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Note on Floquet-Hubbard mean field

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Abstract:

In this note we provide a mean-field treatment to the Floquet-Hubbard model derived from some resonant shaken optical lattice at some special cases. Mean-field phase diagram is obtained. In addition to the charge-density wave and spin-density wave order in the usual bipartitle Hubbard model, there is a new phase of coexistence of them. Moreover, there is a free phase with no order to appear. This is also different from an usual Hubbard model on a square lattice at half-filling, where there must be none-zero order even at small interaction due to the nesting of the Fermi Surface. The result indicates that shaking may destroy or support the coexistence of orders.

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1 Floquet-Hubbard model

Through shaking of the optical lattice, a stroboscopically effective Hamiltonian, which is named Floquet-Hubbard Hamiltonian, is obtained after averaging over a full period. The Floquet-Hubbard Hamiltonian is written as[1]

$$
\begin{aligned}
H &= -\sum_{n.n.,\sigma} t_x \left[\mathcal{J}_0(K_0)\hat{a}_{ij\bar{\sigma}} + \mathcal{J}_l(K_0)\hat{b}^l_{ij\bar{\sigma}} \right] c^\dagger_{i\sigma} c_{j\sigma} + h.c. + g\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} \\
&= -\sum_{\substack{i\in A, j\in B \\ n.n.,\sigma}} t_x \Big(\mathcal{J}_0(K_0)\Big[(1-\hat{n}_{i\bar{\sigma}})(1-\hat{n}_{j\bar{\sigma}}) + \hat{n}_{i\bar{\sigma}}\hat{n}_{j\bar{\sigma}}\Big] \\
&\qquad\qquad + \mathcal{J}_l(K_0)\Big[(-1)^l(1-\hat{n}_{i\bar{\sigma}})\hat{n}_{j\bar{\sigma}} + \hat{n}_{i\bar{\sigma}}(1-\hat{n}_{j\bar{\sigma}})\Big]\Big) c^\dagger_{i\sigma} c_{j\sigma} + h.c. \\
&\quad + g\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}
\end{aligned}
\tag{1.1}
$$

where $\sigma \in \{\uparrow, \downarrow\}$ and $\bar{\sigma}$ is the complement of σ in the set.

Here $K_0 = mA\omega d_x$ is determined by the shaken optical lattice. A is shaking amplitude and ω is shaking frequency. d_x is taken as the distance of two nearest neighbouring lattice site. In brief, the Hamiltonian above can be written as

$$
\begin{aligned}
H = -\sum_{\langle i,j\rangle,\sigma} &\Big(t_0\Big[(1-\hat{n}_{i\bar{\sigma}})(1-\hat{n}_{j\bar{\sigma}}) + \hat{n}_{i\bar{\sigma}}\hat{n}_{j\bar{\sigma}}\Big] + t_1\Big[(-1)^l(1-\hat{n}_{i\bar{\sigma}})\hat{n}_{j\bar{\sigma}} + \hat{n}_{i\bar{\sigma}}(1-\hat{n}_{j\bar{\sigma}})\Big]\Big) c^\dagger_{i\sigma} c_{j\sigma} \\
&+ h.c. + g\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}
\end{aligned}
\tag{1.2}
$$

depending on $\{t_0, t_1, g, l\}$.

l is a parameter also determined by the shaking details[1]. There are generally big differences whether l is even or odd. However, when $t_1 = 0$, the two cases reduce to one. Whatever calculation or analysis we do on the even case and the odd case should match at $t_1 = 0$.

2 Mean-field treatment

The Hamiltonian in the even case (l even) possess SO(4) symmetry, the same one that exists in a usual bipartite Hubbard model.[2] However, the SO(4) symmetry that exists in the usual Hubbard is lacked in the odd case. Besides, there are particle-hole symmetries at half-filling at both even and odd cases (defined different by a sublattice exchange operation).[3] Take all these into considerations, we provide a mean-field treatment firstly to the even case at half-filling, following how that is done in an usual Hubbard model.

Order parameters. The bipartite lattice is divided into A/B sublattices. The charge-density wave (CDW) order and spin-density wave (SDW) order, denoted as c and s respectively, is introduced as

$$\langle \hat{n}_A \rangle = 1 + c \qquad \langle \hat{S}^z_A \rangle = s \tag{2.1}$$

Hence

$$\langle \hat{n}_B \rangle = 1 - c \qquad \langle \hat{S}^z_B \rangle = -s \tag{2.2}$$

where we consider total charge density $\langle \hat{n} \rangle = 1$ (half-filling) and total magnetic momentum $\langle \hat{S} \rangle = 0$. Easy to verify that these two quantities are conserved. [4]

Mean-field Hamiltonian. Using a path-integral approach we write down a mean-field Hamiltonian as[1]

$$\begin{aligned} H_{\text{meanF}} = &\sum_k \Big[- P_\uparrow(c,s)Q(k)a^\dagger_{k\uparrow}b_{k\uparrow} - P_\downarrow(c,s)Q(-k)a^\dagger_{k\downarrow}b_{k\downarrow} \Big] + H.c. \\ &+ \frac{gN}{2}(1 + c^2 - s^2) \\ &+ \eta_c \left[c - \frac{(\hat{n}_{A\uparrow} + \hat{n}_{A\downarrow}) - (\hat{n}_{B\uparrow} + \hat{n}_{B\downarrow})}{2} \right] N \\ &+ \eta_s \left[s - \frac{(\hat{n}_{A\uparrow} - \hat{n}_{A\downarrow}) - (\hat{n}_{B\uparrow} - \hat{n}_{B\downarrow})}{2} \right] N \end{aligned} \tag{2.3}$$

[1] Actually it is merely depends on the resonant shaking frequency, [1, 2]

[2] See Appendix A for a detailed discussion. See Ref[3].

[3] See Appendix B.

[4] To simplify the notation, we will sometimes use the without-hat symbols to represent the expectation value of a quantity in the following. Means that the corresponding operators taken expectation value under a "real" self-consistent solution state. For example $n_A := \langle \hat{n}_A \rangle$.

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

$$P_\uparrow(c,s) = \frac{t_0}{2}[1-(c-s)^2] + \frac{t_1}{2}[1+(c-s)^2] \tag{2.4}$$

$$P_\downarrow(c,s) = \frac{t_0}{2}[1-(c+s)^2] + \frac{t_1}{2}[1+(c+s)^2] \tag{2.5}$$

In the representation of Nambu spinors the mean-field Hamiltonian reads

$$H_{\mathrm{meanF}} = \sum_k \left(a^\dagger_{k\uparrow} \; b^\dagger_{k\uparrow} \; a_{-k\downarrow} \; b_{-k\downarrow} \right) \mathcal{H}(k) \begin{pmatrix} a_{k\uparrow} \\ b_{k\uparrow} \\ a^\dagger_{-k\downarrow} \\ b^\dagger_{-k\downarrow} \end{pmatrix} + const.(\text{para.s}) \tag{2.6}$$

where

$$\mathcal{H}(k) = \begin{pmatrix} -\frac{1}{2}\eta_c - \frac{1}{2}\eta_s & -P_\uparrow(c,s)Q(k) & 0 & 0 \\ -P_\uparrow(c,s)Q(-k) & \frac{1}{2}\eta_c + \frac{1}{2}\eta_s & 0 & 0 \\ 0 & 0 & \frac{1}{2}\eta_c - \frac{1}{2}\eta_s & P_\downarrow(c,s)Q(k) \\ 0 & 0 & P_\downarrow(c,s)Q(-k) & -\frac{1}{2}\eta_c + \frac{1}{2}\eta_s \end{pmatrix} \tag{2.7}$$

and

$$const. = \left(\eta_c c + \eta_s s + \frac{g}{2}[1 + c^2 - s^2] \right) N \tag{2.8}$$

Mean-field phase diagram. looks like

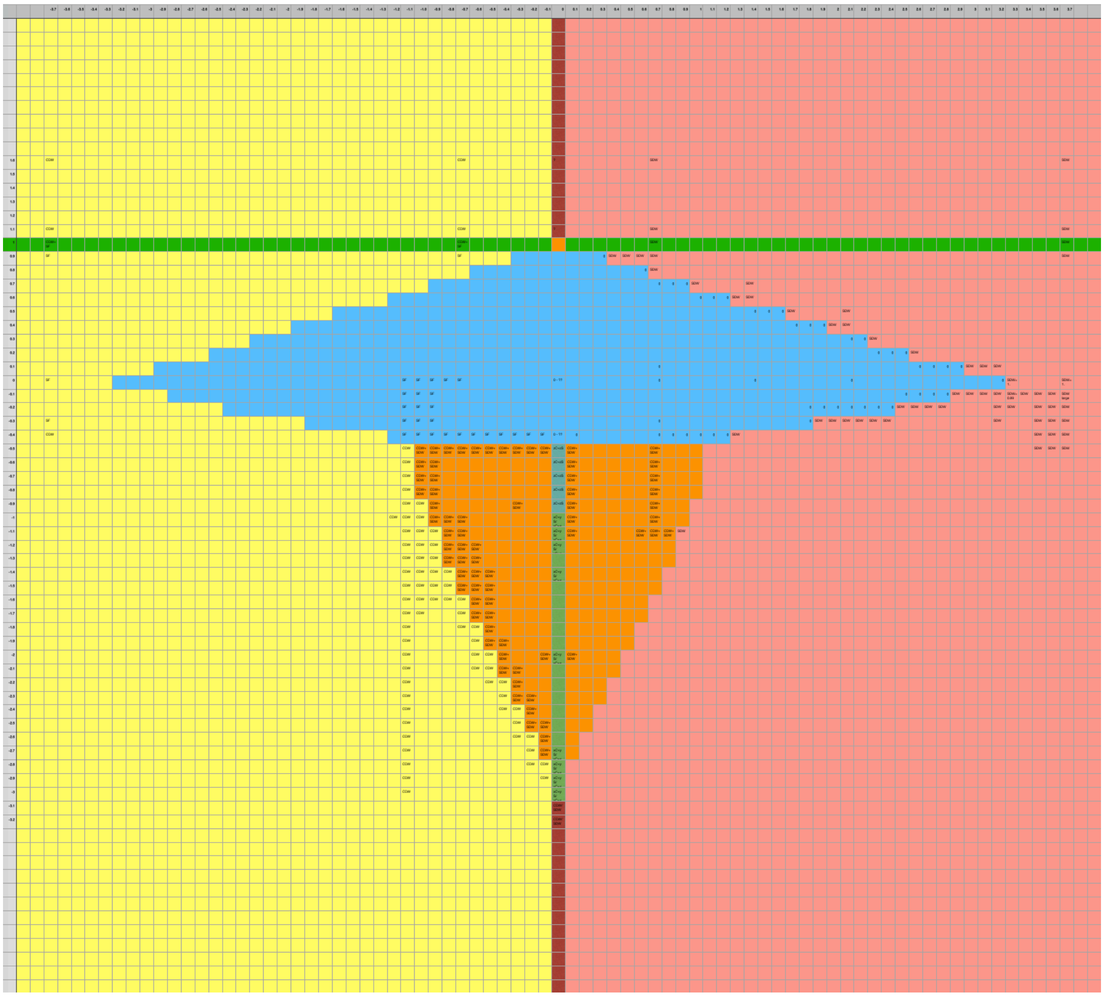

Figure 1: Mean-field phase diagram (in an EXCEL table form). Horizontal axis: interaction strength $g/|t_0|$. Verticle axis: hopping ratio $t_1/|t_0|$. COLOR REGION. Yellow: CDW. Pink: SDW. Orange: CDW+SDW. Blue: free. Dark red line (verticle): first order phase transtion. Green line (horizontal): the usual Hubbard model ($t_1 = t_0$).

A SO(4) symmetry

A.1 The usual bipartite Hubbard model

The usual bipartite Hubbard model, the Hamiltonian of which written as

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + h.c. + g \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) \tag{A.1}$$

possess SO(4) symmetry[3]. The Hamiltonian commutes with two sets of SU(2) generator operators, one of which is the usual spin rotation SU(2) and the other is related to the CDW and SF rotation symmetry which we call it charge SU(2). To show the Hamiltonian commutes with both these two SU(2), we firstly introduce two su(2) algebra as follows.

1. Spin su(2)

   Introduce single particle operators

   $$S_z = \frac{1}{2} \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow} \ , \quad S_+ = \sum_i c_{i\uparrow}^\dagger c_{i\downarrow} \tag{A.2}$$

   Introduce $S_- = (S_+)^\dagger$, $S_x = (S_+ + S_-)/2$, $S_y = (S_+ + S_-)/(2i)$. Easy to verify that $[S_+, S_-] = 2S_z$, and $[S_i, S_j] = \mathrm{i}\epsilon_{ijk} S_k$. Thus $\{S_x, S_y, S_z\}$ form a su(2) algebra.

2. Charge su(2)

   Introduce

   $$L_z = -\frac{1}{2} \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow} + \frac{1}{2} N \ , \quad L_+ = \sum_i (-1)^i c_{i\uparrow} c_{i\downarrow} \tag{A.3}$$

   and $L_- = (L_+)^\dagger$, $L_x = (L_+ + L_-)/2$, $L_y = (L_+ + L_-)/(2i)$. Easy to verify that $[L_+, L_-] = 2L_z$, and $[L_i, L_j] = \mathrm{i}\epsilon_{ijk} L_k$. Thus $\{L_x, L_y, L_z\}$ form a su(2) algebra.

   $(-1)^i$ means that its value is -1 if $i \in A$ or 1 if $i \in B$.

Several things should be noticed.

- The set of S operators and the set of L operators can be transformed to each other via a W transformation:

  $$W^{-1} c_{i\uparrow} W = (-1)^i c_{i\uparrow}^\dagger \tag{A.4}$$
  $$W^{-1} c_{i\downarrow} W = c_{i\downarrow} \tag{A.5}$$

- $W^{-1} H(g) W = H(-g)$. If we define a set $\mathcal{H} = \{H(t_0, g)\}$, we have that $[W, \mathcal{H}] = 0$.
- The spin su(2) symmetry can be easily verified. $[S_z, H] = 0$, $[S_+, H] = 0$.
- The charge su(2) symmetry can either be checked directly, by showing $[L_z, H] = 0$ and $[L_+, H] = 0$ directly, or be deduced using the above 3 points. The logic is since $[S, H] = 0$, meaning $[S, H(g)] = 0$ and $[S, H(-g)] = 0$, then $W^{-1}[S, H(g)]W = [W^{-1} S W, W^{-1} H(g) W] = [L, H(-g)] = 0$.

  This logic is of great use in showing the SO(4) symmetry in Floquet-Hubbard model.

- the charge SU(2) symmetry is the symmetry relates CDW and Cooper pair order in attractive interacting regime. Because of this symmetry, we can select a certain "direction" in the mean-field calculation, assuming the order is along a certain direction. If we choose SDW to along $z-$direction in repulsive regime, we can assume it along $z-$direction also in the attractive regime, which is the CDW order.
- $L_+ = \sum_i (-1)^i c_{i\uparrow} c_{i\downarrow} = \sum_i \exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{x}_i) c_{i\uparrow} c_{i\downarrow}$, with $\boldsymbol{Q} = (\pi, \pi)$.

A.2 Floquet-Hubbard model

The Floquet-Hubbard Hamiltonian in l even case reads

$$H = -\sum_{\langle i,j\rangle,\sigma} \left(t_0 \Big[(1-\hat{n}_{i\bar{\sigma}})(1-\hat{n}_{j\bar{\sigma}}) + \hat{n}_{i\bar{\sigma}}\hat{n}_{j\bar{\sigma}} \Big] + t_1 \Big[(1-\hat{n}_{i\bar{\sigma}})\hat{n}_{j\bar{\sigma}} + \hat{n}_{i\bar{\sigma}}(1-\hat{n}_{j\bar{\sigma}}) \Big] \right) c^\dagger_{i\sigma} c_{j\sigma} \\ + h.c. + g\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} \tag{A.6}$$

It has the same SO(4) symmetry as in the usual bipartite Hubbard model, which can be seen by directly showing $[S, H] = 0$, $[L, H] = 0$.

Or, after showing $[S, H] = 0$, and $W^{-1}H(g)W = H(-g)$, because of

$$W: \quad n_{i\uparrow} \to 1 - n_{i\uparrow} \\ n_{i\downarrow} \to n_{i\downarrow} \tag{A.7}$$

the $[L, H] = 0$ is revealed naturally following the logic above.

To show the spin SU(2) symmetry, consider the very original Hamiltonian from beginning[1, 2]

$$H(t) = -\sum_{\substack{\langle i,j\rangle \\ \sigma=\uparrow,\downarrow}} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \sum_{i,\sigma} f_i(t)\hat{n}_{i\sigma} \tag{A.8}$$

it's a usual bipartite Hubbard model adding a time-dependent term $\sum_{i,\sigma} f_i(t)\hat{n}_{i\sigma}$. Apparently this Hamiltonian possess spin-rotation SU(2) symmetry. Because the term added is a summation over the total particle number at each site. The Floquet-Hubbard Hamiltonian is obtained by doing a unitary transformation U_3[1] and then do time average over one full period. Formally,

$$H_{\text{flHubb}} = \frac{1}{T}\int_0^T dt U_3^\dagger H(t) U_3 \tag{A.9}$$

But $U_3 = R(t) = \exp(\mathrm{i}\sum_j l\omega t \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}) \exp(\mathrm{i}\sum_{j\sigma} F_j(t)\hat{n}_{j\sigma})$ which also depends merely on $\hat{n}_i$ and an interaction term (already shown to commute with S). Thus $[U_3, S] = 0$, the unitary transformation is one that does not break the spin-rotation SU(2) symmetry. Time average does not of course either. Hence $[S, H_{\text{flHubb}}] = 0$.

PS: Notice that what we have shown is that the Floquet-Hubbard Hamiltonian has spin-rotation SU(2) symmetry generally, no matter l is even or odd. But in odd case, the

Hamiltonian does not possess the same SO(4) symmetry as in an usual bipartite Hubbard model, not because of the lack of spin-rotation SU(2) symmetry, but that $[W, \mathcal{H}] \neq 0$. In this case the W transformation does not transform a $H(g)$ to a $H(-g)$, since it does not commutes with the density-dependent tunneling term.

B Particle-hole symmetries at half-filling

l even Define particle-hole transformation $C : c_{i\sigma} \to (-1)^i c^\dagger_{i\sigma}$. Hamiltonian is invariant under C. $[C, H] = 0$.

l odd Define particle-hole transformation $C : c_{i\sigma} \to (-1)^i c^\dagger_{i\sigma}$, and sublattice switching transformation $S : A \leftrightarrow B$. Hamiltonian is invariant under the combination of C and S. $[CS, H] = 0$.

C Self-consistent equations and the iterative solving scheme

Feynman-Hellman theorem tells us $\langle \partial H(\lambda)/\partial\lambda \rangle = \partial E(\lambda)/\partial\lambda$ where the expectation value of l.h.s. is taken under some eigenstates of H while E on r.h.s. is the corresponding eigen energy.

We solve here for the many-body ground state of the Floquet-Hamiltonian. Take partial derivative, successively, with respect to all 16 parameters, and let $\partial E(para.)/\partial para. = 0$, which implies

$$\sum_{k,i} u_i^*(k) \frac{\partial \mathcal{H}(k; para.)}{\partial para.} u_i(k) \Theta(-\epsilon_i(k)) + \frac{\partial const.}{\partial para.} = 0 \tag{C.1}$$

Here are some expressions used in iteratively carry out Eq. (C.1).

$$\frac{\partial P_\uparrow}{\partial c} = (t_1 - t_0)(c - s) = -\frac{\partial P_\uparrow}{\partial s} \tag{C.2}$$

$$\frac{\partial P_\downarrow}{\partial c} = (t_1 - t_0)(c + s) = \frac{\partial P_\downarrow}{\partial s} \tag{C.3}$$

And the Partial derivatives of the Nambu Hamiltonian with respect to η_c, η_s, c, s are:

$$\frac{\partial \mathcal{H}(k)}{\partial \eta_c} = \frac{1}{2} \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} \qquad \frac{\partial const.}{\partial \eta_c} = Nc \tag{C.4}$$

$$\frac{\partial \mathcal{H}(k)}{\partial \eta_s} = \frac{1}{2} \begin{pmatrix} -1 & & & \\ & 1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix} \qquad \frac{\partial const.}{\partial \eta_s} = Ns \tag{C.5}$$

$$\frac{\partial \mathcal{H}(k)}{\partial c} = \begin{pmatrix} 0 & -\frac{\partial P_\uparrow}{\partial c} Q(k) & & \\ -\frac{\partial P_\uparrow}{\partial c} Q(-k) & 0 & & \\ & & 0 & \frac{\partial P_\downarrow}{\partial c} Q(k) \\ & & \frac{\partial P_\downarrow}{\partial c} Q(-k) & 0 \end{pmatrix} \quad \frac{\partial const.}{\partial c} = (gc + \eta_c) N \tag{C.6}$$

$$\frac{\partial \mathcal{H}(k)}{\partial s} = \begin{pmatrix} 0 & -\frac{\partial P_\uparrow}{\partial s} Q(k) & & \\ -\frac{\partial P_\uparrow}{\partial s} Q(-k) & 0 & & \\ & & 0 & \frac{\partial P_\downarrow}{\partial s} Q(k) \\ & & \frac{\partial P_\downarrow}{\partial s} Q(-k) & 0 \end{pmatrix} \quad \frac{\partial const.}{\partial s} = [-gs + \eta_s] N \tag{C.7}$$

Acknowledgments

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References

[1] ns' detailed Note.

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