Effective Hamiltonians for fastly driven many-body lattice systems

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We consider 1D lattices described by Hubbard or Bose-Hubbard models, in the presence of periodic high-frequency perturbations, such as uniform ac force or modulation of tunnelling constants. Effective Hamiltonians for interacting particles are derived using an averaging method resembling classical canonical perturbation theory. Previous studies demonstrated renormalization of tunnelling constants by the high-frequency force leading to interesting phenomena such as coherent destruction of tunnelling and creation of artificial gauge fields. We find explicitly second-order corrections to the effective Hamiltonians due to interactions. These corrections correspond to non-trivial processes such as single-particle density-dependent tunnelling, correlated pair hoppings, nonlocal (extended) pair hopping, nearest neighbour interactions, superexchange interactions. Some of these processes arise also in multiband lattice models, and are capable to give rise to a rich variety of quantum phases. Using a suitable driving protocol, it is possible to suppress or enhance a particular process in the effective Hamiltonian. Our approach and results differ from that of the recent study based on flow equation method [A. Verdeny and coworkers, Phys.Rev.Lett 111, 175301 (2013)], and allow to reproduce known single- and two-particle solutions obtained by multiple time-scale method (e.g., [S. Longhi, Phys. Rev. B 77, 195326 (2008)]). The results may found applications in designing effective Hamiltonian models in experiments with ultracold atoms in optical lattices, e.g. for simulating solid-state phenomena via optical means.

The idea of engineering effective Hamiltonians using high-frequency perturbations probably goes back to the famous Kapitza pendulum \cite{1–4}. In classical and celestial mechanics there are many examples of systems with separation of typical timescales on slow and fast ones, and corresponding perturbation methods were developed long time ago (see, e.g., \cite{5}). It is interesting to extend these methods to the quantum realm, especially to lattice systems, where high-frequency perturbations are often used, e.g. for construction of quantum simulators (well-controllable quantum systems for simulating complicated condensed matter phenomena \cite{6,7}).

Indeed, a suitable driving applied to ultracold atoms in optical lattices allows to realize dynamical localization \cite{8,9}, mimick photoconductivity \cite{10}, simulate artificial gauge fields \cite{11}, classical \cite{12} and quantum magnetism; study transport phenomena \cite{13,14} and the superfluid-to-Mott insulator transition \cite{15,16}. In solid-state physics, ac-driven systems also received a lot of interest in the context of dynamical localization \cite{17,18}, and coherent control of electronic transport in semiconductor superlattices and arrays of coupled quantum dots \cite{19,20}, novel proposals include microwave-induced topological insulators \cite{21}; photoinduced quantum Hall insulators \cite{22}, metal-insulator \cite{23,24} and superconductivity \cite{25}. Apart from the latter (very complicated \cite{24}) solid-state phenomena, the most of the abovementioned applications are in fact based on modifying single-particle tunnelling constants by a high-frequency force, a phenomenon that can be derived by averaging a Hamiltonian of the system (i.e., keeping only zeroth order terms in $\frac{1}{\hbar}$ (inverse frequency of perturbation) and neglecting all higher-order terms). Hower, for many realistic applications of such type, it is important to derive accurate effective Hamiltonians taking into account higher-order terms (see, e.g., \cite{26}).

Here we elaborate a convenient method which allows to determine explicitly higher-order corrections to effective Hamiltonians of driven quantum lattices. These corrections correspond to non-trivial (many-body) processes such as single-particle density-dependent tunnelling, correlated pair hoppings, nonlocal (extended) pair hopping, and so on. Using a suitable driving, we are able to suppress or enhance a particular process in the effective Hamiltonian. Such approach can be very useful for engineering particular Hamiltonians, for simulating solid-state phenomena via optical means, for accurate interpretation of experiments with driven lattice systems, etc.

To clarify our main idea, let us firstly start with a Schrödinger equation for a lattice system (e.g., a single particle in a driven 1D tight-binding model), written in the matrix form:

$$i\dot{X} = \epsilon H X,$$

where $\epsilon = \frac{1}{\hbar}$ is a small parameter, $\omega$ is a frequency of perturbation, $H(t)$ is a time-dependent (matrix) Hamiltonian of the system, $X$ is a column of coefficients of expansion of a quantum state in a certain basis, and fast time was introduced ($t \to t/\epsilon$), resulting in the small coefficient $\epsilon$ in front of r.h.s of Eq. (1), to put high-frequency dependence of the Hamiltonian in explicit form. A particular example, a single particle in a tight-binding model, is
Hermitian time-periodic matrices, which would remove Hamiltonian, the transformation is sought in the form
\[ \mathcal{H} \rightarrow \mathcal{H} + \mathcal{K} \]
where\[ \mathcal{K} = \frac{1}{2} \left\{ K_1 \mathcal{H} K_1 - \frac{i}{2} (\dot{K}_1 \mathcal{K} - \mathcal{K} \dot{K}_1) \right\} \]
and square brackets denote matrix commutation: \([A,B] = AB - BA\).

Eqs. (2) or (6) allow to consider, e.g., a particle in driven tight-binding models with various boundary conditions, as well as with additional external potentials (see 27 and SI). General expressions for higher-order corrections will contain nested commutators (similar to, e.g., 28), but for most practical purposes corrections up to the second order are sufficient. The general equations (6) are also convenient for studying many-body systems. Indeed, in the case of many particles, one can construct a corresponding Hamiltonian matrix and fulfill the same transformations. Moreover, it is not necessary to consider Hamiltonians 33 in the matrix representation: one can use, e.g., creation and annihilation operators.

Indeed, consider now a Bose-Hubbard model with a high-frequency driving:
\[ H(t) = H_{BH} + H_d(t), \]
\[ H_{BH} = J \sum_i (\epsilon_i^c c_{i+1}^c + \epsilon_i^f c_{i+1}^f) + U \sum_i n_i (n_i - 1), \]
\[ H_d(t) = \mathcal{E}(\omega t) \sum_j j n_j, \]
where \( J \) is the hopping parameter, \( U \) is the interaction strength. Later, we will consider also time-dependent \( J(t) \), which can be obtained, e.g., by amplitude modulation of the lattice 10, 33. Following the approach we used in the single-particle case, we make a preliminary transformation \( U^{(0)}(t) = \exp\{\mathcal{C}(t)\} \), \( f(t) \equiv \frac{t}{\mathcal{E}(t')}dt' \), and make rescaling of time, \( t' = \omega t = t/\epsilon \), so that the new Hamiltonian is \( \mathcal{H}(t) = \epsilon (H_{eff}^{(0)} + \delta H(t)) \), where
\[ H_{eff}^{(0)} = \sum_i J_{eff} (\epsilon_i^c c_{i+1}^c + \epsilon_i^f c_{i+1}^f) + U \sum_i n_i (n_i - 1), \]
\[ \delta H(t) = \sum_i [\delta^+(t) \epsilon_i^c c_{i+1}^c + \delta^-(t) \epsilon_i^f c_{i+1}^f], \]
In other words, the new Hamiltonian is \( \mathcal{H}(t) = \epsilon \sum_i \left[ \delta^+(t) \epsilon_i^c c_{i+1}^c + \delta^-(t) \epsilon_i^f c_{i+1}^f \right] + U \sum_i n_i (n_i - 1) \), where \( \delta^\pm = e^{\pm i \delta(t)} \). The unitary transformations we fulfilled in the single-particle case should be done here as well. However, to find Hamiltonians \( K_1, K_2, \mathcal{H}_1, \mathcal{H}_2 \) explicitly, we have to fulfill more complicated many-body calculations. In the first order, we have \( K_1 = -i \{ \mathcal{H}, \mathcal{K} \} = -i \epsilon \sum_i \left[ \delta^+(t) \epsilon_i^c c_{i+1}^c + \delta^-(t) \epsilon_i^f c_{i+1}^f \right] \), and therefore \( K_1 = -i \epsilon \sum_i \left[ \delta^+(t) \epsilon_i^c c_{i+1}^c + \delta^-(t) \epsilon_i^f c_{i+1}^f \right] \). Commutators \([\mathcal{H}, K_1], [\mathcal{H}, K_1], ,\) etc., are derived in SI. We obtain a very interesting result: the first-order correction to the averaged Hamiltonian is \( \langle \mathcal{H}, K_1 \rangle = -2 e i U \sum_j \delta^+_j c_j^f (n_j - n_{j+1}) c_{j+1}^c - \delta^-_j c_j^f (n_j - n_{j+1}) c_{j+1}^c \). This correction resembles somehow the result of the flow equation method calculations 34 (the structure of Hamiltonian is the same, but the coefficients \( \delta^\pm \) are different). However, the main thing is that in our approach this contribution completely disappears during time-averaging (being averaged to zero, \( \mathcal{H}_1 = 0 \), and therefore to find
At the same time, \( \Delta(n) \), we need to consider the next orders of perturbation, exactly as in the single-particle case. This give us (see SI)

\[
\mathcal{H}_2 = U(\Delta_1 a_1 + h.c.) + U(\Delta_2 + \Delta_3^2) a_2, \tag{9}
\]

where

\[
\begin{align*}
\Delta_1 &= \langle \delta_2^+ \delta_2^- + 2\delta_2^- \delta_3^+ \rangle, \\
\Delta_2 &= \langle \delta_3^+ \delta_3^- + 2\delta_3^- \delta_3^+ \rangle, \\
a_1 &= \sum_j \left( c_{j-1}^\dagger (4n_j - n_{j+1} - n_{j-1}) c_{j+1} + 2c_{j+1}^\dagger c_{j+1} c_{j+1} \right), \\
a_2 &= \sum_j \left( (4n_j n_{j+1} - 2n_j (n_j - 1) - c_{j-1}^\dagger c_{j+1} c_j - c_{j-1}^\dagger c_{j+1} c_{j+1} - c_{j-1}^\dagger c_{j+1} c_{j+1} c_{j+1} \right)
\end{align*}
\]

(10)

The effective Hamiltonian contains nearest-neighbour interactions and several types of correlated tunnelling processes (pair tunnelling \( c_{j+1}^\dagger c_{j+1} c_{j+1} c_{j+1} \) and pair 'dissociation'/association' process \( c_{j+1}^\dagger c_{j+1} c_{j+1} c_{j+1} \)). One may expect a rich phase diagram of the driven system. In particular, it is known that extended Bose-Hubbard model, obtained by adding nearest-neighbour interactions to the Bose-Hubbard Hamiltonian, possess a supersolid phase. Analysis of the phase diagram of (9) is beyond the scope of this paper.

We note that in the particular case of harmonic perturbation \( \mathcal{E} = -K \sin t \), we have \( \Delta_1 = 2 \sum_{k=1}^{\infty} (-1)^k \frac{J^2(K)}{K^2} \). This is a decaying oscillatory function of \( K \) which can be either positive or negative, and by varying the amplitude \( K \) one can either maximize its absolute value (e.g., at \( K = 1.77 \)), or put it to zero (e.g., at \( K = 3.33 \)).

At the same time, \( \Delta_2 = 2 \sum_{k=1}^{\infty} \frac{J^2(K)}{K^2} \), which is a non-vanishing oscillatory function of \( K \) with local maxima at \( K = 1.93, 5.32 \), etc. It is not difficult to show that using a more complicated driving with several parameters one can simultaneously put \( \Delta_1 \) and \( \Delta_2 \) to zero, or selectively nullify one of them while maximizing another one. This can be useful for making more precise experiments on dynamical localization. In case of harmonic driving, a single-particle tunnelling is stopped at \( J_0(K) = 0 \). We see that even in the many-body setup, one can construct a more complicated driving which would stop also higher-order processes, using general formulas for the effective Hamiltonian.

Let us now consider the driven Hubbard model

\[
\begin{align*}
H &= H_H + H_d(t), \\
H_H &= J \sum_{i,\sigma} (c_{i+1,\sigma}^\dagger c_{i,\sigma} + c_{i+1,\sigma}^\dagger c_{i,\sigma}) + U \sum_i n_{i,\sigma} n_{i,-\sigma}, \\
H_d(t) &= \mathcal{E}(\omega t) \sum_j j n_j, \tag{11}
\end{align*}
\]

which becomes, after the preliminary transformation discussed above,

\[
\mathcal{H} = \sum_{i,\sigma} \left( \delta_{i+1,\sigma} c_{i+1,\sigma}^\dagger c_{i+1,\sigma} + \delta_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} \right) + U \sum_i n_{i,\sigma} n_{i,-\sigma}
\]

Calculations analogous to the Bose-Hubbard model case give us (see SI)

\[
\begin{align*}
\mathcal{H}_1 &= 0, \\
\mathcal{H}_2 &= \Delta_0 (-2S + A + A^\dagger + 4V - 2V) + \left[ \Delta_0 (4R - 2R + 2R) + H.c. \right],
\end{align*}
\]

where \( \Delta_0 = \langle \delta_2^+ (\delta_0^+ - \frac{1}{2} \delta_2^+) + \delta_2^- (\delta_2^- - \frac{1}{2} \delta_2^-) \rangle, \Delta_0 = \langle \delta_2^- (\delta_0^+ - \frac{1}{2} \delta_2^-) \rangle \), and several types of tunnelling and interaction processes were denoted as \( S, A, R, R, R, V \), and \( V \). \( S \) denotes a correlated tunneling process of two atoms on neighboring sites exchanging their positions ('superexchange'). \( A \) denotes a tunneling process where a pair of atoms at \( j \)th site is dissociated into two atoms at neighboring sites \( (j - 1) \) and \((j + 1) \). \( R \) denotes a corresponding correlated tunneling process of association of two atoms into a pair. \( R \) denotes a correlated tunneling process where an extended pair of atoms is tunnelling to the right neighboring sites, and \( R \) denotes tunnelling to the left. \( R \) denotes tunnelling of a localized pair of atoms to the right, and \( R \) denotes tunnelling to the left. \( R \) denotes single-particle next-nearest-neighbour density-dependent tunnelling to the right, and \( R \) denotes corresponding tunnelling to the left; \( V \) denotes nearest-neighbour interaction, and \( V \) denotes usual local interaction.

\[
\begin{align*}
S &= \sum_j c_{j+1,\sigma}^\dagger c_{j,\sigma} c_{j-1,\sigma}^\dagger c_{j+1,\sigma}, \\
A &= A^\dagger + A^\dagger, \quad A \rightarrow -\sigma = \sum_j c_{j,\sigma}^\dagger c_{j+1,\sigma}^\dagger c_{j-1,\sigma} c_{j+1,\sigma}, \\
R &= R^\dagger + R^\dagger, \quad R \rightarrow -\sigma = \sum_j c_{j,\sigma}^\dagger c_{j-1,\sigma}^\dagger c_{j+1,\sigma} c_{j+1,\sigma}, \\
R &= \sum_j c_{j+1,\sigma}^\dagger c_{j+1,\sigma}^\dagger c_{j,\sigma}^\dagger c_{j,\sigma}, \\
R &= \sum_j c_{j+1,\sigma} c_{j+1,\sigma} c_{j,\sigma}^\dagger c_{j,\sigma}^\dagger, \\
V &= \sum_j n_j n_{j+1,\sigma}, \quad V = \sum_j n_j n_{j+1,\sigma}\tag{12}
\end{align*}
\]

We note that a two-particle problem in a driven asymmetric Hubbard model was recently considered in [35], where formation of a doublet of two fermions residing on nearest-neighbour sites and co-tunnelling along the lattice was found (bare tunnelling constants of the two fermions being different, \( J_1 \neq J_1 \)). This result (obtained in the first order approximation), in fact, is in accordance with our finding that there are no first-order corrections in driven symmetric Hubbard model. Indeed, the first-order correction found in [35] is proportional to \( J_1 = J_1 \); i.e. it completely disappears in the symmetric limit \( J_1 = J_1 \), in accordance with our result.
To conclude, a convenient method based on canonical (unitary) transformations has been elaborated and applied to two different lattice systems: driven 1D Hubbard and Bose-Hubbard models. For a general high-frequency driving, we derive explicitly effective Hamiltonians including corrections from interactions. By a suitable driving, it is possible to cancel particular contributions in these Hamiltonians.

These results, we believe, will be useful for forthcoming experiments with cold atoms in driven optical lattices. In particular, presently in experiments with shaken optical lattices utilizing effective (averaged) tunnelling constants, a frequency of driving is typically chosen in kHz regime, in order to be much higher than all timescales related to trapping potential and interactions, and much lower than interband transition frequency. Explicit knowledge of corrections from trapping potentials and many-body interactions we derived here allow to extend area of applicability of shaken lattice simulations to sub-kHz regime, by choosing driving protocols that cancel second-order corrections. On the other hand, one might want instead to amplify particular contributions from second-order corrections, thereby engineering new model Hamiltonians. Another inspiring direction of application of our theory is photoinduced superconductivity and metal-insulator transitions, where recent studies show importance of induced Kapitza-like effective potentials.

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As a particular example, in the case of a particle in a driven tight-binding chain, one has (see [A.P. Itin, A.I. Neishtadt, in preparation]) $H = J \sum (|n\rangle \langle n + 1| + |n + 1\rangle \langle n|) + e d E(\omega t) \sum \langle n|n\rangle \langle n|$, where $d$ is the intersite distance, $E$ is the applied electric field, $e$ is the charge of the particle, $J$ is the tunnelling constant. The same model can be realized also with neutral particles (in the co-moving frame), by appropriate shaking of the lattice \cite{13}. Expanding a quantum state as $|\psi(t)\rangle = \sum c_n|n\rangle$, we get a system of equations

$$i \dot{c}_n = J(c_{n+1} + c_{n-1}) + E(\omega t) n c_n. \quad (13)$$

We make a transformation $c_n(t) = X_n(t) \exp\left[-i \int_0^t E(t') dt' \right]$, so that equations of motion are

$$i \dot{X}_n = J(X_{n+1} F(t) + X_{n-1} F^*(t)), \quad (14)$$

where $F(t) = \exp\left[-i \int_0^t E(t') dt' \right] = F_0 + \sum F_i \exp(-i \omega t)$, $E = e d E$.

Introducing fast time $t' = \omega t \equiv t/\epsilon$, we get, in the matrix form, Eq. (1), with the Hamiltonian $H$ corresponding to Eq. (13).

In a more general setting, a particle in a driven tight-binding chain subject to an additional external potential $V(n)$, we have

$$i \dot{X}_n = \epsilon [J(X_{n+1} F(t) + X_{n-1} F^*(t)) + V(n) X_n], \quad (15)$$

or

$$i \dot{X}_n = \epsilon H. \quad (16)$$

In the spirit of classical canonical perturbation theory, we are making a unitary transformation $X = C \tilde{X}$ so that equations for the transformed variables are

$$i \dot{\tilde{X}} = [C^{-1} \epsilon H C - i C^{-1} \dot{C}] \tilde{X}. \quad (17)$$

We are searching for a transformation of the form $C = \exp[\epsilon K_1 + \epsilon^2 K_2 + \epsilon^3 K_3]$, where $K_i$ are skew-Hermitian time-periodic matrices, which would remove time-dependent terms from the Hamiltonian, leaving only time-independent terms.

We have

$$C \approx I + \epsilon K_1 + \epsilon^2 \left( \frac{1}{2} K_1^2 + K_2 \right) + \epsilon^3 \left( \frac{1}{6} K_1^3 + \frac{1}{2} K_1 K_2 + K_2 K_1 + K_3 \right),$$

$$C^\dagger \approx I - \epsilon K_1 + \epsilon^2 \left( \frac{1}{2} K_1^2 - K_2 \right) + \epsilon^3 \left( -\frac{1}{6} K_1^3 + \frac{1}{2} K_1 K_2 + K_2 K_1 - K_3 \right), \quad (18)$$

where $I$ is the unity matrix.

In the first order, we have

$$i \dot{\tilde{K}}_1 = H(t) - \langle H(t) \rangle \equiv \{ H \}, \quad (19)$$

and therefore $i \dot{K}_1 = \int (H - \langle H \rangle) dt = \int \{ H \} dt$. We introduce here curly brackets as taking time-periodic part of a time-dependent function: $\{ X \} \equiv X - \langle X(t) \rangle$, where $\langle X(t) \rangle \equiv \frac{1}{2\pi} \int_0^{2\pi} X(t') dt'$.

In the second order,
\[ i\dot{K}_2 = \left\{ HK_1 - K_1 H - \frac{i}{2} (\dot{K}_1 K_1 - K_1 \dot{K}_1) \right\}, \] (20)

and the effective Hamiltonian is

\[ \epsilon H_{eff} = \epsilon H_0 + \epsilon^2 H_1 + \epsilon^3 H_2, \] (21)

where

\[
\begin{align*}
H_0 &= \langle H \rangle \\
H_1 &= \langle HK_1 - K_1 H - \frac{i}{2} (\dot{K}_1 K_1 - K_1 \dot{K}_1) \rangle \\
H_2 &= \langle HK_2 - K_2 H + \frac{1}{2} (HK_1^2 + K_1^2 H) - K_1 H K_1 - \frac{i}{2} (\dot{K}_1 K_1 - K_1 \dot{K}_1) - \frac{i}{6} (\dot{K}_1 K_1^2 + K_1^2 \dot{K}_1 - 2K_1 \dot{K}_1) \rangle
\end{align*}
\]

(22)

In the case of the uniform tight-binding model (without external potential) and open boundary conditions the effective Hamiltonians have the following simple form

\[
H_1 = J^2 DZ_1, \quad H_2 = -\frac{J^3}{3} (L_3 U_1 + L_3^* B_1),
\]

(23)

where \( Z_1 = \delta_{i,j} \delta_{i,1} - \delta_{i,j} \delta_{i,N} \), \( N \) is the number of sites, \( D = \sum_{l=1}^L (|F_l|^2 - |F_{-l}|^2)/l, \) \( U_1 = \delta_{i,i+1} \delta_{i,1} + \delta_{i,i+1} \delta_{i,N-1} \) (the upper co-diagonal with ‘1’ on its ends, and zeros elsewhere), \( B_1 = \delta_{i,i-1} \delta_{i,2} + \delta_{i,i-1} \delta_{i,N} \) (the lower co-diagonal with ‘1’ on its ends), \( L_3 \) is a function of driving defined in [27]. In other words, the first-order correction \( H_1 \) is non-zero only if perturbation has certain broken time symmetry (for a single harmonic perturbation, \( \cos t \), \( H_1 \) disappears), and it localizes near the ends of the chain (near boundaries). More generally, it requires non-uniformity of the coupling constant \( J \), so e.g. in a model with alternating coupling constants \( J_1 - J_2 - J_1 \), or with a more general non-uniform coupling \( J(n) \), the correction will be non-zero throughout the whole chain [26]. For the uniform coupling \( J(n) \), \( H_2 \) is also localized near the boundaries of the open chain. The method of multiple time scales [26] produces the same results in these cases.

A very interesting new result can be obtained for a parabolic external potential \( V(n) = V n^2/2 \): the second-order correction to the averaged Hamiltonian corresponds to an induced uniform next-nearest neighbour coupling, which for the harmonic perturbation with amplitude \( K \) is explicitly given by \( J' = -\epsilon^2 J^2 V \sum_{l=1}^L \frac{(-)^l j^2 l}{l^2} \) [27].

In the case of infinite uniform lattice, or periodic boundary conditions, \( H_1 \) and higher-order corrections are absent.

**B. Bose-Hubbard model**

We have

\[
\begin{align*}
K_1 &= -i \{ H \} = -i \sum_i \left( \delta^+_i c^+_i c^i_{i+1} + \delta^-_i c^i_{i+1} c_i \right), \\
K_1 &= -i \sum_i \left( \delta^+_i c^+_i c^i_{i+1} + \delta^-_i c^i_{i+1} c_i \right)
\end{align*}
\]

(24)

(25)

\[ HK_1 - K_1 H = -i 2U \sum_j \left( \delta^+_j c^j_j (n_j - n_{j+1}) c^i_{j+1} + \delta^-_j c^j_{j+1} (n_{j+1} - n_j) c^i_j \right) \]

(26)

Since \([K_1, K_1] = 0\),
For the second-order corrections we have

\[\begin{align*}
\dot{K}_2 &= \{HK_1 - K_1H\}, \\
K_2 &= -2U \sum_j \left( \delta^+_2 c_j^\dagger(n_j - n_{j+1})c_{j+1} + \delta^-_2 c_{j+1}^\dagger(n_{j+1} - n_j)c_j \right)
\end{align*}\]

(27)

For the second-order corrections we have

\[\begin{align*}
HK_2 - K_2H &= 2U \sum_{\alpha=1}^6 A_\alpha, \\
A_1 &= -\delta^+_2 \delta^-_0 \sum_j \left( c_{j-1}^\dagger(4n_j - n_{j+1} - n_{j-1})c_{j+1} - 2c_j^\dagger c_j c_{j+1}c_{j+1} \right) = -\delta^+_2 \delta^-_0 a_1 \\
A_2 &= -\delta^+_2 \delta^-_0 \sum_j \left( 4n_jn_{j+1} - 2n_j(n_j - 1) - c_{j-1}^\dagger c_{j+1} c_j c_{j+1}c_j - c_j^\dagger c_{j+1}c_{j+1}c_j \right) = -\delta^+_2 \delta^-_0 a_2, \\
A_3 &= \sum_j \left( 4n_jn_{j+1} - 2n_j(n_j - 1) - c_{j-1}^\dagger c_{j+1} c_j c_{j+1}c_j - c_j^\dagger c_{j+1}c_{j+1}c_j \right) = -\delta^+_2 \delta^-_0 a_3, \\
A_4 &= -\delta^+_2 \delta^-_0 \sum_j \left( c_{j+1}^\dagger(4n_j - n_{j+1} - n_{j-1})c_j - 2c_j^\dagger c_j^\dagger c_{j+1}c_{j+1} \right) = -\delta^+_2 \delta^-_0 a_4, \\
A_5 &= -2U\delta^+_2 \sum_j \left( c_j^\dagger(n_j - n_{j+1})^2c_{j+1} \right) = -2U\delta^+_2 a_5, \\
A_6 &= -2U\delta^-_2 \sum_j \left( c_{j+1}^\dagger(n_j - n_{j+1})^2c_j \right) = -2U\delta^-_2 a_6,
\end{align*}\]

(28)

\[\begin{align*}
-\frac{i}{2} \left( \dot{K}_1K_2 - K_2\dot{K}_1 \right) &= U \sum_{\alpha=1}^4 B_\alpha, \\
B_1 &= \delta^+ \delta^-_0 a_1, \\
B_2 &= \delta^+ \delta^-_2 a_2, \\
B_3 &= \delta^- \delta^-_2 a_3, \\
B_4 &= \delta^- \delta^-_4 a_4,
\end{align*}\]

(29)

\[\begin{align*}
-\frac{i}{2} \left( \dot{K}_2K_1 - K_1\dot{K}_2 \right) &= U \sum_{\alpha=1}^4 C_\alpha, \\
C_1 &= -(\delta^+)^2 a_1, \\
C_2 &= -\delta^+ \delta^-_1 a_2, \\
C_3 &= -\delta^- \delta^-_1 a_3, \\
C_4 &= -(\delta^-)^2 a_4,
\end{align*}\]

(30)

\[\begin{align*}
\frac{1}{2} \left[ [H, K_1], K_1 \right] &= U \sum_{\alpha=1}^4 D_\alpha, \\
D_1 &= (\delta^+)^2 a_1, \\
D_2 &= \delta^+ \delta^-_1 a_2, \\
D_3 &= \delta^- \delta^-_1 a_3, \\
D_4 &= (\delta^-)^2 a_4,
\end{align*}\]

(31)

We note that \(D_k = -C_k\) and time-averages of the coefficients \(A_5\) and \(A_6\) are equal to zero. Also, \([\dot{K}_1, K_1] = 0\).
We therefore get the effective second-order correction

\[ H_2 = U \sum_{\alpha=1}^{4} \Delta_\alpha a_\alpha, \]

\[ \Delta_1 = \langle \delta_2^+ \delta^- - 2 \delta_2^+ \delta_0^+ \rangle, \]

\[ \Delta_2 = \langle \delta_2^+ \delta_2^- - 2 \delta_2^+ \delta_0^- \rangle, \]

\[ \Delta_3 = \langle \delta_2^- \delta_2^- - 2 \delta_2^- \delta_0^+ \rangle, \]

\[ \Delta_4 = \langle \delta_2^- \delta_2^- - 2 \delta_2^- \delta_0^- \rangle, \] (32)

where \( a_\alpha \) are given by

\[ a_1 = \sum_j (c_{j-1}^\dagger (4n_j - n_{j+1} - n_{j-1}) c_{j+1}^\dagger - 2c_{j}^\dagger c_{j+1} c_{j+1}) \]

\[ a_2 = \sum_j (4n_j n_{j+1} - 2n_j (n_j - 1) - c_{j-1}^\dagger c_{j+1} c_j c_j - c_{j}^\dagger c_{j+1} c_{j+1}) \] (33)

\[ a_3 = \sum_j (4n_j n_{j+1} - 2n_j (n_j - 1) - c_{j-1}^\dagger c_{j+1} c_j c_j - c_{j}^\dagger c_{j+1} c_{j+1}) \]

\[ a_4 = \sum_j (c_{j+1}^\dagger (4n_j - n_{j+1} - n_{j-1}) c_{j-1} - 2c_{j+1}^\dagger c_{j+1} c_j c_j) \]

We can simplify it further:

\[ H_2 = U(\Delta_1 a_1 + h.c) + U(\Delta_2 + \Delta_3) a_2 \] (34)

C. Hubbard model

We have:

\[ H = \sum_{i,\sigma} \left( \delta_{ij}^+ c_{i,\sigma}^\dagger c_{j+1,\sigma} + \delta_{ij}^- c_{i+1,\sigma}^\dagger c_{i,\sigma} \right) + U \sum_i n_{i,\sigma} n_{i,-\sigma} \]

\[ = T^\dagger + T^\dagger + U \]

\[ \hat{K}_1 = -i \{ H \} = -i \sum_{j,\sigma} \left( \delta_{ij}^+ c_{j,\sigma}^\dagger c_{j+1,\sigma} + \delta_{ij}^- c_{j+1,\sigma} c_{j,\sigma} \right), \]

\[ K_1 = -i \sum_{j,\sigma} \left( \delta_{ij}^+ c_{j,\sigma}^\dagger c_{j+1,\sigma} + \delta_{ij}^- c_{j+1,\sigma} c_{j,\sigma} \right) \equiv K_{1}^\dagger + K_{1}^\dagger, \]

\[ HHK_1 - K_1 H = [T^\dagger, K_{1}^\dagger] + [T^\dagger, K_{1}^\dagger] + [U, K_{1}^\dagger] + [U, K_{1}^\dagger], \]

\[ T^\dagger K_{1}^\dagger - K_{1}^\dagger T^\dagger = -i(\delta_{ij}^+ \delta_{ij}^+ - \delta_{ij}^- \delta_{ij}^-) \sum_i (n_{i+1,\uparrow} - n_{i,\uparrow}) \]

\[ T^\dagger K_{1}^\dagger - K_{1}^\dagger T^\dagger = -i(\delta_{ij}^+ \delta_{ij}^+ - \delta_{ij}^- \delta_{ij}^-) \sum_i (n_{i+1,\downarrow} - n_{i,\downarrow}) \]

\[ U K_{1}^\dagger - K_{1}^\dagger U = -i U \sum_j (\delta_{ij}^+ c_{j+1,\uparrow} c_{j,\uparrow} (n_{j,\downarrow} - n_{j+1,\downarrow}) - \delta_{ij}^- c_{j+1,\downarrow} c_{j,\downarrow} (n_{j,\uparrow} - n_{j+1,\uparrow})) \]

\[ U K_{1}^\dagger - K_{1}^\dagger U = -i U \sum_j (\delta_{ij}^+ c_{j+1,\uparrow} c_{j,\uparrow} (n_{j,\uparrow} - n_{j+1,\uparrow}) - \delta_{ij}^- c_{j+1,\downarrow} c_{j,\downarrow} (n_{j,\downarrow} - n_{j+1,\downarrow})) \]

We have also \([\hat{K}_1, K_1] = 0\), therefore

\[ i\hat{K}_2 = \{ HHK_1 - K_1 H \}, \] (36)

\[ \hat{K}_2 = \delta_{01} \sum_{j,\sigma} (n_{j,\sigma} - n_{j+1,\sigma}) + U \sum_{j,\sigma} \left( \delta_{ij}^- c_{j+1,\sigma} c_{j,\sigma} - \delta_{ij}^+ c_{j,\sigma} c_{j+1,\sigma} \right) (n_{j,-\sigma} - n_{j+1,-\sigma}) = K_{\delta}^\dagger + K_{\delta}^\dagger + K_{\delta}^\dagger + K_{\delta}^\dagger. \]
To calculate commutator of $H$ and $K_2$, we proceed as follows:

$$
[H, K_2] = \left[ T^\dagger, K_2^\dagger \right] + \left[ T^\dagger, K_2 \right] + \left[ T^i, K_2^\dagger \right] + \left[ T^i, K_2 \right] + \left[ U, K_2^\dagger \right] + \left[ U, K_2 \right] \tag{37}
$$

$$
T^i K_2^\dagger - K_2^\dagger T^i = U \sum_j \left( \delta_0^i \delta_2^i c_{j+1,\uparrow} c_{j+1,\downarrow} + \delta_0^i \delta_2^i c_{j-1,\uparrow} c_{j+1,\downarrow} \right) (n_{j,\downarrow}^\dagger n_{j,\downarrow} - n_{j,\uparrow} n_{j+1,\downarrow})
+ U \sum_j \left( \delta_0^i \delta_2^i c_{j+1,\uparrow} c_{j-1,\uparrow} c_{j+1,\downarrow} + \delta_0^i \delta_2^i c_{j-1,\uparrow} c_{j+1,\downarrow} \right) (n_{j,\downarrow} - 2n_{j,\downarrow}^\dagger + n_{j+1,\downarrow})
\tag{38}
$$

The last two terms in Eq.(37) will produce zero time-average and are not important for us. Let us introduce $[H, K_2]_U = \left[ T^\dagger, K_2^\dagger \right] + \left[ T^\dagger, K_2 \right] + \left[ T^i, K_2^\dagger \right] + \left[ T^i, K_2 \right]$, i.e. the expression (37) without the last two terms. Expressions above represent several fundamental processes. We introduce the following notation for them:

$$
S = S_{\uparrow, \downarrow} + S_{\downarrow, \uparrow}, \quad S_{\sigma, -\sigma} = \sum_j c_{j+1, \sigma}^\dagger c_{j, -\sigma} c_{j+1, -\sigma}^\dagger c_{j, \sigma}, \quad \tag{39}
$$

$$
A = A_{\uparrow, \downarrow} + A_{\downarrow, \uparrow}, \quad A_{\sigma, -\sigma} = \sum_j c_{j, \sigma}^\dagger c_{j-1, -\sigma} c_{j, -\sigma}^\dagger c_{j-1, \sigma}, \quad \tag{40}
$$

$$
R = R_{\uparrow, \downarrow} + R_{\downarrow, \uparrow}, \quad R_{\sigma, -\sigma} = \sum_j c_{j, \sigma}^\dagger c_{j-1, -\sigma} c_{j+1, -\sigma}^\dagger c_{j-1, \sigma}, \quad \tag{41}
$$

$$
R_2 = R_{2, \uparrow} + R_{2, \downarrow}, \quad R_{2, \sigma} = \sum_j c_{j+1, \sigma}^\dagger c_{j-1, \sigma} (n_{j-1, -\sigma} - 2n_{j, -\sigma} + n_{j+1, -\sigma}), \quad \tag{42}
$$

$$
V = \sum \delta_0^i + \delta_2^i V_{\sigma}, \quad V_{\sigma} = \sum_j n_{j, \sigma} n_{j+1, -\sigma}, \quad \tag{43}
$$

$$
V = \sum_j n_{j, \downarrow} n_{j, \uparrow} \quad \tag{44}
$$
There are several different types of tunnelling and interaction processes here ($S, A, R, R_2, V, \text{ and } V$). $S$ denotes a correlated tunnelling process of two atoms on neighboring sites exchanging their positions ('superexchange'). $A^\dagger$ denotes a tunnelling process where a pair of atoms at $j$th site is dissociated into two atoms at neighboring sites ($j - 1$ and $j + 1$). $A$ denotes a corresponding correlated tunneling process of association of two atoms into a pair. $R$ denotes a correlated tunnelling process where an extended pair of atoms is tunnelling to the right neighboring sites, and $R^\dagger$ denotes tunnelling to the left. $R$ denotes tunnelling of a localised pair of atoms to the right, and $R^\dagger$ denotes corresponding tunnelling to the left. $R_2$ denotes single-particle next-nearest-neighbour density-dependent tunnelling to the right, and $R_2^\dagger$ denotes corresponding tunnelling to the left. $V$ denotes nearest-neighbour interaction, and $V$ denotes usual local interaction. We can rewrite $[H, K_2]_{\mu \ell}$ in terms of these fundamental processes:

$$[H, K_2]_{\mu \ell} = U[(\delta_0^+ \delta_2^- (4R - 2R + R_2) + H.c.) + (\delta_0^+ \delta_2^- + \delta_0^- \delta_2^+)(-2S + A + A^\dagger + 4V - 2V)]$$

Now, let us consider the term $\frac{1}{2}[H, K_1, K_1]$. It can be shown $\frac{1}{2}[H, K_1, K_1] = \frac{1}{2}P(\delta_0^+ \rightarrow \delta_1^x, \delta_2^+ \rightarrow -\delta_1^x)[H, K_2]_{\mu \ell}$. Also,

$$-\frac{i}{2}[\dot{K}_2, K_1] = \frac{1}{2}P(\delta_0^+ \rightarrow \delta_1^+, \delta_2^+ \rightarrow \delta_1^x)[H, K_2]_{\mu \ell} = -\frac{1}{2}[[H, K_1], K_1],$$

and

$$-\frac{i}{2}[\dot{K}_1, K_2] = -\frac{1}{2}P(\delta_0^+ \rightarrow \delta^x)[H, K_2]_{\mu \ell}$$

We have finally

$$\mathcal{H}_2 = \Delta_0(-2S + A + A^\dagger + 4V - 2V) + \left[\Delta^-(4R - 2R + R_2) + H.c.\right],$$

where

$$\Delta_0 = \langle \delta_2^+ \left(\delta_0^+ - \frac{1}{2}\delta^+\right) + \delta_2^+ \left(\delta_0^- - \frac{1}{2}\delta^-\right)\rangle$$

$$\Delta^- = \langle \delta_2^- \left(\delta_0^- - \frac{1}{2}\delta^-\right)\rangle$$