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Effective Hamiltonians for fastly driven tight-binding chains

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ABSTRACT

We consider a single particle tunnelling in a tight-binding model with nearest-neighbour couplings, in the presence of a periodic high-frequency force. An effective Hamiltonian for the particle is derived using an averaging method resembling classical canonical perturbation theory. Three cases are considered: uniform lattice with periodic and open boundary conditions, and lattice with a parabolic potential. We find that in the latter case, interplay of the potential and driving leads to appearance of the effective next-nearest neighbour couplings. In the uniform case with periodic boundary conditions the second- and third-order corrections to the averaged Hamiltonian are completely absent, while in the case with open boundary conditions they have a very simple form, found before in some particular cases by S. Longhi (2008) [10]. These general results may found applications in designing effective Hamiltonian models in experiments with ultracold atoms in optical lattices, e.g. for simulating solid-state phenomena.

1. Introduction

Effective Hamiltonians created by high-frequency perturbations have many interesting applications in physics; a well-known counterintuitive example of induced effective potential is provided by Kapitza pendulum [1,2]. We are interested in applying averaging methods of classical Hamiltonian mechanics (see, e.g., [3]) to quantum tight-binding models, which often arise in solid-state and, more generally, condensed-matter physics.

In solid-state physics, unusual transport phenomena may arise when an ac electric field is applied to the system, e.g. coherent destruction of tunnelling and dynamic localisation [4,5]. Corresponding applications to coherent control of tunnelling and electronic transport in semiconductor superlattices and arrays of coupled quantum dots have been receiving a lot of interest lately [6,7]. Very recently, in many experiments with atoms in optical lattices, effective Hamiltonians were created using high-frequency perturbations [5,8,9]. A particle in a deep optical lattice potential can be described by a tight-binding model. Applying a high-frequency force, one can engineer effective tunnelling constants in the model, which can be useful to mimic certain solid-state phenomena [8]. For many realistic applications of such type, it is important to derive accurate effective Hamiltonians taking into account higher-order terms [10]. Here we find a useful method for such derivation in the spirit of canonical perturbation theory, and apply it for several tight-binding systems. Our approach is based on idea of canonical transformations removing time-dependence from the Hamiltonian, which in the present context means unitary transformations of square matrices. Similar ideas have been applied to transport in classical periodic potentials [11–13]. In the next section, the general method is outlined. In Section 3, it is applied to three different tight-binding models. Our approach is actually not limited to tight-binding systems, but it becomes especially transparent and elegant for such kind of systems. Section 4 gives concluding remarks.

2. The averaging method

Consider a tight-binding model with the Hamiltonian

$$H = J\sum\big(|n\rangle\langle n+1| + |n+1\rangle\langle n|\big) + \sum_n V(n)|n\rangle\langle n| + edE(\omega t)\sum_n n|n\rangle\langle n|, \tag{1}$$

where J is the hopping parameter, $V(n)$ is the external potential (we consider only parabolic potential in this paper, $V(n) = V\frac{n^2}{2}$), d is the intersite distance, E is the applied electric field, e is the charge of the particle. The same model can be realised also with neutral particles, by appropriate shaking of the lattice.

Expanding a quantum state as $|\psi(t)\rangle = \sum c_n|n\rangle$, one gets a system of equations

$$i\dot{c}_n = J(c_{n+1} + c_{n-1}) + V(n)c_n + \mathcal{E}(\omega t)nc_n. \tag{2}$$

It is convenient to make a transformation $c_n(t) = x_n(t) \times \exp[-in\int_0^t \mathcal{E}(t')\,dt']$, so that equations of motion are

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$$i\dot{x}_n = J\left(x_{n+1}F(t) + x_{n-1}F^*(t)\right) + V(n)c_n, \tag{3}$$

where $F(t) = \exp[-i\int_0^t \mathcal{E}(t')\,dt'] = F_0 + \sum F_l \exp(-il\omega t)$, $\mathcal{E} = edE$.

Introducing fast time $t' = \omega t \equiv t/\epsilon$, we get, in the matrix form,

$$i\dot{X} = \epsilon H X, \tag{4}$$

where

$$H = J\begin{pmatrix} 0 & F & \cdots & 0 \\ F^* & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & F \\ 0 & \cdots & F^* & 0 \end{pmatrix} \equiv J\left(F\mathcal{U} + F^*\mathcal{B}\right), \tag{5}$$

where $\mathcal{U}$, $\mathcal{B}$ are matrices with unities on the first upper- and lower-co-diagonals, correspondingly ($\mathcal{U}_{mn} = \delta_{m,n+1}$, $\mathcal{B}_{mn} = \delta_{m,n-1}$).

Secondly, consider the case of the chain with periodic boundary conditions, with the Hamiltonian

$$H_p = J\begin{pmatrix} 0 & F & 0 & \cdots & F^* \\ F^* & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & 0 & F \\ F & 0 & \cdots & F^* & 0 \end{pmatrix}. \tag{6}$$

Thirdly, in the case of a lattice with additional parabolic potential ($V(n) = V\frac{n^2}{2}$) often employed in applications with ultracold atoms, the Hamiltonian is

$$H_{pp} = J\begin{pmatrix} \frac{N^2V}{2J} & F & 0 & \cdots & 0 \\ F^* & \frac{(N-1)^2V}{2J} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & \frac{(N-1)^2V}{2J} & F \\ 0 & 0 & \cdots & F^* & \frac{N^2V}{2J} \end{pmatrix}, \tag{7}$$

where V is the strength of the parabolic potential, and the lattice has $(2N+1)$ sites.

In the spirit of the Hamiltonian averaging method in classical mechanics, we are making a unitary transformation $X = C\tilde{X}$ so that equations for the transformed variables are

$$i\dot{\tilde{X}} = \left[C^{-1}\epsilon HC - iC^{-1}\dot{C}\right]\tilde{X}. \tag{8}$$

We are looking 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.

Generally, we have

$$\begin{aligned} C &\approx I + \epsilon K_1 + \epsilon^2\left(\frac{1}{2}K_1^2 + K_2\right) \\ &\quad + \epsilon^3\left(\frac{1}{6}K_1^3 + \frac{1}{2}(K_1K_2 + K_2K_1) + K_3\right), \\ C^\dagger &\approx I - \epsilon K_1 + \epsilon^2\left(\frac{1}{2}K_1^2 - K_2\right) \\ &\quad + \epsilon^3\left(-\frac{1}{6}K_1^3 + \frac{1}{2}(K_1K_2 + K_2K_1) - K_3\right), \end{aligned} \tag{9}$$

where I is the unity matrix.

In the first order, we have

$$i\dot{K}_1 = H(t) - \langle H(t)\rangle \equiv \{H\}, \tag{10}$$

and therefore $iK_1 = \int (H - \langle H\rangle)\,dt = \int \{H\}\,dt$. 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,

$$i\dot{K}_2 = \left\{HK_1 - K_1H - \frac{i}{2}(\dot{K}_1K_1 - K_1\dot{K}_1)\right\}. \tag{11}$$

In the third order, we finally get

$$\epsilon H_{eff} = \epsilon H_1 + \epsilon^2 H_2 + \epsilon^3 H_3, \tag{12}$$

where

$$\begin{aligned} H_1 &= \langle H\rangle, \\ H_2 &= \left\langle HK_1 - K_1H - \frac{i}{2}(\dot{K}_1K_1 - K_1\dot{K}_1)\right\rangle, \\ H_3 &= \left\langle HK_2 - K_2H + \frac{1}{2}\left(HK_1^2 + K_1^2H\right) - K_1HK_1\right. \\ &\quad - \frac{i}{2}(\dot{K}_1K_2 - K_1\dot{K}_2 + \dot{K}_2K_1 - K_2\dot{K}_1) \\ &\quad \left. - \frac{i}{6}\left(\dot{K}_1K_1^2 + K_1^2\dot{K}_1 - 2K_1\dot{K}_1K_1\right)\right\rangle. \end{aligned} \tag{13}$$

These general formulas can be easily applied to particular models, as done in the next section.

One can also write expressions Eq. (13) in a more compact way:

$$\begin{aligned} H_1 &= \langle H\rangle, \\ H_2 &= \frac{1}{2}\langle[\{H\}, K_1]\rangle, \\ H_3 &= \left\langle [H, K_2] + \frac{1}{2}\left[[H, K_1], K_1\right] - \frac{i}{2}\left([\dot{K}_1, K_2] + [\dot{K}_2, K_1]\right)\right. \\ &\quad \left. - \frac{i}{6}\left[[\dot{K}_1, K_1], K_1\right]\right\rangle, \end{aligned} \tag{14}$$

where square brackets denote matrix commutation: $[A, B] = AB - BA$.

3. Applications to particular models

For the uniform model with periodic boundary conditions (6), we get a very interesting and important result: $H_2 = H_3 = 0$. First- and second-order corrections are completely absent in this case (note that, since the Hamiltonian ϵH_1 contains ϵ, H_2 and H_3 define the first- and the second-order corrections, correspondingly).

For the uniform model with open boundary conditions (5), we have

$$K_1 = -i\int \{H\}\,dt = J\begin{pmatrix} 0 & L & \cdots & 0 \\ -L^* & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & L \\ 0 & \cdots & -L^* & 0 \end{pmatrix} = J\left(L\mathcal{U} - L^*\mathcal{B}\right),$$

$$L \equiv \sum_{l\neq 0} \frac{F_l}{l}\exp(-ilt),$$

$$\dot{K}_1 = -i\{H\} = -iJ\begin{pmatrix} 0 & \tilde{F} & \cdots & 0 \\ \tilde{F}^* & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \tilde{F} \\ 0 & \cdots & \tilde{F}^* & 0 \end{pmatrix} = -iJ\left(\tilde{F}\mathcal{U} + \tilde{F}^*\mathcal{B}\right),$$

$$\tilde{F} \equiv \{F\} = \sum_{l\neq 0} F_l \exp(-ilt),$$