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Note on Floquet-Hubbard: details

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ABSTRACT:

Contents

1 Floquet approach: the Effective Hamiltonian of a shaking lattice

1.1 preparing knowledge

A shaking lattice in the cold atom laboratory appears often in such a form:

$$x \to \ \tilde{x} = x - A\cos(\omega t) \tag{1.1}$$

$$V(x, y, z) \to \ V(\tilde{x}, y, z) = V(x - A\cos(\omega t), y, z) \tag{1.2}$$

or similar.

Unitary transformation:

$$\psi(t) \to \ \tilde{\psi}(t) = U(t)\psi(t) \tag{1.3}$$

$$H \to \ \tilde{H} = UHU^{\dagger} + (\mathrm{i}\partial_t U)U^{\dagger} \tag{1.4}$$

To obtain this, just substitute the unitary transformation into the Shrödinger equation.

1.2 deriving the Floquet-Hubbard Hamiltonian

Consider Hamiltonian $H(t) = \dfrac{p^2}{2m} + V(x - x_0(t))$ where

$$x_0(t) = A\cos(\omega t) \tag{1.5}$$
$$\dot{x}_0(t) = -\omega A \sin(\omega t) = \frac{p_0(t)}{m} \tag{1.6}$$
$$p_0(t) = -m\omega A \sin(\omega t) \tag{1.7}$$
$$\dot{p}_0(t) = -m\omega^2 A \cos(\omega t) \tag{1.8}$$

Unitary 1: translation in $\hat{x}$-rep. tramsform to co-moving frame.

$$U_1(t) = \exp(\mathrm{i}\hat{p}x_0(t)) \tag{1.9}$$
$$U_1 x U_1^\dagger = \exp(\mathrm{i}\hat{p}x_0)x\exp(-\mathrm{i}\hat{p}x_0) = x + x_0 \tag{1.10}$$

$$\begin{aligned}
U_1 H U_1^\dagger &= \exp(\mathrm{i}px_0(t))V(x - x_0(t))\exp(-\mathrm{i}px_0(t)) + \frac{p^2}{2m} \\
&= \frac{p^2}{2m} + V(x) && (1.11) \\
\mathrm{i}\partial_t U_1(t) &= \mathrm{i}\partial_t \exp(\mathrm{i}px_0(t)) \\
&= -p\dot{x}_0(t) \\
&= \omega A \sin(\omega t)p && (1.12)
\end{aligned}$$

$$\begin{aligned}
\therefore H_1(t) &= U_1 H U_1^\dagger + (\mathrm{i}\partial_t U_1)U_1^\dagger \\
&= \frac{(p - p_0(t))^2}{2m} + V(x) && (1.13)
\end{aligned}$$

Unitary 2: translation in $\hat{p}$-rep. gauge transformation

$$U_2(t) = \exp(-\mathrm{i}\hat{x}p_0(t)) \tag{1.14}$$
$$U_2 p U_2^\dagger = p + p_0 \tag{1.15}$$

$$\begin{aligned}
U_2 H_1 U_2^\dagger &= \exp(-\mathrm{i}xp_0(t))\frac{(p - p_0(t))^2}{2m}\exp(\mathrm{i}xp_0(t)) + V(x) \\
&= \frac{p^2}{2m} + V(x) && (1.16) \\
\mathrm{i}\partial_t U_2(t) &= \mathrm{i}\partial_t \exp(-\mathrm{i}xp_0(t)) \\
&= x\dot{p}_0(t) \\
&= -m\omega^2 A\cos(\omega t)x && (1.17)
\end{aligned}$$

$$\begin{aligned}
\therefore H_2(t) &= U_2 H_1 U_2 + (\mathrm{i}\partial_t U_2)U_2^\dagger \\
&= \frac{p^2}{2m} + V(x) - m\omega^2 A\cos(\omega t)x && (1.18)
\end{aligned}$$

After these two unitary transformation, and taking the single-band approximation and maintain merely onsite interaction, we reach a model similar to Eq.(1) in [1], written as a tight-binding model:

$$H(t) = -\sum_{\substack{\langle i,j\rangle \\ \sigma=\uparrow,\downarrow}} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \sum_{i,\sigma} f_i(t)\hat{n}_{i\sigma} \tag{1.19}$$

Here $f_i(t) = m\omega^2 A\cos(\omega t)x_i$, to be consistent with [1].

Unitary 3: rotating frame

$$R(t) = \exp(\mathrm{i}\sum_j l\omega t\hat{n}_{j\uparrow}\hat{n}_{j\downarrow})\exp(\mathrm{i}\sum_{j\sigma} F_j(t)\hat{n}_{j\sigma}) \tag{1.20}$$

Here $F_j(t) = \int^t f_j(t')dt'$. $l = 0$ or $l \neq 0$.

1. $l = 0$. $R_0(t) = \exp(i\sum_{j,\sigma} F_j(t)\hat{n}_{j\sigma}) = \exp(i\sum_{j,\sigma}\int^t dt' f_j(t')\hat{n}_{j\sigma})$

$$\begin{aligned} \mathrm{i}\partial_t R_0(t) &= \mathrm{i}\partial_t \exp(\mathrm{i}\sum_{j\sigma}\int^t dt' f_j(t')\hat{n}_{j\sigma}) \\ &= (-\sum_{j\sigma} f_j(t)\hat{n}_{j,\sigma})R_0(t) \end{aligned} \tag{1.21}$$

So the second term $(\mathrm{i}\partial_t U)U^\dagger$ is just to shift the onsite energy by $-\sum_{j\sigma} f_j(t)\hat{n}_{j,\sigma}$ at each site such that it cancels the last term in Eq.(1.19). And it does this no matter whether $l = 0$ or not.

Now consider the first term RHR^{-1}. R commutes with the interaction term. $[R, H_{\mathrm{int}}] = 0$. So we just need to calculate $RH_{\mathrm{kin}}R^{-1}$.

$$\begin{aligned} &\exp(\mathrm{i}\sum_{j\sigma} F_j(t)\hat{n}_{j\sigma}) t_{ij} c^\dagger_{i\sigma} c_{j\sigma} \exp(-\mathrm{i}\sum_{j\sigma} F_j(t)\hat{n}_{j\sigma}) \\ =&\exp(\mathrm{i}\sum_{j\sigma} F_j(t)\hat{n}_{j\sigma}) t_{ij} c^\dagger_{i\sigma} \exp(-\mathrm{i}\sum_{j'\sigma'} F_{j'}(t)(\hat{n}_{j'\sigma'} + \delta_{j'j}\delta_{\sigma'\sigma}))c_{j\sigma} \\ =&t_{ij}\exp[\mathrm{i}(F_i(t) - F_j(t))]c^\dagger_{i\sigma}c_{j\sigma} \\ =&t_{ij}\exp(-\mathrm{i}mA\omega(x_i - x_j)\sin(\omega t))c^\dagger_{i\sigma}c_{j\sigma} \\ =&t_{ij}\exp(-\mathrm{i}mA\omega d_x\sin(\omega t))c^\dagger_{i\sigma}c_{j\sigma} \end{aligned}$$

where $d_x = x_i - x_j$ is the distance between the center of neareast-neighbour Wannier functions. (see Ref[1])

Hence we derive the time-dependent Hamiltonian in rotating frame:

$$H_{\mathrm{rot}}(t) = -\sum_{n.n.,\sigma}\tilde{t}_{ij}(t)c^\dagger_{i\sigma}c_{j\sigma} + h.c. + U\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} \tag{1.22}$$

$$\text{with} \qquad \tilde{t}_{ij}(t) = t_{ij}\exp(-\mathrm{i}mA\omega d_x\sin(\omega t)) \tag{1.23}$$

2. $l \neq 0$. $R(t) = R_l(t) R_0(t)$.

$$R_l(t) = \exp(\mathrm{i}\sum_j l\omega t \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}) \tag{1.24}$$

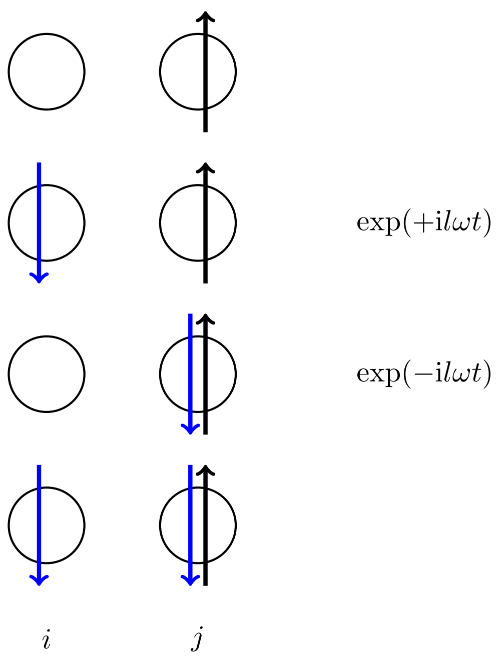
$$R_0(t) = \exp(\mathrm{i}\sum_{j\sigma} F_j(t)\hat{n}_{j\sigma}) \tag{1.25}$$

the effect of $R_0(t)$ is derived above. Left only $R_l(t)$ to be considered. Apparently $R_l(t)$ commutes with the last two terms in Eq. (1.19). We need to calculate only $R_l H_{\mathrm{kin}} R_l^\dagger$ and $\mathrm{i}\partial_t R_l(t)$.

$$\mathrm{i}\partial_t R_l(t) = \mathrm{i}\partial_t \exp(\mathrm{i}\sum_j l\omega t \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}) \tag{1.26}$$

$$= -l\omega \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} R_l(t) \tag{1.27}$$

$$\begin{aligned}
&R_l(t) t_{ij} c^\dagger_{i\uparrow} c_{j\uparrow} R_l^{-1}(t) \\
=&\exp(\mathrm{i}\sum_j l\omega t \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}) t_{ij} c^\dagger_{i\uparrow} c_{j\uparrow} \exp(-\mathrm{i}\sum_j l\omega t \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}) \\
=&t_{ij} c^\dagger_{i\uparrow} c_{j\uparrow} \exp(\mathrm{i}\sum_{j'} l\omega t(\hat{n}_{j'\uparrow} + \delta_{ij'} - \delta_{jj'})\hat{n}_{j'\downarrow}) \exp(-\mathrm{i}\sum_j l\omega t \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}) \\
=&t_{ij} c^\dagger_{i\uparrow} c_{j\uparrow} \exp(\mathrm{i} l\omega t(\hat{n}_{i\downarrow} - \hat{n}_{j\downarrow}))
\end{aligned}$$



Hence we derive the time-dependent Hamiltonian in rotating frame when $l \neq 0$:

$$H_{\mathrm{rot}}(t) = -\sum_{n.n.,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} \exp[\mathrm{i} l\omega t(\hat{n}_{i\bar{\sigma}} - \hat{n}_{j\bar{\sigma}}) - \mathrm{i} mA\omega d_x \sin(\omega t)] + (U - l\omega)\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} \tag{1.28}$$

High-frequency approximation The Hamiltonian for a periodic driven system writes

$$H(t) = H_0 + H_1 e^{\mathrm{i}\omega t} + H_{-1} e^{-\mathrm{i}\omega t} + \dots \tag{1.29}$$

where

$$H_m = \frac{1}{T}\int_{t_0}^{t_0+T} dt H(t) e^{\mathrm{i}m\omega t} \tag{1.30}$$

When ω is much larger than any energy scale in the system, that is $\omega \gg t_{ij}, U$ in Eq. (1.22) or $\omega \gg t_{ij}, \delta = U - l\omega$ in Eq. (1.28), we make high-frequency expansion [1] of $H(t)$ to obtain the stroboscopically effective Hamiltonian $e^{-\mathrm{i}H_{\mathrm{eff}}T} := U(t+T, t)$. Maintain only the lowest order in high-frequency approximation, namely $H_0 = \frac{1}{T}\int^T H(t)dt$ and $H_{\mathrm{eff}} \simeq H_0$, we end up with the effective Hamiltonian for $l = 0$ and $l \neq 0$, respectively, written as follows.

$$l = 0 \qquad H_{\mathrm{eff}} = -\sum_{n.n.,\sigma} t_x \mathcal{J}_0(K_0) c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + U\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} \tag{1.31}$$

$$l \neq 0 \qquad H_{\mathrm{eff}} = -\sum_{n.n.,\sigma} t_x \Big[\mathcal{J}_0(K_0)\hat{a}_{ij\bar{\sigma}} + \mathcal{J}_l(K_0)\hat{b}^l_{ij\bar{\sigma}}\Big] c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + \delta\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} \tag{1.32}$$

where we have omitted writing the t_y, t_z hopping term for conciseness, and

$$\begin{aligned} \hat{a}_{ij\sigma} &= (1 - \hat{n}_{i\sigma})(1 - \hat{n}_{j\sigma}) + \hat{n}_{i\sigma}\hat{n}_{j\sigma} \\ \hat{b}^l_{ij\sigma} &= (-1)^l (1 - \hat{n}_{i\sigma})\hat{n}_{j\sigma} + \hat{n}_{i\sigma}(1 - \hat{n}_{j\sigma}) \\ K_0 &= mA\omega d_x \end{aligned}$$

In deriving Eq. (1.31) and (1.32) we have made use of the integral def. of Bessel function:

$$\mathcal{J}_l(x) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{\mathrm{i}(lt - x\sin t)} dt \tag{1.33}$$

$$\mathcal{J}_l(x) = (-1)^l \mathcal{J}_{-l}(x) \tag{1.34}$$

The effective Hamiltonian of $l = 0$ case is an usual Hubbard model.[2] We focus on that of the $l \neq 0$ cases in the following. We name it the Floquet-Hubbard Hamiltonian.

[1] see Ref[3, 4]

[2] Notice also that when $\mathcal{J}_0(K_0) = \mathcal{J}_1(K_0)$ and l is even, the model reduces to an usual Fermi-Hubbard model too.

2 Mean-field calculation: CDW and superfluid in Floquet-Hubbard model

Floquet-Hubbard Hamiltonian writes:

$$
\begin{aligned}
H &= -\sum_{n.n.,\sigma} t_x \Big[\mathcal{J}_0(K_0)\hat{a}_{ij\bar{\sigma}} + \mathcal{J}_l(K_0)\hat{b}^l_{ij\bar{\sigma}}\Big] c^\dagger_{i\sigma} c_{j\sigma} + h.c. + g\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} && (2.1)\\
&= -\sum_{\substack{i\in A, j\in B\\ n.n.,\sigma}} t_x \bigg(\mathcal{J}_0(K_0)\Big[(1-\hat{n}_{i\bar{\sigma}})(1-\hat{n}_{j\bar{\sigma}}) + \hat{n}_{i\bar{\sigma}}\hat{n}_{j\bar{\sigma}}\Big] && (2.2)\\
&\qquad + \mathcal{J}_l(K_0)\Big[(-1)^l(1-\hat{n}_{i\bar{\sigma}})\hat{n}_{j\bar{\sigma}} + \hat{n}_{i\bar{\sigma}}(1-\hat{n}_{j\bar{\sigma}})\Big]\bigg) c^\dagger_{i\bar{\sigma}} c_{j\bar{\sigma}} + h.c. \\
&\quad + g\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}
\end{aligned}
$$

where the last equation Eq. (2.2) is because the honeycomb lattice is bipartite and there are two sites in one unit cell. Note that the model will reduce to an usual Fermi-Hubbard model when $\mathcal{J}_0(K_0) = \mathcal{J}_1(K_0)$ and l even.

2.1 Mean field Hamiltonian (I)

By introducing two sets of order parameters, namely the superfluid order parameters $\{\Delta\}$ and CDW order parameters $\{n\}$, we could write down some mean field Hamiltonian in these order parameters in a bilinear form, which we are able to solve. Then we solve the ground state (for zero temperature) and find the extreme value for all the order parameters. Just like what we do as in an usual Hubbard model. But how to derive the mean field Hamiltonian? We use a path integral approach. Similar to Hubbard-Stratonovich transformation, we firstly introduce some other dynamical fields in the path integral (that is the Δs and ns here together with some Lagrangian multipliers) which will give rise to the former action, hopefully, when integrated out. However, rather than integrate it indeed, we instead replace the dynamical fields we introduced with some numbers. From the Lagrangian we obtain the Hamiltonian, in a power of at most 2 in the field operators (bilinear). This is the mean field Hamiltonian. But what are the numbers we shall replace with in the previous step? They are actually the extreme value of the parameters we introduced that we should carry out from the mean field Hamiltonian. And this can be done iteratively in numerics. By differentiating the Lagrangian/Hamiltonian with respect to all the parameters we introduced (order parameters and Lagrangian multipliers) combined with the Feynman-Hellman theorem some more equations relates parameters to parameters or parameters to observables could also be obtained. And this step helps in the iterative solving precedure.

The details of the derivation is omitted here. See appendix A for reference.

Here we just write down the mean field Hamiltonian as

$$
\begin{aligned}
&H_{\mathrm{meanF}}(n_{o\uparrow}, n_{o\downarrow}, n_{e\uparrow}, n_{e\downarrow}, \eta_{o\uparrow}, \eta_{o\downarrow}, \eta_{e\uparrow}, \eta_{e\downarrow}, \Delta_o, \bar{\Delta}_o, \Delta_e, \bar{\Delta}_e, \lambda_o, \bar{\lambda}_o, \lambda_e, \bar{\lambda}_e) \\
&\quad = -\sum_{\substack{\langle i,j\rangle \\ i\in A, j\in B}} \Bigg[\Big(t_0[(1-n_{o\downarrow})(1-n_{e\downarrow}) + n_{o\downarrow}n_{e\downarrow}] + t_1[(-1)^l(1-n_{o\downarrow})n_{e\downarrow} + n_{o\downarrow}(1-n_{e\downarrow})] \Big) c^\dagger_{i\uparrow}c_{j\uparrow} \\
&\qquad\qquad + \Big(t_0[(1-n_{o\uparrow})(1-n_{e\uparrow}) + n_{o\uparrow}n_{e\uparrow}] + t_1[(-1)^l(1-n_{o\uparrow})n_{e\uparrow} + n_{o\uparrow}(1-n_{e\uparrow})] \Big) c^\dagger_{i\downarrow}c_{j\downarrow} \Bigg] \\
&\qquad\qquad + H.c. \\
&\qquad\qquad + gN(\bar{\Delta}_o\Delta_o + \bar{\Delta}_e\Delta_e) \\
&\qquad\qquad + \lambda_o(N\Delta_o - \sum_{i\in A} c_{i\downarrow}c_{i\uparrow}) + \bar{\lambda}_o(N\bar{\Delta}_o - \sum_{i\in A} c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}) \\
&\qquad\qquad + \lambda_e(N\Delta_e - \sum_{j\in B} c_{j\downarrow}c_{j\uparrow}) + \bar{\lambda}_e(N\bar{\Delta}_e - \sum_{j\in B} c^\dagger_{j\uparrow}c^\dagger_{j\downarrow}) \qquad (2.3) \\
&\qquad\qquad + gN(n_{o\uparrow}n_{o\downarrow} + n_{e\uparrow}n_{e\downarrow}) \\
&\qquad\qquad + \eta_{o\uparrow}(Nn_{o\uparrow} - \sum_{i\in A} c^\dagger_{i\uparrow}c_{i\uparrow}) + \eta_{o\downarrow}(Nn_{o\downarrow} - \sum_{i\in A} c^\dagger_{i\downarrow}c_{i\downarrow}) \\
&\qquad\qquad + \eta_{e\uparrow}(Nn_{e\uparrow} - \sum_{j\in B} c^\dagger_{j\uparrow}c_{j\uparrow}) + \eta_{\downarrow}(Nn_{e\downarrow} - \sum_{j\in B} c^\dagger_{j\downarrow}c_{j\downarrow})
\end{aligned}
$$

Here $n_{o\uparrow}, n_{o\downarrow}, n_{e\uparrow}, n_{e\downarrow}$ are order parameters in the density channel with $\eta_{o\uparrow}, \eta_{o\downarrow}, \eta_{e\uparrow}, \eta_{e\downarrow}$ the corresponding lagrangian multipliers, and $\Delta_o, \bar{\Delta}_o, \Delta_e, \bar{\Delta}_e$ are order parameters in the Cooper channel and $\lambda_o, \bar{\lambda}_o, \lambda_e, \bar{\lambda}_e$ the corresponding lagrangian multipliers. We assume the lattice is bipartite, in particular, a honeycomb lattice. Hence we could change the notation from $o(odd)/e(even)$ to $a(A)/b(B)$, that is A/B sublattice. And $t_0 = t_x\mathcal{J}_0(K_0)$, $t_1 = t_x\mathcal{J}_l(K_0)$, $g = U - l\omega$ if compared with the model parameters derived in last section.

With the Fourier transformation

$$
\begin{aligned}
A: &\qquad c_{i\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{\mathrm{i}ki} a_{k\sigma} \\
B: &\qquad c_{j\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{\mathrm{i}kj} b_{k\sigma}
\end{aligned}
$$

we write the mean field Hamiltonian in momentum space,

$$
\begin{aligned}
H_{\text{meanF}} = & \sum_k \Big[- P_\uparrow(n_{A\downarrow}, n_{B\downarrow})Q(k)a^\dagger_{k\uparrow}b_{k\uparrow} - P_\downarrow(n_{A\uparrow}, n_{B\uparrow})Q(-k)a^\dagger_{k\downarrow}b_{k\downarrow}\Big] + H.c. \\
& + gN(\bar{\Delta}_A\Delta_A + \bar{\Delta}_B\Delta_B) \\
& + \lambda_A(N\Delta_A - \sum_k a_{-k\downarrow}a_{k\uparrow}) + \bar{\lambda}_A(N\bar{\Delta}_A - \sum_k a^\dagger_{k\uparrow}a^\dagger_{-k\downarrow}) \\
& + \lambda_B(N\Delta_B - \sum_k b_{-k\downarrow}b_{k\uparrow}) + \bar{\lambda}_B(N\bar{\Delta}_B - \sum_k b^\dagger_{k\uparrow}b^\dagger_{-k\downarrow}) \\
& + gN(n_{A\uparrow}n_{A\downarrow} + n_{B\uparrow}n_{B\downarrow}) \\
& + \eta_{A\uparrow}(Nn_{A\uparrow} - \sum_k a^\dagger_{k\uparrow}a_{k\uparrow}) + \eta_{A\downarrow}(Nn_{A\downarrow} - \sum_k a^\dagger_{k\downarrow}a_{k\downarrow}) \\
& + \eta_{B\uparrow}(Nn_{B\uparrow} - \sum_k b^\dagger_{k\uparrow}b_{k\uparrow}) + \eta_{B\downarrow}(Nn_{B\downarrow} - \sum_k b^\dagger_{k\downarrow}b_{k\downarrow})
\end{aligned}
\tag{2.4}
$$

Or in the representation of Nambu spinors writes

$$
H_{\text{meanF}} = \sum_k \begin{pmatrix} a^\dagger_{k\uparrow} & b^\dagger_{k\uparrow} & a_{-k\downarrow} & b_{-k\downarrow} \end{pmatrix} \mathcal{H}(k) \begin{pmatrix} a_{k\uparrow} \\ b_{k\uparrow} \\ a^\dagger_{-k\downarrow} \\ b^\dagger_{-k\downarrow} \end{pmatrix} + const.(\text{parameters.}) \tag{2.5}
$$

Here

$$
\mathcal{H}(k) = \begin{pmatrix} -\eta_{A\uparrow} & -P_\uparrow(n_{A\downarrow}, n_{B\downarrow})Q(k) & -\bar{\lambda}_A & 0 \\ -P_\uparrow(n_{A\downarrow}, n_{B\downarrow})Q(-k) & -\eta_{B\uparrow} & 0 & -\bar{\lambda}_B \\ -\lambda_A & 0 & \eta_{A\downarrow} & P_\downarrow(n_{A\uparrow}, n_{B\uparrow})Q(k) \\ 0 & -\lambda_B & P_\downarrow(n_{A\uparrow}, n_{B\uparrow})Q(-k) & \eta_{B\downarrow} \end{pmatrix} \tag{2.6}
$$

where we introduce the notation:

$$
Q(k) = \sum_i \exp(k \cdot d_i) \tag{2.7}
$$

$$
P_{\bar{\sigma}}(n_{A\sigma}, n_{B\sigma}) = t_0[(1 - n_{A\sigma})(1 - n_{B\sigma}) + n_{A\sigma}n_{B\sigma}] + t_1[(-1)^l(1 - n_{A\sigma})n_{B\sigma} + n_{A\sigma}(1 - n_{B\sigma})] \tag{2.8}
$$

and the *const.* term is some energy constant depends on the order parameters and lagrangian multipliers we introduced.

$$
\begin{aligned}
const. = \; & gN(\bar{\Delta}_A\Delta_A + \bar{\Delta}_B\Delta_B) \\
& + N[\lambda_A\Delta_A + \bar{\lambda}_A\bar{\Delta}_A + \lambda_B\Delta_B + \bar{\lambda}_B\bar{\Delta}_B] \\
& + gN(n_{A\uparrow}n_{A\downarrow} + n_{B\uparrow}n_{B\downarrow}) \\
& + N[\eta_{A\uparrow}n_{A\uparrow} + \eta_{B\uparrow}n_{B\uparrow} + \eta_{A\downarrow}(n_{A\downarrow} - 1) + \eta_{B\downarrow}(n_{B\downarrow} - 1)]
\end{aligned}
\tag{2.9}
$$

2.2 Iterative renewed self-consistent solving procedure

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 ground state of the many-body Hamiltonian (2.4), or written as (2.5). Take partial derivative, successively, with respect to all 16 parameters, and let $\partial E(para.)/\partial para. = 0$, which implies

$$\sum_{k,i} u_i^*(k)\frac{\partial \mathcal{H}(k;para.)}{\partial para.}u_i(k)\Theta(-\epsilon_i(k)) + \frac{\partial const.}{\partial para.} = 0 \tag{2.10}$$

In above equation, the i in the summation denotes the band index with ϵ_i its eigen energy and u_i the eigenvector, while k indicates quasi-momentum in the first Brillioun zone.

$$\frac{\partial \mathcal{H}(k)}{\partial \Delta_A} = 0 \qquad\qquad \frac{\partial const.}{\partial \Delta_A} = \lambda_A N + gN\bar{\Delta}_A \tag{2.11}$$

$$\frac{\partial \mathcal{H}(k)}{\partial \bar{\Delta}_A} = 0 \qquad\qquad \frac{\partial const.}{\partial \bar{\Delta}_A} = \bar{\lambda}_A N + gN\Delta_A \tag{2.12}$$

$$\frac{\partial \mathcal{H}(k)}{\partial \Delta_B} = 0 \qquad\qquad \frac{\partial const.}{\partial \Delta_B} = \lambda_B N + gN\bar{\Delta}_B \tag{2.13}$$

$$\frac{\partial \mathcal{H}(k)}{\partial \bar{\Delta}_B} = 0 \qquad\qquad \frac{\partial const.}{\partial \bar{\Delta}_B} = \bar{\lambda}_A N + gN\Delta_B \tag{2.14}$$

This set of equations implies the lagrangian multipliers for the superfluid order parameters are the order parameters themselves. That is,

$$\lambda_A = -g\bar{\Delta}_A \tag{2.15}$$

$$\bar{\lambda}_A = -g\Delta_A \tag{2.16}$$

$$\lambda_B = -g\bar{\Delta}_B \tag{2.17}$$

$$\bar{\lambda}_B = -g\Delta_B \tag{2.18}$$

Equations derived from derivatives with respect to 4 λs:

$$\frac{\partial \mathcal{H}(k)}{\partial_{\lambda_A}} = \begin{pmatrix} 0 & & & \\ 0 & & & \\ -1 & 0 & 0 & 0 \\ 0 & & & \end{pmatrix} \qquad \frac{\partial const.}{\partial_{\lambda_A}} = N\Delta_A \tag{2.19}$$

$$\frac{\partial \mathcal{H}(k)}{\partial_{\bar{\lambda}_A}} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ & & 0 & \\ & & 0 & \\ & & 0 & \end{pmatrix} \qquad \frac{\partial const.}{\partial_{\bar{\lambda}_A}} = N\bar{\Delta}_A \tag{2.20}$$

$$\frac{\partial \mathcal{H}(k)}{\partial_{\lambda_B}} = \begin{pmatrix} & 0 & & \\ & 0 & & \\ & 0 & & \\ 0 & -1 & 0 & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial_{\lambda_B}} = N\Delta_B \tag{2.21}$$

$$\frac{\partial \mathcal{H}(k)}{\partial_{\bar{\lambda}_B}} = \begin{pmatrix} & & & 0 \\ 0 & 0 & 0 & -1 \\ & & & 0 \\ & & & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial_{\bar{\lambda}_B}} = N\bar{\Delta}_B \tag{2.22}$$

from 4 ηs:

$$\frac{\partial \mathcal{H}(k)}{\partial \eta_{A\uparrow}} = \begin{pmatrix} -1 & & & \\ & 0 & & \\ & & 0 & \\ & & & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial \eta_{A\uparrow}} = Nn_{A\uparrow} \tag{2.23}$$

$$\frac{\partial \mathcal{H}(k)}{\partial \eta_{B\uparrow}} = \begin{pmatrix} 0 & & & \\ & -1 & & \\ & & 0 & \\ & & & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial \eta_{B\uparrow}} = Nn_{B\uparrow} \tag{2.24}$$

$$\frac{\partial \mathcal{H}(k)}{\partial \eta_{A\downarrow}} = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 1 & \\ & & & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial \eta_{A\downarrow}} = N(n_{A\downarrow} - 1) \tag{2.25}$$

$$\frac{\partial \mathcal{H}(k)}{\partial \eta_{B\downarrow}} = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 0 & \\ & & & 1 \end{pmatrix} \qquad \frac{\partial const.}{\partial \eta_{B\downarrow}} = N(n_{B\downarrow} - 1) \tag{2.26}$$

from 4 ns:

$$\frac{\partial\mathcal{H}(k)}{\partial n_{A\uparrow}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial P_\downarrow}{\partial n_{A\uparrow}}Q(k) \\ 0 & 0 & \frac{\partial P_\downarrow}{\partial n_{A\uparrow}}Q(-k) & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial n_{A\uparrow}} = N(\eta_{A\uparrow} + g n_{A\downarrow}) \tag{2.27}$$

$$\frac{\partial\mathcal{H}(k)}{\partial n_{B\uparrow}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial P_\downarrow}{\partial n_{B\uparrow}}Q(k) \\ 0 & 0 & \frac{\partial P_\downarrow}{\partial n_{B\uparrow}}Q(-k) & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial n_{B\uparrow}} = N(\eta_{B\uparrow} + g n_{B\downarrow}) \tag{2.28}$$

$$\frac{\partial\mathcal{H}(k)}{\partial n_{A\downarrow}} = \begin{pmatrix} 0 & -\frac{\partial P_\uparrow}{\partial n_{A\downarrow}}Q(k) & 0 & 0 \\ -\frac{\partial P_\uparrow}{\partial n_{A\downarrow}}Q(-k) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial n_{A\downarrow}} = N(\eta_{A\downarrow} + g n_{A\uparrow}) \tag{2.29}$$

$$\frac{\partial\mathcal{H}(k)}{\partial n_{B\downarrow}} = \begin{pmatrix} 0 & -\frac{\partial P_\uparrow}{\partial n_{B\downarrow}}Q(k) & 0 & 0 \\ -\frac{\partial P_\uparrow}{\partial n_{B\downarrow}}Q(-k) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial n_{B\downarrow}} = N(\eta_{B\downarrow} + g n_{B\uparrow}) \tag{2.30}$$

where

$$\frac{\partial P_{\bar\sigma}}{\partial n_{A\sigma}} = t_0[2n_{B\sigma} - 1] + t_1[-(-1)^l n_{B\sigma} + (1 - n_{B\sigma})] \tag{2.31}$$

$$\frac{\partial P_{\bar\sigma}}{\partial n_{B\sigma}} = t_0[2n_{A\sigma} - 1] + t_1[(-1)^l(1 - n_{A\sigma}) - n_{A\sigma}] \tag{2.32}$$

or specifically,

$$l \text{ odd}: \qquad \frac{\partial P_{\bar\sigma}}{\partial n_{A\sigma}} = t_0(2n_{B\sigma} - 1) + t_1 \tag{2.33}$$

$$\frac{\partial P_{\bar\sigma}}{\partial n_{B\sigma}} = t_0(2n_{A\sigma} - 1) - t_1 \tag{2.34}$$

$$l \text{ even}: \qquad \frac{\partial P_{\bar\sigma}}{\partial n_{A\sigma}} = (t_1 - t_0)(1 - 2n_{B\sigma}) \tag{2.35}$$

$$\frac{\partial P_{\bar\sigma}}{\partial n_{B\sigma}} = (t_1 - t_0)(1 - 2n_{A\sigma}) \tag{2.36}$$

$$\tag{2.37}$$

2.3 Charge density order and Spin density order: Mean field Hamiltonian (II)

The previous decoupling encounters difficulties in practical iterative solving process. We hence add some constraints on it.

Firstly we do some vaviable substitution. Define 4 new variables:

$$n_A = n_{A\uparrow} + n_{A\downarrow} \qquad S_A^z = n_{A\uparrow} - n_{A\downarrow}$$
$$n_B = n_{B\uparrow} + n_{B\downarrow} \qquad S_B^z = n_{B\uparrow} - n_{B\downarrow}$$

Then we pose two constraints (half-filling & total spin zero):

$$n_A + n_B = 2 \tag{2.38}$$
$$S_A^z + S_B^Z = 0 \tag{2.39}$$

such that these for new defined variables can be written as

$$n_A = 1 + c \qquad S_A^z = s \tag{2.40}$$
$$n_B = 1 - c \qquad S_B^z = -s \tag{2.41}$$

Then we have actually two orders: c and s.[3] Hence

$$n_{A\uparrow} = \frac{n_A + S_A^z}{2} = \frac{1 + c + s}{2} \tag{2.42}$$
$$n_{A\downarrow} = \frac{n_A - S_A^z}{2} = \frac{1 + c - s}{2} \tag{2.43}$$
$$n_{B\uparrow} = \frac{n_B + S_B^z}{2} = \frac{1 - c - s}{2} \tag{2.44}$$
$$n_{B\downarrow} = \frac{n_B - S_B^z}{2} = \frac{1 - c + s}{2} \tag{2.45}$$

- The decoupling of the interaction part is

$$g n_{A\uparrow} n_{A\downarrow} + g n_{B\uparrow} n_{B\downarrow} = \frac{g}{2}(1 + c^2 - s^2) \tag{2.46}$$

- The kinetic part is just substitute c and s into P_σ function: $P_{\bar{\sigma}}(c, s) = P_{\bar{\sigma}}(n_{A\sigma}(c, s), n_{B\sigma}(c, s))$

$$\begin{aligned}
P_\uparrow &= t_0(2n_{A\downarrow}n_{B\downarrow}) + t_1[(-1)^l n_{B\downarrow}^2 + n_{A\downarrow}^2] \\
&= t_0 \cdot \frac{1-(c-s)^2}{2} + t_1 \cdot \begin{cases} \frac{1}{2}(c-s) & l \ \text{odd} \\ \frac{1}{2}[1+(c-s)^2] & l \ \text{even} \end{cases} \\
P_\downarrow &= t_0(2n_{A\uparrow}n_{B\uparrow}) + t_1[(-1)^l n_{B\uparrow}^2 + n_{A\uparrow}^2] \\
&= t_0 \cdot \frac{1-(c+s)^2}{2} + t_1 \cdot \begin{cases} \frac{1}{2}(c+s) & l \ \text{odd} \\ \frac{1}{2}[1+(c+s)^2] & l \ \text{even} \end{cases}
\end{aligned}$$

[3] implies charge density wave and spin density wave for interactions $g > 0$ or < 0 respectively, in the usual Hubbard model.

- Moreover,

$$
\begin{aligned}
\frac{\partial P_\uparrow}{\partial c} &= -t_0(c-s) + t_1 \cdot \begin{cases} \frac{1}{2} & l \ \text{odd} \\ \frac{1}{2}(c-s) & l \ \text{even} \end{cases} \\
&= \begin{cases} -t_0(c-s) + \frac{1}{2}t_1 \\ (t_1 - t_0)(c-s) \end{cases} \\
&= -\frac{\partial P_\uparrow}{\partial s} \\
\frac{\partial P_\downarrow}{\partial c} &= -t_0(c+s) + t_1 \cdot \begin{cases} \frac{1}{2} & l \ \text{odd} \\ \frac{1}{2}(c+s) & l \ \text{even} \end{cases} \\
&= \begin{cases} -t_0(c+s) + \frac{1}{2}t_1 \\ (t_1 - t_0)(c+s) \end{cases} \\
&= \frac{\partial P_\downarrow}{\partial s}
\end{aligned}
$$

- The Lagrangian multiplier terms added:

$$\eta_c \left[c - \frac{(\hat{n}_{A\uparrow} + \hat{n}_{A\downarrow}) - (\hat{n}_{B\uparrow} + \hat{n}_{B\downarrow})}{2} \right] N \tag{2.47}$$

$$\eta_s \left[s - \frac{(\hat{n}_{A\uparrow} - \hat{n}_{A\downarrow}) - (\hat{n}_{B\uparrow} - \hat{n}_{B\downarrow})}{2} \right] N \tag{2.48}$$

coefficients:

$$\hat{n}_{A\uparrow} : \qquad -\frac{1}{2}\eta_c - \frac{1}{2}\eta_s \tag{2.49}$$

$$\hat{n}_{B\uparrow} : \qquad +\frac{1}{2}\eta_c + \frac{1}{2}\eta_s \tag{2.50}$$

$$\hat{n}_{A\downarrow} : \qquad -\frac{1}{2}\eta_c + \frac{1}{2}\eta_s \tag{2.51}$$

$$\hat{n}_{B\downarrow} : \qquad +\frac{1}{2}\eta_c - \frac{1}{2}\eta_s \tag{2.52}$$

$$consts. \qquad \eta_c c + \eta_s s \tag{2.53}$$

Thus, the mean field Hamiltonian (for the density order part) is written as

$$
\begin{aligned}
H_{\text{meanF}} =& \sum_k \Big[-P_\uparrow(c,s)Q(k)a^\dagger_{k\uparrow}b_{k\uparrow} - P_\downarrow(c,s)Q(-k)a^\dagger_{k\downarrow}b_{k\downarrow}\Big] + H.c.\\
&+ gN(\bar{\Delta}_A\Delta_A + \bar{\Delta}_B\Delta_B)\\
&+ \lambda_A(N\Delta_A - \sum_k a_{-k\downarrow}a_{k\uparrow}) + \bar{\lambda}_A(N\bar{\Delta}_A - \sum_k a^\dagger_{k\uparrow}a^\dagger_{-k\downarrow})\\
&+ \lambda_B(N\Delta_B - \sum_k b_{-k\downarrow}b_{k\uparrow}) + \bar{\lambda}_B(N\bar{\Delta}_B - \sum_k b^\dagger_{k\uparrow}b^\dagger_{-k\downarrow})\\
&+ \frac{gN}{2}(1+c^2-s^2)\\
&+ \eta_c\Big[c - \frac{(\hat{n}_{A\uparrow}+\hat{n}_{A\downarrow})-(\hat{n}_{B\uparrow}+\hat{n}_{B\downarrow})}{2}\Big]N\\
&+ \eta_s\Big[s - \frac{(\hat{n}_{A\uparrow}-\hat{n}_{A\downarrow})-(\hat{n}_{B\uparrow}-\hat{n}_{B\downarrow})}{2}\Big]N
\end{aligned}
\tag{2.54}
$$

Or in the representation of Nambu spinors writes

$$
H_{\text{meanF}} = \sum_k \begin{pmatrix} a^\dagger_{k\uparrow} & b^\dagger_{k\uparrow} & a_{-k\downarrow} & b_{-k\downarrow}\end{pmatrix} \mathcal{H}(k) \begin{pmatrix} a_{k\uparrow} \\ b_{k\uparrow} \\ a^\dagger_{-k\downarrow} \\ b^\dagger_{-k\downarrow}\end{pmatrix} + const.(\text{para.s}) \tag{2.55}
$$

where

$$
\mathcal{H}(k) = \begin{pmatrix}
-\frac{1}{2}\eta_c - \frac{1}{2}\eta_s & -P_\uparrow(c,s)Q(k) & -\bar{\lambda}_A & 0\\
-P_\uparrow(c,s)Q(-k) & \frac{1}{2}\eta_c + \frac{1}{2}\eta_s & 0 & -\bar{\lambda}_B\\
-\lambda_A & 0 & \frac{1}{2}\eta_c - \frac{1}{2}\eta_s & P_\downarrow(c,s)Q(k)\\
0 & -\lambda_B & P_\downarrow(c,s)Q(-k) & -\frac{1}{2}\eta_c + \frac{1}{2}\eta_s
\end{pmatrix} \tag{2.56}
$$

and

$$
const. = \Big[-g(\bar{\Delta}_A\Delta_A + \bar{\Delta}_B\Delta_B) + \frac{g}{2}(1+c^2-s^2) + \eta_c c + \eta_s s\Big]N \tag{2.57}
$$

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

$$\frac{\partial\mathcal{H}(k)}{\partial\eta_c} = \frac{1}{2}\begin{pmatrix} -1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} \qquad \frac{\partial const.}{\partial\eta_c} = Nc \tag{2.58}$$

$$\frac{\partial\mathcal{H}(k)}{\partial\eta_s} = \frac{1}{2}\begin{pmatrix} -1 & & & \\ & 1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix} \qquad \frac{\partial const.}{\partial\eta_s} = Ns \tag{2.59}$$

$$\frac{\partial\mathcal{H}(k)}{\partial c} = \begin{pmatrix} 0 & -\frac{\partial P_\uparrow}{\partial c}Q(k) & & \\ -\frac{\partial P_\uparrow}{\partial c}Q(-k) & 0 & & \\ & & 0 & \frac{\partial P_\downarrow}{\partial c}Q(k) \\ & & \frac{\partial P_\downarrow}{\partial c}Q(-k) & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial c} = (gc+\eta_c)N \tag{2.60}$$

$$\frac{\partial\mathcal{H}(k)}{\partial s} = \begin{pmatrix} 0 & -\frac{\partial P_\uparrow}{\partial s}Q(k) & & \\ -\frac{\partial P_\uparrow}{\partial s}Q(-k) & 0 & & \\ & & 0 & \frac{\partial P_\downarrow}{\partial s}Q(k) \\ & & \frac{\partial P_\downarrow}{\partial s}Q(-k) & 0 \end{pmatrix} \qquad \frac{\partial const.}{\partial s} = [-gs+\eta_s]N \tag{2.61}$$

2.3.1 total particle number and total magnetic momentum conservation.

Total particle number (density) operator is

$$\hat{\mathcal{N}} = \hat{n}_{A\uparrow} + \hat{n}_{B\uparrow} + \hat{n}_{A\downarrow} + \hat{n}_{B\downarrow} \tag{2.62}$$

$$= \sum_k \left(a^\dagger_{k\uparrow}\; b^\dagger_{k\uparrow}\; a_{-k\downarrow}\; b_{-k\downarrow}\right) \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} \begin{pmatrix} a_{k\uparrow} \\ b_{k\uparrow} \\ a^\dagger_{-k\downarrow} \\ b^\dagger_{-k\downarrow} \end{pmatrix} + 2N \tag{2.63}$$

again, N is the number of unit cells.

Total magnetic momentum is

$$\hat{\mathcal{S}}_z = \hat{n}_{A\uparrow} + \hat{n}_{B\uparrow} - (\hat{n}_{A\downarrow} + \hat{n}_{B\downarrow}) \tag{2.64}$$

$$= \sum_k \left(a^\dagger_{k\uparrow}\; b^\dagger_{k\uparrow}\; a_{-k\downarrow}\; b_{-k\downarrow}\right) \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \begin{pmatrix} a_{k\uparrow} \\ b_{k\uparrow} \\ a^\dagger_{-k\downarrow} \\ b^\dagger_{-k\downarrow} \end{pmatrix} - 2N \tag{2.65}$$

To ensure $\mathcal{N} = 2$ and $\mathcal{S}_z = 0$, one way is to add two more lagrangian-multiplier terms

$$\eta_{\mathcal{N}} \left[2 - (\hat{n}_{A\uparrow} + \hat{n}_{A\downarrow} + \hat{n}_{B\uparrow} + \hat{n}_{B\downarrow}) \right] N \tag{2.66}$$

$$\eta_{\mathcal{S}} \left[0 - (\hat{n}_{A\uparrow} - \hat{n}_{A\downarrow} + \hat{n}_{B\uparrow} - \hat{n}_{B\downarrow}) \right] N \tag{2.67}$$

onto the mean field Hamiltonian Eq. (2.54), (2.55). Or we can check these expectation values after we reach a self-consistent solution of (2.54), (2.55). Some symmetries of the system assure us the satisfiction of them. They are

1) Particle-hole symmetry when l is even. $c_{i\sigma} \to c_{i\sigma}^{\dagger}$

2) Particle-hole-sublattice symmetry when l is odd. $a_{i\sigma} \to b_{i\sigma}^{\dagger}$

2.4 Phase diagram: Shaking induced

2.4.1 square lattice & l even

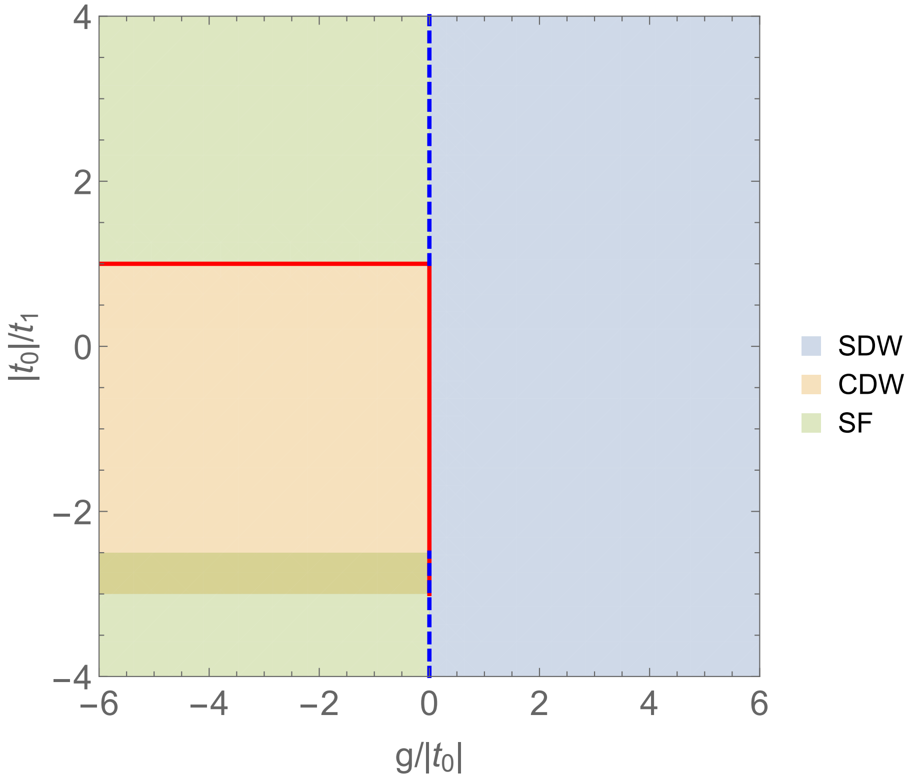


Figure 1: Red full line: 1st order phase transition. Blue dashed line: 2nd order phase transition. Shaded area: undetermined, working on it.

We see that the added term $\sum_i f_i(t)\hat{n}_i$ in Eq. (1.19), and the resulting averaged Floquet-Hubbard Hamiltonian (2.1), breaks the symmetry of CDW and superfluid order in an usual attractive Hubbard model. But it is still spin rotation invariant. Thus the SDW phase in the repulsive case is not affected.

Note also, $t_0 = t_1$ reduces to exactly an usual Hubbard model.

2.4.2 square lattice & l odd

2.4.3 honeycomb lattice & l even

2.4.4 honeycomb lattice & l even

A Mean field theory: a path integral approach.

Given a Hamiltonian H, the Lagrangian is $L = \bar{\psi} \mathrm{i}\partial_t \psi - H$. Also, from a Lagrangian L the Hamiltonian H can be obtained.

So how do we derive, or construct, from a many-body interacting Hamiltonian, a mean field Hamiltonian that is bilinear such that we are able to solve? Path integral formalism gives an approach.

The precedure is:

(1)

(2)

See Ref[5] as a reference.

Acknowledgments

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