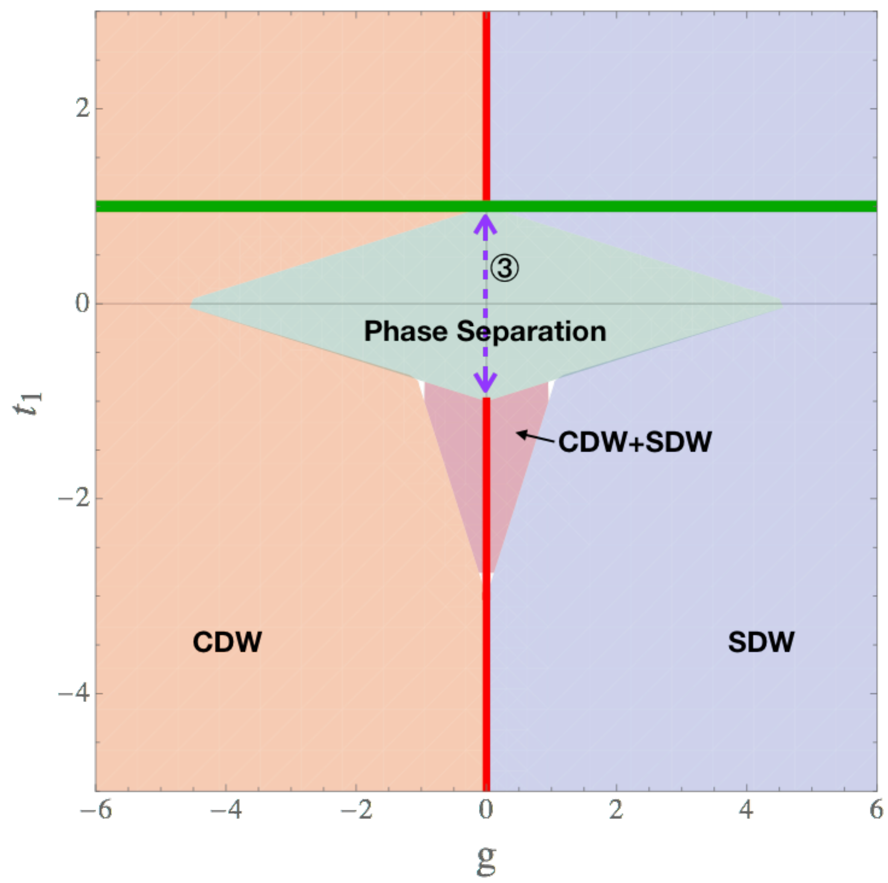

Figure 4: Mean-field phase diagram (II). ③: correlated tunneling induced phase seperation regime (g=0).

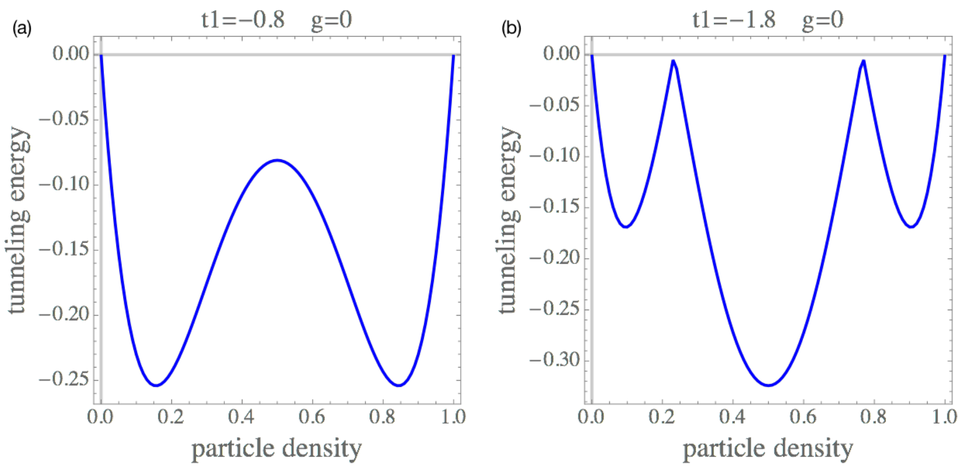

Figure 5: Total energy as a function of particle density (for one spin species) when $g = 0$. On segment shown in Fig.4 ③, system favors phase separation as manifested.

Summary The result of this work is interesting in:

- coexistance of CDW and SDW
- the first-order phase transion in g approaching 0 (while usual Fermi-Hubbard model therein is second-order.)
- phase separation region

References

[1] ETH group, Enhancement and sign reversal of magnetic correlations in a driven quantum many-body system, Nature **553**, 481485 (2018).

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