Eur. Phys. J. B (2024) 97:119
https://doi.org/10.1140/epjb/s10051-024-00757-6

THE EUROPEAN PHYSICAL JOURNAL B

Regular Article - Solid State and Materials

Exact ground states for pentagon chains with spin–orbit interaction

Zsolt Gulacsi[a]

Department of Theoretical Physics, University of Debrecen, Bem ter 18/B, Debrecen 4010, Hungary

Received 7 May 2024 / Accepted 20 July 2024 / Published online 12 August 2024

Abstract. Exact ground states (GS) are deduced for conducting polymers possessing pentagon type of unit cell. The study is done in the presence of many-body spin–orbit interaction (SOI), local and nearest-neighbor Coulomb repulsion (CR), and presence of external E electric and B magnetic fields (EF). The simultaneous presence of SOI, CR, and EF in the exact conducting polymer GS is a novelty, so the development of the technique for the treatment possibility of such strongly correlated cases is presented in detail. The deduced GS show a broad spectrum of physical characteristics ranging from charge density waves doubling the system periodicity, metal–insulator transitions, to interesting external field-driven effects as, e.g., modification possibility of a static charge distribution by a static EF.

1 Introduction

Given by multi-functional characteristics as simplistic synthesis, environmental stability, beneficial electronic, mechanical and optical properties, low cost and weight, or bio-compatibility, the conducting polymers are largely used on a broad spectrum of applications in advanced technologies such as electrochemistry applications, electrochemical sensing, energy storage, supercapacitors, batteries, sensors, fuel or solar cells, or drug delivery, etc [1].

From the other side, the many-body spin–orbit interaction (SOI) is a basic interaction in several fields of extreme interest today, as for example, nanophysics [2], flat band characteristics [3], or topological phases [4].

Coupling the presented two fields, one observes that given by the SOI presence in organic periodic materials [5], the applicability of conducting polymers is enlarged, and new properties come in, e.g., applications in spintronics become possible [6]; the possibilities to relax the rigid mathematical conditions leading to flat bands become available [3], the emergence of different ordered phases by small perturbations becomes possible, spin orbitronics in plastic materials appears, and even inverse spin Hall effect emerges, opening the doors for topological behavior [6]. It must be underlined that even if the SOI coupling (λ) sometimes is small in some organic materials, it can be substantially enhanced (even continuously tuned) by external fields [3], pulsed ferromagnetic resonance [6], or introduction of intrachain atoms that considerably enhance the spin–orbit coupling (e.g., platinum) [7].

[a] e-mail: gulacsi@phys.unideb.hu (corresponding author)

The importance of SOI is stressed as well by the fact that even in the case when $\lambda << 1$, its effect is major, because it breaks the spin-projection double degeneracy of each band [8]. Furthermore, usually the conducting polymers are interacting systems; hence, the leading term of the Coulomb interaction in many-body systems, the on-site Coulomb repulsion $U > 0$, attains even high values in organic materials [9], and introduces strong correlation effects as well. Furthermore, in these conditions also, the nearest-neighbor Coulomb repulsion $V > 0$ satisfying $V < U$ influences the physical behavior. In the description of these systems, the two extreme characteristic parameters (λ, U) satisfy the $U >> \lambda$ relation. Consequently, the perturbative treatment becomes questionable in both low and high coupling constant limits, enforcing special treatment for obtaining exact results for a good quality description. The special treatment is accentuated here because these systems are non-integrable, so Bethe-anzats type of treatment in such cases is inapplicable. In these conditions, exact results for conducting polymers in the presence of SOI till present are not known. The aim of this paper is to break this state of facts, and to present the first exact results for conducting polymers in the enumerated conditions (non-zero λ, V and U, $U >> \lambda$) in many-body, strongly correlated case. It is noted that one particle type of exact solutions in the presence of SOI has been already published in the bosonic 1D situations [10], but many-body interacting fermionic exact solutions in the presence of SOI for conducting polymers are not known at the moment.

An often studied representative of conducting polymers is the polyaminotriazole type of chain with pentagon unit cell, as shown in Fig. 1, which will be analyzed also here. The procedure we use is based on positive semidefinite operator properties. In its initial form, the technique has been initiated many decades ago [11,12], has substantially evolved in time, and for its presently used procedure, you can find detailed description, e.g., Ref. [13] or even review papers as Ref. [14]. This technique can be used also in the case of non-integrable systems, and works as follows: First, without to add extension terms, the Hamiltonian of the system is transformed in exact terms in a positive semidefinite form $\hat{H} = \sum_\nu \hat{P}_\nu + C$, where C is a scalar, and $\hat{P}_\nu$ are positive semidefinite operators. The transformation of the Hamiltonian connects the parameters of the Hamiltonian to the parameters of the $\hat{P}_\nu$ operators via a non-linear system of matching equations, which must be solved to complete the transformation process. The positive semidefinite operators by definition satisfy the $\langle\Psi|\hat{P}_\nu|\Psi\rangle \geq 0$ relation, hence their minimum possible eigenvalue is zero. This property underlines the advantages, and force of attraction of the positive semidefinite operator procedure: instead to try to deduce an arbitrary valued ground state energy, we can concentrate on the deduction of a ground state energy which has a well defined position. This usually represents a doable task. This job not requires (as it seems at first view) to "a priory" know, or guess the value of the C scalar (e.g., the ground-state energy) from the transformation expression. This is because C is connected by several equations to the parameters of the $\hat{P}_\nu$ operators, and to the finally deduced ground state; hence, the C expression becomes to be known only at the end of the calculation.

The exact ground state is deduced as follows: $\hat{H}' = \hat{H} - C$ has the minimum possible eigenvalue zero corresponding to the ground state eigenfunction $|\Psi_0\rangle$, which is obtained from $(\sum_\nu \hat{P}_\nu)|\Psi_0\rangle = 0$, using elevated techniques, see e.g., Refs. [13,14]. Once $|\Psi_0\rangle$ is known, the ground-state energy becomes $E_g = C$. The procedure provides valuable results even in three dimensions [15], 2D Hubbard case [16], or two-dimensional disordered systems [17].

Concerning the pentagon chains, till now only nearest-neighbor hoppings and the Hubbard interactions have been considered in such tasks. The novelty in the present paper is that besides the Hamiltonian terms mentioned above, in deducing the exact ground states, we also consider SOI, nearest-neighbor Coulomb repulsion, and presence of external fields.

The presented deduced physical properties underline a broad spectrum of interesting characteristics, e.g., emerging charge density wave phase accompanied by the doubling of the system periodicity, modification possibility of a static charge distribution by an external static magnetic field, switching possibilities between insulating and conducting phases by external fields, etc.

The remaining part of the paper is structured as follows: Sect. 2 presents the studied system, the transformation of the Hamiltonian in positive semidefinite form, and the solutions of the matching equations in the presence and absence of external fields. Section 3 presents the deduction procedure of the exact ground states, and the obtained ground states themselves. Section 4 presents the summary and conclusion.

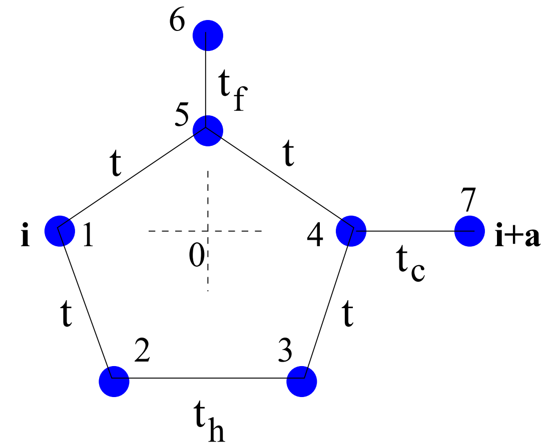

Fig. 1 The pentagon unit cell. The numbers denote the n value, the cell numbering of sites. The origin of the system of coordinates from where one analyses the cell is denoted by 0. The hopping matrix elements t, t_c, t_h, t_f are indicated on bonds, **i** denotes the lattice site to which the cell corresponds, and **a** is the lattice constant

2 The system analyzed

2.1 The case of the zero external magnetic field

2.1.1 The transformation of the Hamiltonian

The Hamilton of the system is $\hat{H} = \hat{H}_K + \hat{H}_U + \hat{H}_V$, where one has

$$\begin{aligned}
\hat{H}_K &= \sum_i \sum_{\sigma,\sigma'} [t^{\sigma,\sigma'} (\hat{c}^\dagger_{i,1,\sigma}\hat{c}_{i,5,\sigma'} + \hat{c}^\dagger_{i,2,\sigma}\hat{c}_{i,1,\sigma'} \\
&\quad + \hat{c}^\dagger_{i,4,\sigma}\hat{c}_{i,3,\sigma'} + \hat{c}^\dagger_{i,5,\sigma}\hat{c}_{i,4,\sigma'}) + t_h^{\sigma,\sigma'}\hat{c}^\dagger_{i,3,\sigma}\hat{c}_{i,2,\sigma'} \\
&\quad + t_f^{\sigma,\sigma'}\hat{c}^\dagger_{i,6,\sigma}\hat{c}_{i,5,\sigma'} + t_c^{\sigma,\sigma'}\hat{c}^\dagger_{i+a,7,\sigma}\hat{c}_{i,4,\sigma'} + h.c.] \\
&\quad + \hat{H}_\epsilon, \\
\hat{H}_\epsilon &= \sum_{i,n} \epsilon^{\sigma,\sigma'}\hat{c}^\dagger_{i,n,\sigma}\hat{c}_{i,n,\sigma'}, \\
\hat{H}_U &= \sum_i \sum_{n=1,2,..6} U_n \hat{n}^\uparrow_{i,n}\hat{n}^\downarrow_{i,n}, \\
\hat{H}_V &= V \sum_{<i,j>} \sum_{<n,n'>} \hat{n}_{i,n}\hat{n}_{j,n'}
\end{aligned} \tag{1}$$

In Fig. 1, one presents the unit cell of the system containing the in cell numbering of sites index ($n = 1, 2, .., 6$). The hopping matrix elements, and the on-site one-particle potentials have (σ, σ') spin projection indices to allow the presence of the many-body SOI. To match better the experimental situations, the antenna (describing the upper connected atoms), i.e., bond 5–6, the lower flank (bond 2–3), and the inter-cell connection (bond 4–7) are such taken to allow different hopping matrix elements, again for allowing comparison to different experimental realizations of the pentagon chain. The $\hat{H}_\epsilon$ term collects the on-site one-particle potential terms. The $U_n > 0$ coefficients are representing the on-site Coulomb repulsions (Hubbard interaction), while $V \geq 0$ represents the nearest-neighbor Coulomb interaction.

To transform in exact terms $\hat{H}$ in a positive semidefinite form, one introduces ten block operators $\hat{B}_{i,z,\sigma}$, $z = 1, 2, \ldots 5$ as follows:

$$\begin{aligned}
\hat{B}_{i,1,\uparrow} &= a_{1,1}\hat{c}_{i,1,\uparrow} + a_{1,2}\hat{c}_{i,2,\uparrow} + a_{1,5}\hat{c}_{i,5,\uparrow} + b_{1,1}\hat{c}_{i,1,\downarrow}, \\
\hat{B}_{i,1,\downarrow} &= a_{1,1}\hat{c}_{i,1,\downarrow} + a_{1,2}\hat{c}_{i,2,\downarrow} + a_{1,5}\hat{c}_{i,5,\downarrow} + b'_{1,1}\hat{c}_{i,1,\uparrow}, \\
\hat{B}_{i,2,\uparrow} &= a_{2,2}\hat{c}_{i,2,\uparrow} + a_{2,3}\hat{c}_{i,3,\uparrow} + a_{2,5}\hat{c}_{i,5,\uparrow}, \\
\hat{B}_{i,2,\downarrow} &= a_{2,2}\hat{c}_{i,2,\downarrow} + a_{2,3}\hat{c}_{i,3,\downarrow} + a_{2,5}\hat{c}_{i,5,\downarrow}, \\
\hat{B}_{i,3,\uparrow} &= a_{3,3}\hat{c}_{i,3,\uparrow} + a_{3,4}\hat{c}_{i,4,\uparrow} + a_{3,5}\hat{c}_{i,5,\uparrow} + b_{3,4}\hat{c}_{i,4,\downarrow}, \\
\hat{B}_{i,4,\uparrow} &= a_{4,5}\hat{c}_{i,5,\uparrow} + a_{4,6}\hat{c}_{i,6,\uparrow}, \\
\hat{B}_{i,3,\downarrow} &= a_{3,3}\hat{c}_{i,3,\downarrow} + a_{3,4}\hat{c}_{i,4,\downarrow} + a_{3,5}\hat{c}_{i,5,\downarrow} + b'_{3,4}\hat{c}_{i,4,\uparrow}, \\
\hat{B}_{i,4,\downarrow} &= a_{4,5}\hat{c}_{i,5,\downarrow} + a_{4,6}\hat{c}_{i,6,\downarrow}, \\
\hat{B}_{i,5,\uparrow} &= a_{5,4}\hat{c}_{i,4,\uparrow} + a_{5,7}\hat{c}_{i+a,7,\uparrow} \\
&\quad + b_{5,4}\hat{c}_{i,4,\downarrow} + b_{5,7}\hat{c}_{i+a,7,\downarrow}, \\
\hat{B}_{i,5,\downarrow} &= a_{5,4}\hat{c}_{i,4,\downarrow} + a_{5,7}\hat{c}_{i+a,7,\downarrow} \\
&\quad + b'_{5,4}\hat{c}_{i,4,\uparrow} + b'_{5,7}\hat{c}_{i+a,7,\uparrow}.
\end{aligned} \tag{2}$$

Here i represents the lattice site, z denotes the block operator index ($z = 1, 2, \ldots 5$), so (z, σ) has ten different values, while σ represents the spin projection. The coefficients, $a_{z,n}$ and $b_{z,n}$ called block operator parameters, are indexed by the block operator index z, and in cell position n on which the operator following the coefficient acts. The coefficients $a_{z,n}$ are present in terms whose spin projection is equal to the spin projection of the block operator, while the $b_{z,n}$ coefficients denote terms whose spin projection is opposite to the spin projection of the block operator. One has totally 21 block operator parameters ($a_{z,n}$ values: 13; and $b_{z,n}$ values: 8), which at the moment are unknown, but can be determined from the transformation of the starting Hamiltonian (1) to the positive semidefinite Hamiltonian

$$\hat{H} = \sum_{i,z,\sigma} \hat{B}^\dagger_{i,z,\sigma}\hat{B}_{i,z,\sigma} + \hat{H}_U + \hat{H}_V. \tag{3}$$

At this step, it must be noted that the presented expression of the block operators in (2) has been optimized for the analyzed problem. This optimization has in fact two main aspects, namely: (i) because of the translational symmetry, the block operator parameters are the same in each unit cell, i.e., are i independent. (ii) The opposite spin components in the block operators are optimized to minimally describe the requirements raised by the presence of SOI which leads to spin-flip hoppings. Given by this, we have much less $b_{z,n}$ coefficients in block operators than $a_{z,n}$ coefficients, which simplifies and helps the mathematical treatment.

If (3) is the same relation as (1), it must be a relationship in between the block operator parameters and the starting parameters of the Hamiltonian (1). These relations called the matching equations are presented in the following subsection.

2.1.2 Matching equations in zero external magnetic field

The matching equations are obtained by effectuating the $\hat{B}^\dagger_{i,z,\sigma}\hat{B}_{i,z,\sigma}$ product together with the $\sum_{i,z,\sigma}$ sum operation in (3), and equating each obtained term to the corresponding term in (1), e.g., the coefficient of the operator $\hat{c}^\dagger_{i,1,\uparrow}\hat{c}_{i,5,\uparrow}$ in (3) is $a^*_{1,1}a_{1,5}$, while in (1) is $t^{\uparrow,\uparrow}_{1,5}$, the relation being spin projection independent, from where the first equality of the third line of (4) follows, etc.

For the hoppings without spin-flip, one obtains ten equations:

$$\begin{aligned}
&0 = t^{\uparrow,\uparrow}_{2,5} = t^{\downarrow,\downarrow}_{2,5} = a^*_{1,2}a_{1,5} + a^*_{2,2}a_{2,5}, \\
&0 = t^{\uparrow,\uparrow}_{3,5} = t^{\downarrow,\downarrow}_{3,5} = a^*_{3,3}a_{3,5} + a^*_{2,3}a_{2,5}, \\
&t = t^{\uparrow,\uparrow}_{1,5} = t^{\downarrow,\downarrow}_{1,5} = a^*_{1,1}a_{1,5}, \quad t = t^{\uparrow,\uparrow}_{2,1} = t^{\downarrow,\downarrow}_{2,1} = a^*_{1,2}a_{1,1}, \\
&t = t^{\uparrow,\uparrow}_{4,3} = t^{\downarrow,\downarrow}_{4,3} = a^*_{3,4}a_{3,3}, \\
&t = t^{\uparrow,\uparrow}_{5,4} = t^{\downarrow,\downarrow}_{5,4} = a^*_{3,5}a_{3,4}, \quad t_h = t^{\uparrow,\uparrow}_{3,2} = t^{\downarrow,\downarrow}_{3,2} = a^*_{2,3}a_{2,2}, \\
&t_f = t^{\uparrow,\uparrow}_{6,5} = t^{\downarrow,\downarrow}_{6,5} = a^*_{4,6}a_{4,5}, \\
&t_c = t^{\uparrow,\uparrow}_c = t^{\uparrow,\uparrow}_{7,4} = a^*_{5,7}a_{5,4} + b'^*_{5,7}b'_{5,4}, \\
&t_c = t^{\downarrow,\downarrow}_c = t^{\downarrow,\downarrow}_{7,4} = a^*_{5,7}a_{5,4} + b^*_{5,7}b_{5,4}.
\end{aligned} \tag{4}$$

The spin-flip hoppings provide ten equations as follows

$$\begin{aligned}
&t^{\uparrow,\downarrow}_{1,5} = b'^*_{1,1}a_{1,5}, \quad t^{\downarrow,\uparrow}_{1,5} = \frac{t^{\uparrow,\downarrow}_{1,5}}{\alpha} = b^*_{1,1}a_{1,5}, \\
&t^{\uparrow,\downarrow}_{2,1} = a^*_{1,2}b_{1,1}, \\
&t^{\downarrow,\uparrow}_{2,1} = \frac{t^{\uparrow,\downarrow}_{2,1}}{\alpha} = a^*_{1,2}b'_{1,1}, \\
&t^{\uparrow,\downarrow}_{5,4} = a^*_{3,5}b_{3,4}, \\
&t^{\downarrow,\uparrow}_{5,4} = \frac{t^{\uparrow,\downarrow}_{5,4}}{\alpha} = a^*_{3,5}b'_{3,4}, \quad t^{\uparrow,\downarrow}_{4,3} = b'^*_{3,4}a_{3,3}, \\
&t^{\downarrow,\uparrow}_{4,3} = \frac{t^{\uparrow,\downarrow}_{4,3}}{\alpha} = b^*_{3,4}a_{3,3}, \\
&t^{\uparrow,\downarrow}_c = t^{\uparrow,\downarrow}_{7,4} = b'^*_{5,7}a_{5,4} + a^*_{5,7}b_{5,4}, \\
&t^{\downarrow,\uparrow}_c = t^{\downarrow,\uparrow}_{7,4} = \frac{t^{\uparrow,\downarrow}_{7,4}}{\alpha_c} = b^*_{5,7}a_{5,4} + a^*_{5,7}b'_{5,4}.
\end{aligned} \tag{5}$$

In Eq. (5), the coefficients α, α_c take into consideration the difference between the hoppings $t^{\uparrow,\downarrow}_{n,n'}$ and $t^{\downarrow,\uparrow}_{n,n'}$ given by the SOI. In the present case, taking into account only the Rashba term for conducting polymers [18], one has $\alpha = \alpha_c = -1$.

The non-spin-flip on-site one-particle potentials provide eight matching equations as follows:

$$\begin{aligned}
&\epsilon_4 = \epsilon_6^{\uparrow,\uparrow} = \epsilon_6^{\downarrow,\downarrow} = |a_{4,6}|^2, \quad \epsilon_3 = \epsilon_5^{\uparrow,\uparrow} = \epsilon_5^{\downarrow,\downarrow}\\
&\quad = |a_{4,5}|^2 + |a_{1,5}|^2 + |a_{2,5}|^2 + |a_{3,5}|^2,\\
&\epsilon_2 = \epsilon_2^{\uparrow,\uparrow} = \epsilon_2^{\downarrow,\downarrow} = |a_{1,2}|^2 + |a_{2,2}|^2, \quad \epsilon_2 = \epsilon_3^{\uparrow,\uparrow} = \epsilon_3^{\downarrow,\downarrow}\\
&\quad = |a_{2,3}|^2 + |a_{3,3}|^2,\\
&\epsilon_1 = \epsilon_1^{\uparrow,\uparrow} = |a_{1,1}|^2 + |a_{5,7}|^2 + |b'_{1,1}|^2 + |b'_{5,7}|^2,\\
&\epsilon_1 = \epsilon_1^{\downarrow,\downarrow} = |a_{1,1}|^2 + |a_{5,7}|^2 + |b_{1,1}|^2 + |b_{5,7}|^2,\\
&\epsilon_1 = \epsilon_4^{\uparrow,\uparrow} = |a_{3,4}|^2 + |a_{5,4}|^2 + |b'_{3,4}|^2 + |b'_{5,4}|^2,\\
&\epsilon_1 = \epsilon_4^{\downarrow,\downarrow} = |a_{3,4}|^2 + |a_{5,4}|^2 + |b_{3,4}|^2 + |b_{5,4}|^2. \qquad (6)
\end{aligned}$$

For spin-flip on-site one-particle potential, one automatically has $\epsilon_6^{\uparrow,\downarrow} = \epsilon_6^{\downarrow,\uparrow} = 0$, $\epsilon_5^{\uparrow,\downarrow} = \epsilon_5^{\downarrow,\uparrow} = 0$, $\epsilon_3^{\uparrow,\downarrow} = \epsilon_3^{\downarrow,\uparrow} = 0$, $\epsilon_2^{\uparrow,\downarrow} = \epsilon_2^{\downarrow,\uparrow} = 0$, while $\epsilon_1^{\downarrow,\uparrow} = (\epsilon_1^{\uparrow,\downarrow})^*$, $\epsilon_4^{\downarrow,\uparrow} = (\epsilon_4^{\uparrow,\downarrow})^*$ is satisfied. The last two relations further provide two matching equations:

$$\begin{aligned}
&\epsilon_1^{\uparrow,\downarrow} = a^*_{1,1} b_{1,1} + a^*_{5,7} b_{5,7} + b'^*_{1,1} a_{1,1} + b'^*_{5,7} a_{5,7},\\
&\epsilon_4^{\uparrow,\downarrow} = a^*_{3,4} b_{3,4} + a^*_{5,4} b_{5,4} + b'^*_{3,4} a_{3,4} + b'^*_{5,4} a_{5,4}, \quad (7)
\end{aligned}$$

where $\epsilon_1^{\uparrow,\downarrow} = \epsilon_4^{\uparrow,\downarrow} = 0$ holds. Consequently, one has totally 30 matching equations. These are coupled, complex algebraic and non-linear equations, which must be solved for the block operator parameters to indeed transform in exact terms the Hamiltonian from Eq. (1) to the Hamiltonian from Eq. (3).

The detailed solution of the matching Eqs. (4–7) is presented below:

$$\begin{aligned}
a_{1,1} &= \frac{|t| e^{i\theta_1}}{\sqrt{\epsilon_2 - t_h}}, \; a_{1,2} = a_{1,5}\\
&= sign(t)\sqrt{\epsilon_2 - t_h}\, e^{i\theta_1}, \; a_{2,5} = \frac{-\epsilon_2 + t_h}{\sqrt{t_h}} e^{i\theta_2},\\
a_{2,2} &= a_{2,3} = \sqrt{t_h}\, e^{i\theta_2},\\
a_{3,4} &= \frac{|t|}{\sqrt{\epsilon_2 - t_h}} e^{i\theta_3}, \; a_{3,3} = a_{3,5}\\
&= \mathrm{sign}(t)\sqrt{\epsilon_2 - t_h}\, e^{i\theta_3}, \; a_{4,6} = \sqrt{\epsilon_4}\, e^{i\theta_4},\\
a_{4,5} &= \frac{t_f}{\sqrt{\epsilon_4}}\, e^{i\theta_4},\\
a_{5,4} &= \frac{\sqrt{\gamma_1}}{\sqrt{1 + \frac{(\sqrt{\gamma_1\gamma_2} - t_c)^2}{t_c^{\uparrow,\downarrow\,2}}}} e^{i\theta_5},\\
a_{5,7} &= \frac{\sqrt{\gamma_2}}{\sqrt{1 + \frac{(\sqrt{\gamma_1\gamma_2} - t_c)^2}{t_c^{\uparrow,\downarrow\,2}}}} e^{i\theta_5},\\
b_{1,1} &= \mathrm{sign}(t)\frac{t_{2,1}^{\uparrow,\downarrow}}{\sqrt{\epsilon_2 - t_h}} e^{i\theta_1},\\
b'_{1,1} &= -\mathrm{sign}(t)\frac{t_{2,1}^{\uparrow,\downarrow}}{\sqrt{\epsilon_2 - t_h}} e^{i\theta_1},\\
b_{3,4} &= \mathrm{sign}(t)\frac{t_{5,4}^{\uparrow,\downarrow}}{\sqrt{\epsilon_2 - t_h}} e^{i\theta_3},\\
b'_{3,4} &= -\mathrm{sign}(t)\frac{t_{5,4}^{\uparrow,\downarrow}}{\sqrt{\epsilon_2 - t_h}} e^{i\theta_3},\\
b_{5,4} &= \frac{\gamma_1\sqrt{\gamma_2} - t_c\sqrt{\gamma_1}}{t_c^{\uparrow,\downarrow}\sqrt{1 + \frac{(\sqrt{\gamma_1\gamma_2} - t_c)^2}{t_c^{\uparrow,\downarrow\,2}}}} e^{i\theta_5},\\
b'_{5,4} &= -\frac{\gamma_1\sqrt{\gamma_2} - t_c\sqrt{\gamma_1}}{t_c^{\uparrow,\downarrow}\sqrt{1 + \frac{(\sqrt{\gamma_1\gamma_2} - t_c)^2}{t_c^{\uparrow,\downarrow\,2}}}} e^{i\theta_5},\\
b_{5,7} &= \frac{t_c\sqrt{\gamma_2} - \gamma_2\sqrt{\gamma_1}}{t_c^{\uparrow,\downarrow}\sqrt{1 + \frac{(\sqrt{\gamma_1\gamma_2} - t_c)^2}{t_c^{\uparrow,\downarrow\,2}}}} e^{i\theta_5},\\
b'_{5,7} &= -\frac{t_c\sqrt{\gamma_2} - \gamma_2\sqrt{\gamma_1}}{t_c^{\uparrow,\downarrow}\sqrt{1 + \frac{(\sqrt{\gamma_1\gamma_2} - t_c)^2}{t_c^{\uparrow,\downarrow\,2}}}} e^{i\theta_5}, \qquad (8)
\end{aligned}$$

where $\theta_1, \theta_2, \ldots \theta_5$ are arbitrary phases. The deduced solution needs the following conditions:

$$\begin{aligned}
&\epsilon_1 > 0,\; \epsilon_2 > 0,\; \epsilon_3 > 0,\; \epsilon_4 > 0,\; t_h > 0,\; \epsilon_2 - t_h > 0,\\
&\gamma_1 = \epsilon_1 - \frac{t^2 + t_{2,1}^{\uparrow,\downarrow\,2}}{\epsilon_2 - t_h} > 0,\\
&\gamma_2 = \epsilon_1 - \frac{t^2 + t_{5,4}^{\uparrow,\downarrow\,2}}{\epsilon_2 - t_h} > 0,\\
&\epsilon_3 = \frac{t_f^2}{\epsilon_4} + \frac{\epsilon_2^2 - t_h^2}{t_h},\; \gamma_1\gamma_2 = t_c^2 + t_c^{\uparrow,\downarrow\,2}. \qquad (9)
\end{aligned}$$

The author underlines that (8, 9) provides the solutions of the matching equations for the transformed positive semidefinite Hamiltonian in (3).

2.2 The case of the non-zero external magnetic field

2.2.1 The transformation of the Hamiltonian

We analyze also the case when an external magnetic field acts on the system perpendicular to the plane containing the polymer, i.e, perpendicular to the unit cell. The effect of the magnetic field is taken into account via (i) the Peierls phase factors attached to the hopping matrix elements in describing the action on the orbital motion, and for completeness, (ii) the Zeeman term describing the effect on the spin degrees of freedom. To be explicitly clear, for $B \neq 0$ introducing the notation $\hat{H}_1 = \hat{H}_K - \hat{H}_\epsilon$, one must transcribe carefully the $\hat{H}_1$ part of the one-particle Hamiltonian as follows

$$\hat{H}_1 = \sum_i \sum_{\sigma,\sigma'} [t_{1,5}^{\sigma,\sigma'} e^{i\phi_{1,5}} \hat{c}^\dagger_{i,1,\sigma} \hat{c}_{i,5,\sigma'} + t_{2,1}^{\sigma,\sigma'} e^{i\phi_{2,1}} \hat{c}^\dagger_{i,2,\sigma} \hat{c}_{i,1,\sigma'}$$

$$+t_{4,3}^{\sigma,\sigma'}e^{i\phi_{4,3}}\hat{c}_{i,4,\sigma}^{\dagger}\hat{c}_{i,3,\sigma'}+t_{5,4}^{\sigma,\sigma'}e^{i\phi_{5,4}}\hat{c}_{i,5,\sigma}^{\dagger}\hat{c}_{i,4,\sigma'}$$
$$+t_{7,4}^{\sigma,\sigma'}e^{i\phi_{7,4}}\hat{c}_{i+a,7,\sigma}^{\dagger}\hat{c}_{i,4,\sigma'}+t_{3,2}^{\sigma,\sigma'}e^{i\phi_{3,2}}\hat{c}_{i,3,\sigma}^{\dagger}\hat{c}_{i,2,\sigma'}$$
$$+t_{6,5}^{\sigma,\sigma'}e^{i\phi_{6,5}}\hat{c}_{i,6,\sigma}^{\dagger}\hat{c}_{i,5,\sigma'}+h.c.], \quad (10)$$

hence the total Hamiltonian becomes

$$\hat{H}=\hat{H}_1+\hat{H}_{\epsilon}+\hat{H}_U+\hat{H}_V+\hat{H}_Z. \quad (11)$$

For the Peierls phase factors, one has $\phi_{3,2}=\phi_1$, $\phi_{4,3}=\phi_{2,1}=\phi_2$, $\phi_{5,4}=\phi_{1,5}=\phi_3$, $\phi_{5,6}=\phi_{7,4}=0$, and $\phi=\phi_1+2\phi_2+2\phi_3=2\pi\Phi/\Phi_0$, where Φ is the magnetic flux threading the unit cell, and $\Phi_0=hc/e$ is the flux quantum. Separately for each phase, one has $\phi_\alpha=2\pi BS_\alpha/\Phi_0$, where $\alpha=1,2,3$, furthermore $S_1=A(0,2,3)$, $S_2=A(0,3,4)$, $S_3=A(0,4,5)$, where $A(i,j,k)$ represents the area of the triangle defined by the points (i,j,k) in Fig. 1 presenting the unit cell. One trivially has $S=S_1+2S_2+2S_3$. The Zeeman term in Eq. (11) has the standard form $\hat{H}_Z=-h\sum_{i,n}(\hat{n}_{i,n,\uparrow}-\hat{n}_{i,n,\downarrow})$. It is noted that in the presence of $\hat{H}_Z$, in the matching equations written for $\hat{H}_Z=0$, in fact one renormalizes the on-site one-particle potentials by $\epsilon_i^{\sigma,\sigma}\to\epsilon_i^{\sigma,\sigma}+\mu h$, where $\mu=-1$ for $\sigma=\uparrow$ and $\mu=+1$ for $\sigma=\downarrow$.

2.2.2 Matching equations in non-zero external magnetic field

To transform the Hamiltonian (11) in positive semidefinite form, one uses the same block operators as before, given in (2), but for the block operator parameters $a_{k,n}$ (which become to be different for $\hat{B}_{i,k,\uparrow}$ and $\hat{B}_{i,k,\downarrow}$), we must introduce a supplementary index u,d as follows: The transformation in positive semidefinite form of the $\hat{H}$ can be given with the condition to consider in Eq. (2) $a_{k,n,u}$ in $\hat{B}_{i,k,\uparrow}$, and $a_{k,n,d}$ in $\hat{B}_{i,k,\downarrow}$. Note that $a_{k,n,d}\neq a_{k,n,u}$ holds, and in (2) we have e.g.,

$$\hat{B}_{i,1,\uparrow}=a_{1,1,u}\hat{c}_{i,1,\uparrow}+a_{1,2,u}\hat{c}_{i,2,\uparrow}+a_{1,5,u}\hat{c}_{i,5,\uparrow}+b_{1,1}\hat{c}_{i,1,\downarrow},$$
$$\hat{B}_{i,1,\downarrow}=a_{1,1,d}\hat{c}_{i,1,\downarrow}+a_{1,2,d}\hat{c}_{i,2,\downarrow}+a_{1,5,d}\hat{c}_{i,5,\downarrow}+b'_{1,1}\hat{c}_{i,1,\uparrow},\ etc. \quad (12)$$

The transformation in the positive semidefinite form given in (3) requires the following matching equations:

The first 10 matching equations from (4) for hoppings without spin-flip become now 18 equations (18, since also in Eq. (4) $t_c^{\uparrow,\uparrow}$ and $t_c^{\downarrow,\downarrow}$ have different equations) as follows

$$t_{1,5}^{\uparrow,\uparrow}e^{i\phi_{1,5}}=te^{i\phi_3}=a^*_{1,1,u}a_{1,5,u},\ t_{1,5}^{\downarrow,\downarrow}e^{i\phi_{1,5}}=te^{i\phi_3}=a^*_{1,1,d}a_{1,5,d},\ t_{2,1}^{\uparrow,\uparrow}e^{i\phi_{2,1}}=te^{i\phi_2}=a^*_{1,2,u}a_{1,1,u},$$
$$t_{2,1}^{\downarrow,\downarrow}e^{i\phi_{2,1}}=te^{i\phi_2}=a^*_{1,2,d}a_{1,1,d},\ t_{4,3}^{\uparrow,\uparrow}e^{i\phi_{4,3}}=te^{i\phi_2}=a^*_{3,4,u}a_{3,3,u},\ t_{4,3}^{\downarrow,\downarrow}e^{i\phi_{4,3}}=te^{i\phi_2}=a^*_{3,4,d}a_{3,3,d},$$
$$t_{5,4}^{\uparrow,\uparrow}e^{i\phi_{5,4}}=te^{i\phi_3}=a^*_{3,5,u}a_{3,4,u},\ t_{5,4}^{\downarrow,\downarrow}e^{i\phi_{5,4}}=te^{i\phi_3}=a^*_{3,5,d}a_{3,4,d},\ t_{3,2}^{\uparrow,\uparrow}e^{i\phi_{3,2}}=t_he^{i\phi_1}=a^*_{2,3,u}a_{2,2,u},$$
$$t_{3,2}^{\downarrow,\downarrow}e^{i\phi_{3,2}}=t_he^{i\phi_1}=a^*_{2,3,d}a_{2,2,d},\ t_{6,5}^{\uparrow,\uparrow}e^{i\phi_{6,5}}=t_f=a^*_{4,6,u}a_{4,5,u},\ t_{6,5}^{\downarrow,\downarrow}e^{i\phi_{6,5}}=t_f=a^*_{4,6,d}a_{4,5,d},$$
$$t_{7,4}^{\uparrow,\uparrow}e^{i\phi_{7,4}}=t_c=a^*_{5,7,u}a_{5,4,u}+b'^*_{5,7}b'_{5,4},\ t_{7,4}^{\downarrow,\downarrow}e^{i\phi_{7,4}}=t_c=a^*_{5,7,d}a_{5,4,d}+b^*_{5,7}b_{5,4},$$
$$0=t_{2,5}^{\uparrow,\uparrow}=a^*_{1,2,u}a_{1,5,u}+a^*_{2,2,u}a_{2,5,u},\ 0=t_{2,5}^{\downarrow,\downarrow}=a^*_{1,2,d}a_{1,5,d}+a^*_{2,2,d}a_{2,5,d},$$
$$0=t_{3,5}^{\uparrow,\uparrow}=a^*_{3,3,u}a_{3,5,u}+a^*_{2,3,u}a_{2,5,u},\ 0=t_{3,5}^{\downarrow,\downarrow}=a^*_{3,3,d}a_{3,5,d}+a^*_{2,3,d}a_{2,5,d}. \quad (13)$$

The second group of ten matching equations relating the spin-flip contributions describing the SOI interaction, and substituting (5), become

$$t_{1,5}^{\uparrow,\downarrow}e^{i\phi_{1,5}}=-\lambda e^{i\phi_3}=b'^*_{1,1}a_{1,5,d},\ t_{1,5}^{\downarrow,\uparrow}e^{i\phi_{1,5}}=\frac{t_{1,5}^{\uparrow,\downarrow}e^{i\phi_{1,5}}}{\alpha}=\lambda e^{i\phi_3}=b^*_{1,1}a_{1,5,u},$$
$$t_{2,1}^{\uparrow,\downarrow}e^{i\phi_{2,1}}=\lambda e^{i\phi_2}=a^*_{1,2,u}b_{1,1},\ t_{2,1}^{\downarrow,\uparrow}e^{i\phi_{2,1}}=\frac{t_{2,1}^{\uparrow,\downarrow}e^{i\phi_{2,1}}}{\alpha}=-\lambda e^{i\phi_2}=a^*_{1,2,d}b'_{1,1},$$
$$t_{5,4}^{\uparrow,\downarrow}e^{i\phi_{5,4}}=-\lambda e^{i\phi_3}=a^*_{3,5,u}b_{3,4},\ t_{5,4}^{\downarrow,\uparrow}e^{i\phi_{5,4}}=\frac{t_{5,4}^{\uparrow,\downarrow}e^{i\phi_{5,4}}}{\alpha}=\lambda e^{i\phi_3}=a^*_{3,5,d}b'_{3,4},$$
$$t_{4,3}^{\uparrow,\downarrow}e^{i\phi_{4,3}}=\lambda e^{i\phi_2}=b'^*_{3,4}a_{3,3,d},\ t_{4,3}^{\downarrow,\uparrow}e^{i\phi_{4,3}}=\frac{t_{4,3}^{\uparrow,\downarrow}e^{i\phi_{4,3}}}{\alpha}=-\lambda e^{i\phi_2}=b^*_{3,4}a_{3,3,u},$$
$$t_{7,4}^{\uparrow,\downarrow}e^{i\phi_{4,7}}=\lambda_c=b'^*_{5,7}a_{5,4,d}+a^*_{5,7,u}b_{5,4},$$
$$t_{7,4}^{\downarrow,\uparrow}e^{i\phi_{7,4}}=\frac{t_{7,4}^{\uparrow,\downarrow}e^{i\phi_{7,4}}}{\alpha_c}=-\lambda_c=b^*_{5,7}a_{5,4,u}+a^*_{5,7,d}b'_{5,4}. \quad (14)$$

Here, taking into account symmetry considerations, we denoted the spin-flip hopping strengths by λ and λ_c according to the relations $t_{1,5}^{\uparrow,\downarrow}e^{i\phi_{1,5}}=-\lambda e^{i\phi_3}$, $t_{5,4}^{\uparrow,\downarrow}e^{i\phi_{5,4}}=-\lambda e^{i\phi_3}$, $t_{2,1}^{\uparrow,\downarrow}e^{i\phi_{2,1}}=\lambda e^{i\phi_2}$, $t_{4,3}^{\uparrow,\downarrow}e^{i\phi_{4,3}}=\lambda e^{i\phi_2}$, $t_{7,4}^{\uparrow,\downarrow}e^{i\phi_{7,4}}=\lambda_c e^{i\phi_{7,4}}=\lambda_c$. Finally, the last ten matching equations connected to on-site one-particle potentials become 14 equations:

$$\epsilon_6^{\uparrow,\uparrow}=\epsilon_6-h=|a_{4,6,u}|^2,\quad \epsilon_6^{\downarrow,\downarrow}=\epsilon_6+h=|a_{4,6,d}|^2,$$
$$\epsilon_5^{\uparrow,\uparrow}=\epsilon_5-h=|a_{4,5,u}|^2+|a_{1,5,u}|^2+|a_{2,5,u}|^2+|a_{3,5,u}|^2,$$
$$\epsilon_5^{\downarrow,\downarrow}=\epsilon_5+h=|a_{4,5,d}|^2+|a_{1,5,d}|^2+|a_{2,5,d}|^2+|a_{3,5,d}|^2,$$

$$
\begin{aligned}
\epsilon_2^{\uparrow,\uparrow} &= \epsilon_2 - h = |a_{1,2,u}|^2 + |a_{2,2,u}|^2, \\
\epsilon_2^{\downarrow,\downarrow} &= \epsilon_2 + h = |a_{1,2,d}|^2 + |a_{2,2,d}|^2, \\
\epsilon_3^{\uparrow,\uparrow} &= \epsilon_3 - h = |a_{2,3,u}|^2 + |a_{3,3,u}|^2, \\
\epsilon_3^{\downarrow,\downarrow} &= \epsilon_3 + h = |a_{2,3,d}|^2 + |a_{3,3,d}|^2, \\
\epsilon_1^{\uparrow,\uparrow} &= \epsilon_1 - h = |a_{1,1,u}|^2 + |a_{5,7,u}|^2 + |b'_{1,1}|^2 + |b'_{5,7}|^2, \\
\epsilon_1^{\downarrow,\downarrow} &= \epsilon_1 + h = |a_{1,1,d}|^2 + |a_{5,7,d}|^2 + |b_{1,1}|^2 + |b_{5,7}|^2, \\
\epsilon_4^{\uparrow,\uparrow} &= \epsilon_4 - h = |a_{3,4,u}|^2 + |a_{5,4,u}|^2 + |b'_{3,4}|^2 + |b'_{5,4}|^2, \\
\epsilon_4^{\downarrow,\downarrow} &= \epsilon_4 + h = |a_{3,4,d}|^2 + |a_{5,4,d}|^2 + |b_{3,4}|^2 + |b_{5,4}|^2, \\
\epsilon_1^{\uparrow,\downarrow} &= 0 = a^*_{1,1,u} b_{1,1} + a^*_{5,7,u} b_{5,7} \\
&\quad + b'^*_{1,1} a_{1,1,d} + b'^*_{5,7} a_{5,7,d}, \\
\epsilon_4^{\uparrow,\downarrow} &= 0 = a^*_{3,4,u} b_{3,4} + a^*_{5,4,u} b_{5,4} \\
&\quad + b'^*_{3,4} a_{3,4,d} + b'^*_{5,4} a_{5,4,d}. \qquad (15)
\end{aligned}
$$

Consequently, one has, in the $\mathbf{B} \neq 0$ case, 42 coupled, non-linear complex algebraic matching equations. I only mention that numerical software for solving such system of equations is not present today.

The matching equations at $\mathbf{B} \neq 0$ (13–15) provide analytically the following solutions:

In the case of the first eight block operators, the block operator parameters are given by the following relations: The coefficients of the $z = 1$ block operators $\hat{B}_{i,z=1,\sigma}$ are given by

$$
\begin{aligned}
a_{1,1,u} &= \left[\frac{t^2(T_h + \epsilon_3 - h)}{(\epsilon_2 - h)(\epsilon_3 - h) - t_h^2}\right]^{1/2} e^{i\chi_{1,u}}, \\
a_{1,1,d} &= \left[\frac{t^2(T_h + \epsilon_3 + h)}{(\epsilon_2 + h)(\epsilon_3 + h) - t_h^2}\right]^{1/2} e^{i\chi_{1,d}}, \\
a_{1,5,u} &= t e^{i\phi_3} \left[\frac{(\epsilon_2 - h)(\epsilon_3 - h) - t_h^2}{t^2(T_h + \epsilon_3 - h)}\right]^{1/2} e^{i\chi_{1,u}}, \\
a_{1,5,d} &= t e^{i\phi_3} \left[\frac{(\epsilon_2 + h)(\epsilon_3 + h) - t_h^2}{t^2(T_h + \epsilon_3 + h)}\right]^{1/2} e^{i\chi_{1,d}}, \\
a_{1,2,u} &= t e^{-i\phi_2} \left[\frac{(\epsilon_2 - h)(\epsilon_3 - h) - t_h^2}{t^2(T_h + \epsilon_3 - h)}\right]^{1/2} e^{i\chi_{1,u}}, \\
a_{1,2,d} &= t e^{-i\phi_2} \left[\frac{(\epsilon_2 + h)(\epsilon_3 + h) - t_h^2}{t^2(T_h + \epsilon_3 + h)}\right]^{1/2} e^{i\chi_{1,d}}, \\
b_{1,1} &= \frac{\lambda}{t} \left[\frac{t^2(T_h + \epsilon_3 - h)}{(\epsilon_2 - h)(\epsilon_3 - h) - t_h^2}\right]^{1/2} e^{i\chi_{1,u}}, \\
b'_{1,1} &= -\frac{\lambda}{t} \left[\frac{t^2(T_h + \epsilon_3 + h)}{(\epsilon_2 + h)(\epsilon_3 + h) - t_h^2}\right]^{1/2} e^{i\chi_{1,d}}, \qquad (16)
\end{aligned}
$$

where $T_h = t_h e^{-i\phi} \geq 0$ must be satisfied. The coefficients of the $z = 2$ block operators become

$$
\begin{aligned}
a_{2,2,u} &= \left[\frac{(\epsilon_3 - h)T_h + t_h^2}{T_h + \epsilon_3 - h}\right]^{1/2} e^{i\chi_{2,u}}, \\
a_{2,2,d} &= \left[\frac{(\epsilon_3 + h)T_h + t_h^2}{T_h + \epsilon_3 + h}\right]^{1/2} e^{i\chi_{2,d}}, \\
a_{2,3,u} &= t_h e^{-i\phi_1} \left[\frac{T_h + \epsilon_3 - h}{(\epsilon_3 - h)T_h + t_h^2}\right]^{1/2} e^{i\chi_{2,u}}, \\
a_{2,3,d} &= t_h e^{-i\phi_1} \left[\frac{T_h + \epsilon_3 + h}{(\epsilon_3 + h)T_h + t_h^2}\right]^{1/2} e^{i\chi_{2,d}}, \\
a_{2,5,u} &= -e^{i(\phi_2 + \phi_3)} \\
&\quad \frac{[(\epsilon_2 - h)(\epsilon_3 - h) - t_h^2]}{\sqrt{T_h(\epsilon_2 - h) + t_h^2}\sqrt{\epsilon_3 - h + T_h}} e^{i\chi_{2,u}}, \\
a_{2,5,d} &= -e^{i(\phi_2 + \phi_3)} \\
&\quad \frac{[(\epsilon_2 + h)(\epsilon_3 + h) - t_h^2]}{\sqrt{T_h(\epsilon_2 + h) + t_h^2}\sqrt{\epsilon_3 + h + T_h}} e^{i\chi_{2,d}}. \qquad (17)
\end{aligned}
$$

The coefficients of the $z = 3$ block operators become

$$
\begin{aligned}
a_{3,3,u} &= t e^{i\phi_2} \left[\frac{T_h[(\epsilon_2 - h)(\epsilon_3 - h) - t_h^2]}{t^2[T_h(\epsilon_2 - h) + t_h^2]}\right]^{1/2} e^{i\chi_{3,u}}, \\
a_{3,3,d} &= t e^{i\phi_2} \left[\frac{T_h[(\epsilon_2 + h)(\epsilon_3 + h) - t_h^2]}{t^2[T_h(\epsilon_2 + h) + t_h^2]}\right]^{1/2} e^{i\chi_{3,d}}, \\
a_{3,4,u} &= \left[\frac{t^2[T_h(\epsilon_2 - h) + t_h^2]}{T_h[(\epsilon_2 - h)(\epsilon_3 - h) - t_h^2]}\right]^{1/2} e^{i\chi_{3,u}}, \\
a_{3,4,d} &= \left[\frac{t^2[T_h(\epsilon_2 + h) + t_h^2]}{T_h[(\epsilon_2 + h)(\epsilon_3 + h) - t_h^2]}\right]^{1/2} e^{i\chi_{3,d}}, \\
a_{3,5,u} &= t e^{-i\phi_3} \left[\frac{T_h[(\epsilon_2 - h)(\epsilon_3 - h) - t_h^2]}{t^2[T_h(\epsilon_2 - h) + t_h^2]}\right]^{1/2} e^{i\chi_{3,u}}, \\
a_{3,5,d} &= t e^{-i\phi_3} \left[\frac{T_h[(\epsilon_2 + h)(\epsilon_3 + h) - t_h^2]}{t^2[T_h(\epsilon_2 + h) + t_h^2]}\right]^{1/2} e^{i\chi_{3,d}}, \\
b_{3,4} &= -\frac{\lambda}{t} \left[\frac{t^2[T_h(\epsilon_2 - h) + t_h^2]}{T_h[(\epsilon_2 - h)(\epsilon_3 - h) - t_h^2]}\right]^{1/2} e^{i\chi_{3,u}}, \\
b'_{3,4} &= \frac{\lambda}{t} \left[\frac{t^2[T_h(\epsilon_2 + h) + t_h^2]}{T_h[(\epsilon_2 + h)(\epsilon_3 + h) - t_h^2]}\right]^{1/2} e^{i\chi_{3,d}}. \qquad (18)
\end{aligned}
$$

The coefficients of the $z = 4$ block operators are the following ones

$$
\begin{aligned}
a_{4,5,u} &= \frac{t_f e^{i\chi_{4,u}}}{\sqrt{\epsilon_6 - h}}, \; a_{4,5,d} = \frac{t_f e^{i\chi_{4,d}}}{\sqrt{\epsilon_6 + h}}, \\
a_{4,6,u} &= \sqrt{\epsilon_6 - h} e^{i\chi_{4,u}}, \\
a_{4,6,d} &= \sqrt{\epsilon_6 + h} e^{i\chi_{4,d}}. \qquad (19)
\end{aligned}
$$

The calculation of the block operator coefficients connected to the block operators $\hat{B}_{i,5,\sigma}$, i.e., $z = 5$ is much more tricky. First we should introduce the following notations

$$\begin{aligned}
I_{1,u} &= \epsilon_1 - h - |a_{1,1,u}|^2 - |b'_{1,1}|^2, \\
I_{1,d} &= \epsilon_1 + h - |a_{1,1,d}|^2 - |b_{1,1}|^2, \\
I_{2,u} &= \epsilon_4 - h - |a_{3,4,u}|^2 - |b'_{3,4}|^2, \\
I_{2,d} &= \epsilon_4 + h - |a_{3,4,d}|^2 - |b_{3,4}|^2, \\
V_1 &= -a^*_{1,1,u} b_{1,1} - b'^*_{1,1} a_{1,1,d}, \\
V_2 &= -a^*_{3,4,u} b_{3,4} - b'^*_{3,4} a_{3,4,d}.
\end{aligned} \quad (20)$$

Given by (16–19), all quantities from (20) have known and real values. Now, based on (20), one defines $y = (v\lambda_c - V_2)/(\lambda_c + vV_1)$ and the expressions

$$\begin{aligned}
W_1 &= \frac{t_c - vI_{1,u}}{V_2 - v\lambda_c},\ W_2 = \frac{vt_c - I_{2,u}}{v\lambda_c - V_2}, \\
W_3 &= \frac{t_c - yI_{1,d}}{V_2 + y\lambda_c},\ W_4 = \frac{I_{2,d} - yt_c}{V_2 + y\lambda_c}.
\end{aligned} \quad (21)$$

Based on (21), the following relations providing the requested remaining block operator parameters hold

$$\begin{aligned}
b'_{5,7} &= W_1 a_{5,4,d}, \quad b'_{5,4} = W_2 a_{5,4,d}, \\
b^*_{5,7} &= W_3 a^*_{5,4,u}, \quad b^*_{5,4} = W_4 a^*_{5,4,u}, \\
a^*_{5,7,u} &= \frac{a^*_{5,4,u}}{v}, \quad a_{5,7,d} = \frac{a_{5,4,d}}{y}
\end{aligned} \quad (22)$$

The remaining two block operator parameters are given by

$$\begin{aligned}
a_{5,4,u} &= \left[\frac{V_2 W_1 - yV_1 W_2}{W_4 W_1 - W_3 W_2 (y/v)}\right]^{1/2} e^{i\chi_{5,u}}, \\
a_{5,4,d} &= \left[\frac{V_2 W_3 - vV_1 W_4}{W_2 W_3 - W_1 W_4 (v/y)}\right]^{1/2} e^{i\chi_{5,d}},
\end{aligned} \quad (23)$$

In the presented Eqs. (16–23), the phases $\chi_{k,u}, \chi_{k,d}$, $k = 1, 2, \ldots 5$ are arbitrary, and v is an arbitrary real parameter restricted by the conditions $|a_{5,4,u}|^2, |a_{5,4,d}|^2 > 0$.

The parameter space region where the solution is valid is fixed by the relations $I_{\alpha,\nu} \geq 0$, where $\alpha = 1, 2$, $\nu = u, d$. These relations provide lower limits for the on-site one particle potentials ϵ_1 and ϵ_4. Furthermore one has $T_h \geq 0$, and two remaining matching equations from (15), namely $\epsilon_5 + \mu(\nu)h = |a_{4,5,\nu}|^2 + |a_{1,5,\nu}|^2 + |a_{2,5,\nu}|^2 + |a_{3,5,\nu}|^2$, where $\mu(u) = -1$ and $\mu(d) = +1$ which relates the ϵ_5 value. This last equation must be separately analyzed for the two possible σ values u and d. In the case $h = 0$ analyzed below, from the above ϵ_5 equation, we obtain only a required restriction for ϵ_5 emerging at $a_{k,n,u} = a_{k,n,d} = a_{k,n}$.

3 Exact ground states

Once we solved the matching equations, the exact transformation of the Hamiltonian in positive semidefinite form has been performed. Now based on the positive semidefinite form of the Hamiltonian, one can deduce the exact ground states corresponding to the transformed Hamiltonian (3). As it will be explained, these ground states emerge in the low density case.

3.1 The deduction technique

3.1.1 Introductory remarks

One concentrates now on the transformed Hamiltonian $\hat{H}$ from (3) used with periodic boundary conditions. The procedure is based on the deduction of a local operator $\hat{X}^\dagger_i$ that satisfies the property

$$\{\hat{B}_{j,z,\sigma}, \hat{X}^\dagger_i\} = 0 \quad (24)$$

for all j, i lattice sites, all $z = 1, 2, ..5$, and all σ. The logic in this choice is that based on (24), one has for $|\Psi\rangle = \prod_i \hat{X}^\dagger_i |0\rangle$, where $|0\rangle$ is the vacuum state with no electrons present, the property

$$\left(\sum_{i,z,\sigma} \hat{B}^\dagger_{i,z,\sigma} \hat{B}_{i,z,\sigma}\right)|\Psi\rangle = 0 \quad (25)$$

This is because all $\hat{B}_{i,z,\sigma}$ can be interchanged with $\hat{X}^\dagger_i$, and $\hat{B}_{i,z,\sigma}|0\rangle = 0$ holds. Consequently, introducing $|\Psi\rangle$ in the kernel of $\hat{H}_U$ (i.e., the Hilbert subspace provided by all $|\chi\rangle$ for which $\hat{H}_U|\chi\rangle = 0$), and in the kernel of $\hat{H}_V$, one has the ground state.

In this job, first the $\hat{X}^\dagger_i$ operators must be deduced. For this reason, one takes into consideration a most general domain defined on two unit cells, as presented in Fig. 2. The operator is defined as

$$\begin{aligned}
\hat{X}^\dagger_i = {} & x^*_{1,\uparrow}\hat{c}^\dagger_{i,1,\uparrow} + x^*_{2,\uparrow}\hat{c}^\dagger_{i,2,\uparrow} + x^*_{3,\uparrow}\hat{c}^\dagger_{i,3,\uparrow} \\
& + x^*_{4,\uparrow}\hat{c}^\dagger_{i,4,\uparrow} + x^*_{5,\uparrow}\hat{c}^\dagger_{i,5,\uparrow} + x^*_{6,\uparrow}\hat{c}^\dagger_{6,1,\uparrow} + x^*_{4',\uparrow}\hat{c}^\dagger_{i+1,1,\uparrow} \\
& + x^*_{2',\uparrow}\hat{c}^\dagger_{i+1,2,\uparrow} + x^*_{3',\uparrow}\hat{c}^\dagger_{i+1,3,\uparrow} + x^*_{5',\uparrow}\hat{c}^\dagger_{i+1,5,\uparrow} \\
& + x^*_{6',\uparrow}\hat{c}^\dagger_{i+1,6,\uparrow} + x^*_{7',\uparrow}\hat{c}^\dagger_{i+1,4,\uparrow} + y^*_{1,\downarrow}\hat{c}^\dagger_{i,1,\downarrow} \\
& + y^*_{2,\downarrow}\hat{c}^\dagger_{i,2,\downarrow} + y^*_{3,\downarrow}\hat{c}^\dagger_{i,3,\downarrow} + y^*_{4,\downarrow}\hat{c}^\dagger_{i,4,\downarrow} + y^*_{5,\downarrow}\hat{c}^\dagger_{i,5,\downarrow} \\
& + y^*_{6,\downarrow}\hat{c}^\dagger_{i,6,\downarrow} + y^*_{4',\downarrow}\hat{c}^\dagger_{i+1,1,\downarrow} + y^*_{2',\downarrow}\hat{c}^\dagger_{i+1,2,\downarrow} \\
& + y^*_{3',\downarrow}\hat{c}^\dagger_{i+1,3,\downarrow} + y^*_{5',\downarrow}\hat{c}^\dagger_{i+1,5,\downarrow} \\
& + y^*_{6',\downarrow}\hat{c}^\dagger_{i+1,6,\downarrow} + y^*_{7',\downarrow}\hat{c}^\dagger_{i+1,4,\downarrow}.
\end{aligned} \quad (26)$$

Now the (24) anticommutators are presented, calculated in order with $\hat{B}_{i,1,\uparrow}, \hat{B}_{i,1,\downarrow}, \hat{B}_{i,2,\uparrow}, \hat{B}_{i,2,\downarrow}, \ldots, \hat{B}_{i,5,\uparrow}$, $\hat{B}_{i,5,\downarrow}, \hat{B}_{i+1,1,\uparrow}, \hat{B}_{i+1,1,\downarrow}, \hat{B}_{i+1,2,\uparrow}, \hat{B}_{i+1,2,\downarrow}, \ldots, \hat{B}_{i+1,5,\uparrow}$,

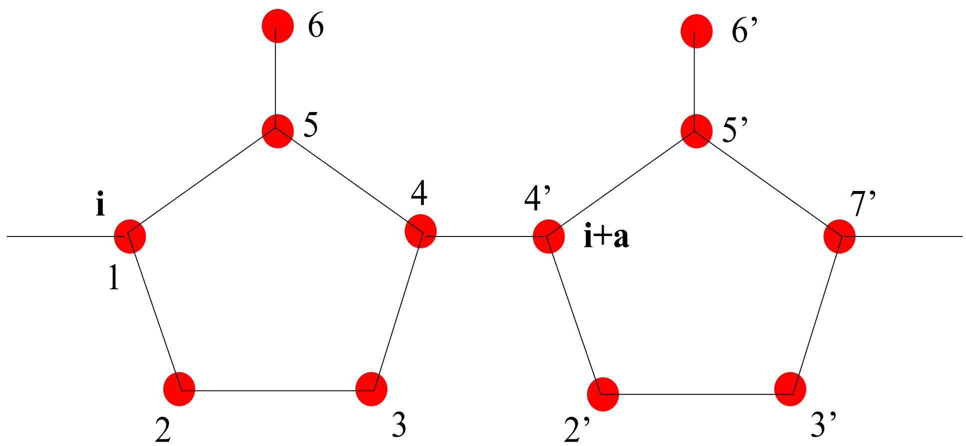

Fig. 2 The $\hat{X}_i^\dagger$ operator connected to the lattice site **i**. The red dotes denote the sites that are belong to $\hat{X}_i^\dagger$

$\hat{B}_{i+1,5,\downarrow}$, $\hat{B}_{i-1,5,\uparrow}$, $\hat{B}_{i-1,5,\downarrow}$, in total 22 equations

$$
\begin{aligned}
&x^*_{2,\uparrow}a_{1,2,u} + x^*_{5,\uparrow}a_{1,5,u} + x^*_{1,\uparrow}a_{1,1,u} + y^*_{1,\downarrow}b_{1,1} = 0,\\
&x^*_{2,\uparrow}a_{2,2,u} + x^*_{3,\uparrow}a_{2,3,u} + x^*_{5,\uparrow}a_{2,5,u} = 0,\\
&y^*_{1,\downarrow}a_{1,1,d} + y^*_{5,\downarrow}a_{1,5,d} + y^*_{2,\downarrow}a_{1,2,d} + x^*_{1,\uparrow}b'_{1,1} = 0,\\
&y^*_{3,\downarrow}a_{2,3,d} + y^*_{5,\downarrow}a_{2,5,d} + y^*_{2,\downarrow}a_{2,2,d} = 0,\\
&x^*_{3,\uparrow}a_{3,3,u} + x^*_{4,\uparrow}a_{3,4,u} + x^*_{5,\uparrow}a_{3,5,u} + y^*_{4,\downarrow}b_{3,4} = 0,\\
&x^*_{5,\uparrow}a_{4,5,u} + x^*_{6,\uparrow}a_{4,6,u} = 0,\\
&y^*_{3,\downarrow}a_{3,3,d} + y^*_{4,\downarrow}a_{3,4,d} + y^*_{5,\downarrow}a_{3,5,d} + x^*_{4,\uparrow}b'_{3,4} = 0,\\
&y^*_{5,\downarrow}a_{4,5,d} + y^*_{6,\downarrow}a_{4,6,d} = 0,\\
&x^*_{4,\uparrow}a_{5,4,u} + x^*_{4',\uparrow}a_{5,7,u} + y^*_{4,\downarrow}b_{5,4} + y^*_{4',\downarrow}b_{5,7} = 0,\\
&x^*_{2',\uparrow}a_{2,2,u} + x^*_{3',\uparrow}a_{2,3,u} + x^*_{5',\uparrow}a_{2,5,u} = 0,\\
&x^*_{4,\uparrow}b'_{5,4} + x^*_{4',\uparrow}b'_{5,7} + y^*_{4,\downarrow}a_{5,4,d} + y^*_{4',\downarrow}a_{5,7,d} = 0,\\
&y^*_{2',\downarrow}a_{2,2,d} + y^*_{3',\downarrow}a_{2,3,d} + y^*_{5',\downarrow}a_{2,5,d} = 0,\\
&x^*_{4',\uparrow}a_{1,1,u} + x^*_{2',\uparrow}a_{1,2,u} + x^*_{5',\uparrow}a_{1,5,u} + y^*_{4',\downarrow}b_{1,1} = 0,\\
&x^*_{4',\uparrow}b'_{1,1} + y^*_{4',\downarrow}a_{1,1,d} + y^*_{2',\downarrow}a_{1,2,d} + y^*_{5',\downarrow}a_{1,5,d} = 0,\\
&x^*_{3',\uparrow}a_{3,3,u} + x^*_{5',\uparrow}a_{3,5,u} + x^*_{7',\uparrow}a_{3,4,u} + y^*_{7',\downarrow}b_{3,4} = 0,\\
&y^*_{3',\downarrow}a_{3,3,d} + y^*_{5',\downarrow}a_{3,5,d} + x^*_{7',\uparrow}b'_{3,4} + y^*_{7',\downarrow}a_{3,4,d} = 0,\\
&x^*_{5',\uparrow}a_{4,5,u} + x^*_{6',\uparrow}a_{4,6,u} = 0,\ y^*_{5',\downarrow}a_{4,5,d} + y^*_{6',\downarrow}a_{4,6,d} = 0,\\
&x^*_{7',\uparrow}a_{5,4,u} + y^*_{7',\downarrow}b_{5,4} = 0,\\
&x^*_{7',\uparrow}b'_{5,4} + y^*_{7',\downarrow}a_{5,4,d} = 0,\ x^*_{1,\uparrow}a_{5,7,u} + y^*_{1,\downarrow}b_{5,7} = 0,\\
&x^*_{1,\uparrow}b'_{5,7} + y^*_{1,\downarrow}a_{5,7,d} = 0,
\end{aligned} \tag{27}
$$

In the $\mathbf{B} = 0$ case when $a_{i,j,u} = a_{i,j,d} = a_{i,j}$, $h = \phi = 0$ holds, because of $b'_{5,4} = -b_{5,4}$ and $b'_{5,7} = -b_{5,7}$, (see (8)), the last four equations from (27) provide $x_{1,\uparrow} = y_{1,\downarrow} = x_{7',\uparrow} = y_{7',\downarrow} = 0$, which is not satisfied automatically at $\mathbf{B} \neq 0$, i.e., $a_{i,j,u} \neq a_{i,j,d}$. That is why, (27) must be separately solved in the presence and in the absence of the external magnetic field.

3.1.2 Solution for $\hat{X}_i^\dagger$ at $\hat{B} = 0$

The solutions of (27) can be given as follows

$$
\begin{aligned}
&x^*_{6,\uparrow} = \frac{t_f}{\epsilon_4}x^*_{2,\uparrow},\ x^*_{6',\uparrow} = \frac{t_f}{\epsilon_4}x^*_{3',\uparrow},\\
&x^*_{5,\uparrow} = -x^*_{2,\uparrow},\ x^*_{5',\uparrow}\\
&\quad = -x^*_{3',\uparrow},\ x^*_{3,\uparrow} = \frac{-\epsilon_2}{t_h}x^*_{2,\uparrow},\ x^*_{1,\uparrow} = 0,\\
&x^*_{2',\uparrow} = \frac{-\epsilon_2}{t_h}x^*_{3',\uparrow},\ x^*_{4,\uparrow} = \frac{\epsilon_2^2 - t_h^2}{t_h(t^2+\lambda^2)}(tx^*_{2,\uparrow} - \lambda y^*_{2,\downarrow}),\\
&x^*_{4',\uparrow} = \frac{\epsilon_2^2 - t_h^2}{t_h(t^2+\lambda^2)}(tx^*_{3',\uparrow} - \lambda y^*_{3',\downarrow}),\\
&x^*_{7',\uparrow} = 0,\ y^*_{1,\downarrow} = 0,\ y^*_{7',\downarrow} = 0,\ y^*_{6,\downarrow} = \frac{t_f}{\epsilon_4}y^*_{2,\downarrow},\\
&y^*_{6',\downarrow} = \frac{t_f}{\epsilon_4}y^*_{3',\downarrow},\ y^*_{5,\downarrow} = -y^*_{2,\downarrow},\ y^*_{5',\downarrow} = -y^*_{3',\downarrow},\\
&y^*_{3,\downarrow} = -\frac{\epsilon_2}{t_h}y^*_{2,\downarrow},\ y^*_{2',\downarrow} = -\frac{\epsilon_2}{t_h}y^*_{3',\downarrow},\\
&y^*_{4,\downarrow} = \frac{\epsilon_2^2 - t_h^2}{t_h(t^2+\lambda^2)}(\lambda x^*_{2,\uparrow} + ty^*_{2,\downarrow}),\\
&y^*_{4',\downarrow} = \frac{\epsilon_2^2 - t_h^2}{t_h(t^2+\lambda^2)}(\lambda x^*_{3',\uparrow} + ty^*_{3',\downarrow}),
\end{aligned} \tag{28}
$$

where the $t^{\uparrow,\downarrow} = \lambda$ notation has been introduced, where λ represents the SOI coupling constant (see (14)). From (28), it is seen that all coefficients of $\hat{X}_i^\dagger$ have been expressed in function of $x^*_{2,\uparrow}, x^*_{3',\uparrow}, y^*_{2,\downarrow}, y^*_{3',\downarrow}$. These can be deduced based on the following relations

$$
\begin{aligned}
x^*_{2,\uparrow} &= \frac{-(\alpha\beta+\gamma\delta)x^*_{3',\uparrow} + (\gamma\beta-\alpha\delta)y^*_{3',\downarrow}}{\alpha^2+\gamma^2},\\
y^*_{2,\downarrow} &= \frac{-(\gamma\beta-\alpha\delta)x^*_{3',\uparrow} - (\alpha\beta+\gamma\delta)y^*_{3',\downarrow}}{\alpha^2+\gamma^2},
\end{aligned} \tag{29}
$$

where $\alpha = ta_{5,4} + \lambda b_{5,4}$, $\beta = ta_{5,7} + \lambda b_{5,7}$, $\gamma = tb_{5,4} - \lambda a_{5,4}$, $\delta = tb_{5,7} - \lambda a_{5,7}$, and $x^*_{3',\uparrow} = p$, $y^*_{3',\downarrow} = q$ are arbitrary parameters.

The physical meaning of these two free p, q parameters can be given as follows: given two set values of these parameters, p_1, q_1 and p_2, q_2, one can construct two linearly independent $\hat{X}^\dagger_{i,1}$ and $\hat{X}^\dagger_{i,2}$ solutions, which provide two linearly independent Hilbert space vectors $|\Psi^0_1\rangle = \hat{X}^\dagger_{i,1}|0\rangle$, and $|\Psi^0_2\rangle = \hat{X}^\dagger_{i,2}|0\rangle$, where $|0\rangle$ is the vacuum state with no fermions present. These can be orthonormalized based on the Gram–Schmidt procedure

$$|\Psi_1\rangle = \frac{|\Psi^0_1\rangle}{\langle\Psi^0_1|\Psi^0_1\rangle}, \quad |\Psi_2\rangle = \frac{|\Psi^0_2\rangle - |v\rangle}{(\langle\Psi^0_2| - \langle v|)(|\Psi^0_2\rangle - |v\rangle)},$$
$$|v\rangle = \langle\Psi^0_2|\Psi_1\rangle|\Psi_1\rangle, \tag{30}$$

obtaining $\langle\Psi_1|\Psi_2\rangle = 0$ together with $\langle\Psi_1|\Psi_1\rangle = \langle\Psi_2|\Psi_2\rangle = 1$. Please note that for this to be done, two free parameters are needed (as obtained here), since only one free parameter mathematically fixes the norm.

3.1.3 Solution for $\hat{X}^\dagger_i$ at $\hat{B} \neq 0$

The here presented solutions occur at

$$a_{5,7,d}a_{5,7,u} \neq b_{5,7}b'_{5,7}, \quad a_{5,4,d}a_{5,4,u} \neq b_{5,4}b'_{5,4}, \tag{31}$$

where from the last four equations of (27), one has $x_{1,\uparrow} = x_{7',\uparrow} = y_{1,\downarrow} = y_{7',\uparrow} = 0$. The deduced coefficients of the operator $\hat{X}^\dagger_i$ are as follows: The first 16 coefficients are given as

$$\begin{aligned}
x^*_{6,\uparrow} &= \frac{t_f}{\epsilon_6 - h} e^{-i(\phi_2+\phi_3)} x^*_{2,\uparrow},\\
y^*_{6,\downarrow} &= \frac{t_f}{\epsilon_6 + h} e^{-i(\phi_2+\phi_3)} y^*_{2,\downarrow},\\
x^*_{6',\uparrow} &= \frac{t_f}{\epsilon_6 - h} e^{i(\phi_2+\phi_3)} x^*_{3',\uparrow},\\
y^*_{6',\downarrow} &= \frac{t_f}{\epsilon_6 + h} e^{i(\phi_2+\phi_3)} y^*_{3',\downarrow},\\
x^*_{5,\uparrow} &= -e^{-i(\phi_2+\phi_3)} x^*_{2,\uparrow},\\
y^*_{5,\downarrow} &= -e^{-i(\phi_2+\phi_3)} y^*_{2,\uparrow},\ x^*_{5',\uparrow} = -e^{i(\phi_2+\phi_3)} x^*_{3',\uparrow},\\
y^*_{5',\downarrow} &= -e^{i(\phi_2+\phi_3)} y^*_{3',\downarrow},\ x^*_{3,\uparrow} = -e^{-i(2\phi_2+2\phi_3)}\\
&\quad \frac{\epsilon_2 - h}{T_h} x^*_{2,\uparrow},\ y^*_{3,\downarrow} = -e^{-i(2\phi_2+2\phi_3)} \frac{\epsilon_2 + h}{T_h} y^*_{2,\downarrow},\\
x^*_{2',\uparrow} &= -e^{i(2\phi_2+2\phi_3)}\\
&\quad \frac{(\epsilon_2 - h)(\epsilon_3 - h) - t_h^2 + T_h(T_h + \epsilon_3 - h)}{T_h(\epsilon_3 - h) + t_h^2} x^*_{3',\uparrow},\\
y^*_{2',\downarrow} &= -e^{i(2\phi_2+2\phi_3)}\\
&\quad \frac{(\epsilon_2 + h)(\epsilon_3 + h) - t_h^2 + T_h(T_h + \epsilon_3 + h)}{T_h(\epsilon_3 + h) + t_h^2} y^*_{3',\downarrow},\\
y^*_{4,\downarrow} &= a x^*_{2,\uparrow} + b y^*_{2,\downarrow},\ x^*_{4,\uparrow} = c x^*_{2,\uparrow} + d y^*_{2,\downarrow},
\end{aligned}$$

$$y^*_{4',\downarrow} = a' x^*_{3',\uparrow} + b' y^*_{3',\downarrow},\ x^*_{4',\uparrow} = c' x^*_{3',\uparrow} + d' y^*_{3',\downarrow}, \tag{32}$$

where one has for the presented prefactors

$$\begin{aligned}
a &= -\lambda e^{-i(\phi_2+2\phi_3)} J_-,\ b = t e^{-i(\phi_2+2\phi_3)} J_+,\\
c &= t e^{-i(\phi_2+2\phi_3)} J_-,\ d = \lambda e^{-i(\phi_2+2\phi_3)} J_+,\\
a' &= \lambda e^{i(\phi_2+2\phi_3)} J_-,\ b' = t e^{i(\phi_2+2\phi_3)} J_+,\\
c' &= t e^{i(\phi_2+2\phi_3)} J_-,\ d' = -\lambda e^{i(\phi_2+2\phi_3)} J_+,\\
J_+ &= \frac{(T_h + \epsilon_2 + h)[(\epsilon_2 + h)^2 - t_h^2]}{(\lambda^2 + t^2)[T_h(\epsilon_2 + h) + t_h^2)]},\\
J_- &= \frac{(T_h + \epsilon_2 - h)[(\epsilon_2 - h)^2 - t_h^2]}{(\lambda^2 + t^2)[T_h(\epsilon_2 - h) + t_h^2)]},
\end{aligned} \tag{33}$$

One notes that in (33), the $\epsilon_2 = \epsilon_3$ equality has been used satisfying the symmetry properties of the system. All presented coefficients are expressed in function of the parameters $x^*_{2,\uparrow}, x^*_{3',\uparrow}, y^*_{2,\downarrow}, y^*_{3',\downarrow}$. These are determined via

$$\begin{aligned}
x^*_{2,\uparrow} &= \frac{Y'\beta' - X'\delta'}{\gamma'\beta' - \alpha'\delta'},\ y^*_{2,\downarrow} = \frac{X'\gamma' - Y'\alpha'}{\gamma'\beta' - \alpha'\delta'},\\
x^*_{3',\uparrow} &= p',\ y^*_{3',\downarrow} = q',\\
\alpha' &= c a_{5,4,u} + a b_{5,4},\ \beta' = d a_{5,4,u} + b b_{5,4},\\
\gamma' &= c b'_{5,4} + a a_{5,4,d},\ \delta' = d b'_{5,4} + b a_{5,4,d},\\
X' &= -p'(a_{5,7,u}c' + b_{5,7}a') - q'(a_{5,7,u}d' + b_{5,7}b'),\\
Y' &= -p'(a_{5,7,d}a' + b'_{5,7}c') - q'(a_{5,7,d}b' + b'_{5,7}d'),
\end{aligned} \tag{34}$$

where p', q' are arbitrary parameters. It is noted that the denominator present on the first line of (34) is non-zero, since $\gamma'\beta' - \alpha'\delta' = e^{-2i(\phi_2+2\phi_3)} J_+ J_- (\lambda^2 + t^2)(b_{5,4}b'_{5,4} - a_{5,4,d}a_{5,4,u}) \neq 0$, see Eq. (31). Concerning p', q', see the observation below (29) relating the p, q parameters.

3.1.4 Other specific solutions for $\hat{X}^\dagger_i$

It can be said that two more specific solutions for $\hat{X}^\dagger_i$ are possible to occur, the first (i) in conditions when the requirement (31) is not satisfied, and the second, in the case when (ii) the domain on which $\hat{X}^\dagger_i$ is defined, differs from the domain presented in Fig. 2. These solutions will not be analyzed in details now and need supplementary interdependences in between the parameters of the Hamiltonian (e.g., (31) taken as equality). These new interdependences not diminish substantially the emergence possibilities of the phases described by the $\hat{X}^\dagger_i$ operators because, e.g., the SOI coupling constants λ, λ_c can be continuously tuned by external electric fields [3].

3.2 The ground-state wave vectors

Once the $\hat{X}_i^\dagger$ operators have been obtained, we deduce now the exact ground states for the Hamiltonian from (3). We start the presentation first for the $\mathbf{B} = 0$ case.

For this reason, let us consider the wave vector

$$|\Phi_1\rangle = \prod_i{}' \hat{X}_i^\dagger |0\rangle = \ldots \hat{X}_i^\dagger \hat{X}_{i+2}^\dagger \hat{X}_{i+4}^\dagger \ldots |0\rangle \quad (35)$$

where $\prod_i'$ represents a product on each second lattice site, and $\hat{X}_i^\dagger$ is taken from (28, 29) deduced at $\mathbf{B} = 0$. Note that $\hat{X}_i^\dagger$ places 1 electron on two nearest-neighbor pentagons excepting their left and right end sites (sites 1 and $7'$ in Fig. 2). I underline that the two cell (two pentagons) extension of the $\hat{X}_i^\dagger$ operator is given by the presence of SOI, which in this manner clearly influences the physical properties of the system.

Inside the block covered by $\hat{X}_i^\dagger$ (sites 2, 3, 4, 5, 6, $4'$, $2'$, $3'$, $5'$, $6'$ in Fig. 2), there are no two electrons present (i.e., double occupancy is not present); hence, $\hat{H}_U|\Phi_1\rangle = 0$ holds. Furthermore, inside this block, there are no two nearest neighboring sites occupied both at least once, so $\hat{H}_V|\Phi_1\rangle = 0$ also holds. In between two nearest-neighbor $\hat{X}_i^\dagger$ and $\hat{X}_{i+2}^\dagger$ operators, two empty sites are present (the horizontal bonds starting to the right from the site $7'$, and starting to the left from the site 1 in Fig. 2, see (28)), so on these sites $\hat{H}_U|\Phi_1\rangle = 0$, and $\hat{H}_V|\Phi_1\rangle = 0$ are also satisfied, consequently

$$(\hat{H}_U + \hat{H}_V)|\Phi_1\rangle = 0 \quad (36)$$

holds. But $\hat{X}_i^\dagger$ was deduced from the condition (25), so (36) type of relation is satisfied also for the first term of the Hamiltonian (3), as a consequence $\hat{H}|\Phi_1\rangle = 0$ holds. But since $\hat{H}$ is build up only from positive semidefinite terms, zero is the smallest possible eigenvalue of $\hat{H}$. As a consequence $|\Phi_1\rangle = |\Phi_{g,1}\rangle$ is the ground state of $\hat{H}$ at a number of $N = N_c/2$ particles in the system. The system has totally $6N_c$ sites, so the maximum number of electrons in the system is $N_{max} = 12N_c$, consequently $N_c/2$ carriers represent $c_0 = N/N_{max} = 1/24$ particle concentration (quarter filled lowest band). This concentration value is placed below system half filling ($6N_c$ electrons), that is why it is called "ground state in the low density" case.

Physically this state represents a charge density wave (CDW) state, since on all second horizontal bonds (e.g., bond $7'$ to $\mathbf{i}+2\mathbf{a}$ in Fig. 2) carriers are missing, and this segment delimited by empty sites periodically repeats along the line of the polymer. This state is insulating, hence is gaped. For the solution to occur, from the point of view of the two-particle interaction terms, $U_n > 0$, $V > 0$, but otherwise arbitrary are needed. One notes that when this state is not present, the lattice periodicity is described by the lattice constant $\mathbf{a}$ whose extent is the length of the unit cell (distance between the sites 1 and $4'$ in Fig. 2). Contrary to this, when the CDW phase appears, since the length of the $\hat{X}$ operator represents the periodicity unit, the system periodicity is doubling, becoming $2\mathbf{a}$. This process is a standard CDW escorting phenomenon which naturally occurs during the presented exact treatment.

Now one turns back to (8), which provide the solution of the matching equations used here, together with the conditions (9), these last providing the parameter space region where the solution is valid. Checking these relations for their meaning in the band structure [see Ref. [3]], one sees, that they give a lowest flat band, which is double degenerate (how this information could be used in flat band engineering for polymers was intensively analyzed in Ref. [3]). Consequently, in $|\Phi_{g,1}\rangle$, one can use at the sites i or $\hat{X}_{i,1}^\dagger$ or $\hat{X}_{i,2}^\dagger$, but not both (in this last case double occupancy appears), maintaining the quarter filling of the lowest band.

A ground state solution of the type (35) holds as well bellow c_0 system filling:

$$|\Phi_{g,1}(c < c_0)\rangle = \prod_{i \in D} \hat{X}_i^\dagger |0\rangle, \quad (37)$$

where D is a manifold of lattice sites containing $N < c_0 N_{\max}$ lattice sites, i.e., $D = i_1, i_2, \ldots i_N$, where the sites contained in the D domain must be at least at a distance $2\mathbf{a}$ from each other. In this case, the charge density wave nature of the ground state is lost, and the ground state is built up from isolated clusters. The insulating nature of the system is maintained.

Increasing the concentration above c_0 (introducing at some sites i both $\hat{X}_{i,1}^\dagger$ and $\hat{X}_{i,2}^\dagger$ in the wave vector), double occupancy appears in between the empty sites placed at sites 1 and $7'$ in Fig. 2, hence a wave vector of the type $|\Phi_1\rangle$ at $c > c_0$ remains a ground state only at $U_n = 0, V > 0$. The insulating nature of the ground state is maintained also in this case.

If we apply electric field on the system, this modifies the SOI interaction strength, and as a consequence, the matching equation solution is no more satisfied, the presented ground state (35) disappears, and the system becomes metallic.

Now let us consider the $\mathbf{B} \neq 0$ case. In this situation, one works with $\hat{X}_i^\dagger$ deduced in (32–34), and we consider here the effect of the external magnetic field described by the Peierls phase factors. In this case, at $c_0 = 1/24$ filling, the ground state expression remains that is given in (35), and at $c < c_0$ filling, that is given in (37). But the situation is that the solution of the matching equations is satisfied only for fixed ϕ values (see Ref. [3]). Hence, when the magnetic field is switched on, the charge density wave phase disappears, and reappears at a fixed external magnetic field values. This is an interesting example which shows how a static magnetic fields can influence a static electric charge distribution. Furthermore, if (35) and (37) are not allowed solutions at $\phi \neq 0$, the lowest band will be dispersive, and the system becomes conducting. This provides a nice example demonstrating that a static magnetic field is able to turn on an insulating phase to a conducting phase. The presented examples may have broad application possibilities in leading technologies.

When at $\mathbf{B} \neq 0$ the conditions from (31) are not satisfied, the expression of the ground-state wave vectors from (35) and (37) remain valid at $V = 0$ only, because in this case, along the horizontal bonds connecting the unit cells, two single occupied nearest-neighbor sites can be present in the system. Because in this case also, the sites 1 and $7'$ in Fig. 2 could be occupied; hence, the charge density wave nature of the ground state is lost.

When the conditions presented in section III.A.4 at point (ii) are present, the $\hat{X}_i^\dagger$ operator acts only on the four middle sites in each unit cell (2, 3, 5, 6 in Fig. 2). Now the (35) and (37) ground-state expressions remain valid also at $V \neq 0$, and could contain even N_c operators, so in this case, the ground state can be written up to a carrier concentration $N/N_{max} = 1/12$. One unit cell will be ferromagnetic, but the cells will be uncorrelated, so the ground state will be paramagnetic. A possible exception from this rule is provided by the situation when the lowest two bands touch each other: this situation will provide a ferromagnetic state based on a similar mechanism as described in Ref. [19].

We note that CDW state in pentagon type of conducting polymers has been observed experimentally in the low concentration limit, see [20]. The measurements were made on polypyrrole, where also the transition to a metallic phase has been detected by increasing the applied electric field value. We note that the study of the emergence of the CDW phase in conducting polymers has also a deeper motivation, since it is considered related to the conduction mechanism (see pg. 5668 from Ref. [21]). Till now, CDW phase in these materials has been deduced only taking into account also the electron–phonon interaction [22] as well, based on approximations. Contrary to this, our result shows that the emergence of the CDW phase in conducting polymers can be deduced even without electron–phonon interaction, based exclusively on interelectronic Coulomb repulsion and SOI.

4 Summary and conclusion

The paper analyzes a pentagon chain type of conducting polymer in the presence of spin–orbit interactions SOI (λ, λ_c), on-site (U) and nearest-neighbor (V) Coulomb repulsions, in the presence of external fields $\mathbf{E}, \mathbf{B}$. Both fields are applied perpendicular to the plane containing the chain. The field $\mathbf{E}$ is able to continuously tune the SOI interaction strength. Usually $\lambda << U$ holds. Besides, if the SOI interaction strength is even small, it has essential effects on the physical properties of the system, since it breaks the spin projection double degeneracy of each band. In these conditions, the perturbative description of the system in both small and high coupling constant limits is questionable; hence, exact methods are used in the study. On the other side, this job has its difficulties because the system is non-integrable, so special technique must be applied to follow this route. On this line, one uses the method based on positive semidefinite operator properties, which provides the first exact ground states for conducting polymers in the presence of SOI. Furthermore, for the first time, this exact procedure is used in the case of conducting polymers in the presence of both U and V Coulomb interactions. In these conditions, the paper concentrates first on the development of the technique used in the presented conditions: the exact transformation of the Hamiltonian in positive semidefinite form, the solution technique of the matching equations, the construction strategy of the exact ground states. The study of the physical properties of the deduced ground states shows a broad spectrum of interesting physical characteristics, e.g., emerging charge density wave phase accompanied by the doubling of the system periodicity, modification possibility of a static charge distribution by an external static magnetic field, transition possibilities between insulating and conducting phases provided by external electric or magnetic fields. The detailed study of all emerging ground states will require future work in the subject.

Funding Information Open access funding provided by University of Debrecen.

Data Availibility Statement The data that support the results are available from the author upon reasonable request.

References

1. S. Tajik, H. Beitollahi, F.G. Nejad, I.S. Shoaie, M.A. Khalilzadeh, M.S. Asi, Q.V. Le, K. Zhang, H.W. Jang, M. Shokouhimehr, Recent developments in conducting polymers: applications for electrochemistry. RSC Adv. **10**, 37834 (2020). Available at https://pubs.rsc.org/en/content/articlehtml/2020/ra/d0ra06160c
2. N. Kucska, Z. Gulacsi, Nanograin ferromagnets from nonmagnetic bulk materials: the case of gold nanoclusters. Int. J. Mod. Phys. B **35**, 2150148 (2021). https://doi.org/10.1142/S0217979221501484

3. N. Kucska, Z. Gulacsi, Spin-orbit interactions may relax the rigid conditions leading to flat bands. Phys. Rev. B **105**, 085103 (2022). https://doi.org/10.1103/PhysRevB.105.085103
4. A. Hijano, E.J. Rodríguez, D. Bercioux, D. Frustaglia, Spin-texture topology in curved circuits driven by spin-orbit interactions. Nat. Comm. Phys. **6**, 186 (2023). Available at https://www.nature.com/articles/s42005-023-01308-8
5. Z.G. Yu, Spin-orbit couplings and its effects in organic solids. Phys. Rev. B **85**, 115201 (2012). https://doi.org/10.1103/PhysRevB.85.115201
6. D. Sun, K.J. van Shooten, M. Kavand et al., Inverse spin Hall effect from pulsed spin current in organic semiconductors with tunable spin-orbit coupling. Nat. Mater. **15**, 863 (2016). Available at https://www.nature.com/articles/nmat4618
7. J.-C. Rojas-Sánchez, N. Reyren, P. Laczkowski, W. Savero, J.-P. Attané, C. Deranlot, M. Jamet, J.-M. George, L. Vila, H. Jaffrès, Spin pumping and inverse spin hall effect in platinum: the essential role of spin-memory loss at metallic interfaces. Phys. Rev. Lett. **112**, 106602 (2014). https://doi.org/10.1103/PhysRevLett.112.106602
8. A. Manchon, H.C. Koo, J. Nitta, S.M. Frolov, R.A. Duine, New perspectives for Rashba spin-orbit coupling. Nat. Matter. **14**, 871 (2015). Available at https://www.nature.com/articles/nmat4360
9. G. Brocks, J. van den Brink, A.F. Morpurgo, Electronic correlations in oligo-acene and -thiopene organic molecular crystals. Phys. Rev. Lett. **93**, 146405 (2004). https://doi.org/10.1103/PhysRevLett.93.146405
10. Y. Luo, X. Wang, J. Yi, W. Li, X. Xie, W. Hai, Exact solutions for spin-orbit coupled bosonic double well system. Available at https://doi.org/10.48550/arXiv.2210.13724
11. U. Brandt, A. Giesekus, Hubbard and Anderson models on perovskitelike lattices: exactly solvable cases. Phys. Rev. Lett. **68**, 2648 (1992). https://doi.org/10.1103/PhysRevLett.68.2648
12. R. Strack, Exact ground-state energy of the periodic Anderson model in d=1 and extended Emery models in d=1,2 for special parameter values. Phys. Rev. Lett. **70**, 833 (1993). https://doi.org/10.1103/PhysRevLett.70.833
13. Z. Gulacsi, A. Kampf, D. Vollhardt, Rout to ferromagnetism in organic polymers. Phys. Rev. Lett. **105**, 266403 (2010). https://doi.org/10.1103/PhysRevLett.105.266403
14. Z. Gulacsi, Exact ground states for correlated electrons on pentagon chains. Int. J. Mod. Phys. B **27**, 1330009 (2013). https://doi.org/10.1142/S0217979213300090
15. Z. Gulacsi, D. Vollhardt, Exact insulating and conducting ground states of a periodic Anderson model in three dimensions. Phys. Rev. Lett. **91**, 186401 (2003). https://doi.org/10.1103/PhysRevLett.91.186401
16. Z. Gulacsi, Delocalization effect of the Hubbard repulsion in exact terms and two dimensions. Phys. Rev. B **77**, 245113 (2008). https://doi.org/10.1103/PhysRevB.77.245113
17. Z. Gulacsi, Exact multielectronic electron-concentration-dependent ground states for disordered two-dimensional two-band systems in the presence of disordered hoppings and finite on-site random interactions. Phys. Rev. B **69**, 054204 (2004). https://doi.org/10.1103/PhysRevB.69.054204
18. H. Lee, M.Y. Zhou, S.Y. Wu, X.R. Zhiang, Research of spin-orbit interactions in organic conjugated polymers. IOP Conf. Ser. Mater. Sci. Eng. **213**, 012005 (2017). https://doi.org/10.1088/1757-899X/213/1/012005
19. M. Gulacsi, Gy. Kovacs, Z. Gulacsi, Flat band ferromagnetism without connectivity conditions in the flat band. Europhys. Lett. **107**, 57005 (2014). Available at https://epljournal.edpsciences.org/articles/epl/abs/2014/17/epl16514/epl16514.html
20. A. Rahman, M.K. Sanyal, Observation of charge density waves characteristics in conducting polymer nanowires: possibility of Wigner crystallization. Phys. Rev. B **76**, 045110 (2007). https://doi.org/10.1103/PhysRevB.76.045111
21. K. Nemsheer, C.S. Rout, Conducting polymers: a comprehensive review on recent advances in synthesis, properties and applications. RSC Adv. **11**, 5659 (2021). Available at https://pubs.rsc.org/en/content/articlelanding/2021/ra/d0ra07800j
22. B. Horovitz, Z. Vardeny, E. Ehrenfreund, O. Brafman, Raman scattering from charge-density waves an application to polyacetylene. J. Phys. C **19**, 7291 (1986). https://doi.org/10.1088/0022-3719/19/36/019/pdf