On some mathematical identities resulting from evaluation of the partition function for an electron moving in a periodic lattice.

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Abstract

We consider a simple model of the dynamics of a single electron in a crystal lattice. Although this is a standard problem in condensed matter physics, alternative ways of evaluating a partition function for such a system lead to equalities, that may be interesting from the point of view of mathematical analysis, combinatorics and graph theory.

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Introduction

In this paper we present results which may be interesting from the point of view of pure mathematics, but originate from some properties of mathematical formalism used to describe certain physical systems. Namely, we derive some generalizations of the integral representation of the modified Bessel function $I_0(2\xi)$,

$$
\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{2\xi \cos(k)} dk = \sum_{\nu=0}^{\infty} \frac{\xi^{2\nu}}{\nu! \nu!},
$$

here given in the form of the Taylor expansion around $\xi = 0$ (see [1], 9.6.16, p. 376). The important observation is that formula (1) describes a partition function of the tight-binding model of a single electron moving in an infinite, one-dimensional chain of atoms. This model and its generalizations are widely used in condensed matter physics and may be found in any standard textbook on that field, (see e.g. [2], p. 11).

If we consider, in the framework of the same model, some $D$-dimensional crystal lattice, and if we write down the corresponding partition function, we obtain equality analogous to (1). Namely, its l.h.s is then a sum or integral over some subset of $\mathbb{R}^D$, having nontrivial symmetry properties. On the other hand, the r.h.s. of both formula (1) and any of its generalizations is a series in one or several complex variables, and can be found with the help of the
method described in detail in the present paper. In that way, we are able to establish several identities, which may be interesting from the point of view of mathematical analysis. What is more important, our method involves some basic techniques and concepts of combinatorics and graph theory, therefore it may be interesting from the point of view those disciplines.

The results presented here have been obtained with the help of a standard mathematical formalism and techniques used in theoretical condensed-matter physics. This fact has two important consequences. First, our notation is generally an usual one for that field. This results in occurrence of additional numerical factors and indices, which may be found redundant, in the formulas presented. Hence, throughout the paper we use units in which Planck constant $\hbar$ and Boltzmann constant $k_B$ are equal unity, $\hbar = k_B = 1$.

Second, our results may be found not rigorous enough from the point of view of pure mathematics. Nonetheless, we believe that they are correct, and they can be given a more formal shape if necessary. This should be one of the subjects of our future investigation.

This paper is organized as follows: in section 1. we introduce some concepts necessary to understand our method and we describe the method itself. In section 2. we analyze various lattice geometries and present the results obtained. Section 3. consists of appendices, where some details, omitted in the main text, are presented.

1 The method

1.1 Preliminaries: physical context

Let us consider a motion of a single electron in a periodic crystal lattice. To construct mathematical model of such a physical system, we have to provide a description of a crystal lattice, as well as to express the quantum dynamics of the electron on that lattice.

To model a crystal lattice, we define first the $D$-dimensional abstract lattice, $\Lambda$, in a standard manner, as a set of lattice vectors $R, r \in \mathbb{R}^D$, being the linear combinations with integral coefficients of $D$ fundamental translation vectors $a_1, a_2, \ldots, a_D$

$$R = \sum_{p=1}^{D} n_p a_p.$$  \hspace{1cm} (2)

However, appropriate model of the real crystal structure is constructed by attaching basis of $M \geq 1$ atoms to each point of the abstract lattice (see e.g. [3], p. 5). We denote positions of atoms by vectors $i$, called lattice sites,
each lattice site has its corresponding lattice vector, $\mathbf{R}(i)$. For lattices with $M = 1$, lattice vectors can be chosen in such a way that they coincide with lattice sites. This is the case of Bravais lattice, and most, although not all, cases analyzed in this paper belong to this class. On the other hand non-Bravais lattices consist of $M > 1$ pairwise disjoint sublattices, with any two points of a given sublattice being equivalent.

It is of crucial importance not to confuse $\Lambda$ with the set of lattice sites $i$, denoted $\Xi$. From now on we use the term lattice only for $\Xi$, whereas $\Lambda$ is always termed abstract lattice, as before. $\Lambda = |\Lambda|$ ($\Xi = |\Xi|$) is the number of the lattice vectors (sites), respectively. Obviously, $\Xi = M\Lambda$, and this number may be finite or not. In the former case the periodic boundary conditions (PBC) have to be imposed to ensure periodicity.

Apart from abstract lattice $\Lambda$ we have to remind the Reader also the notion of the reciprocal lattice, defined as the set of vectors $\mathbf{K}$ having the following property (see e.g. [3], p. 61),

$$e^{i\mathbf{K} \cdot \mathbf{R}} = 1, \quad \text{for any } \mathbf{R} \in \Lambda. \quad (3)$$

Now we return to the question of a quantum-mechanical description of the dynamics of the electron. To be able to give such a description, first we have to specify the Hilbert space $\mathcal{H}$ of the state vectors, and then choose some basis vector set in this space. It turns out that set $\Xi$ in a real space provides the convenient basis in $\mathcal{H}$. Namely, we define state $|i\rangle \in \mathcal{H}$ as describing the electron cloud centered on the lattice site $i$. This is so called Wannier basis or Wannier representation. Such defined states form a complete and orthonormal basis set,

$$\sum_{i \in \Xi} |i\rangle \langle i| = \hat{1}, \quad \langle i|j\rangle = \delta_{ij}. \quad (4)$$

It is convenient to treat our Hilbert space as a subspace of the larger one, called the Fock space, $\mathcal{F}$. This new space, apart from the just defined one-particle states $|i\rangle$, consist of other $N$-particle states, with $N = 0, 2, \ldots, N_{\text{max}}$, $N_{\text{max}} = \Xi$, and may be written as a direct sum of its $N$-particle sectors, $\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \cdots \oplus \mathcal{F}_{N_{\text{max}}}$. Although we are interested in one-particle sector only, $\mathcal{F}_1 \equiv \mathcal{H}$, we use the general formalism of second quantization, as the most convenient for our purposes (compare [4], chapter 1). We introduce electron creation (annihilation) operators $c_i^\dagger$ ($c_j$) for lattice site $i$ ($j$), respectively.

\[\text{It may be also regarded as some kind of coordinate representation of quantum mechanics, but in the discretized, rather than continuous, real space. We use those three terms interchangeably in the following sections.}\]
They obey standard anti-commutation relations

\[ c_j c_i^\dagger + c_i^\dagger c_j = \delta_{ij}, \quad c_j c_i + c_i c_j = 0, \]  

and are related to the basis state vectors \( |i\rangle \) (\langle i|) in the following way

\[ |i\rangle = c_i^\dagger |0\rangle, \quad \langle i| = \langle 0|c_i, \]

where \( |0\rangle \) is a vacuum state, spanning zero-particle sector \( F_0 \subset F \).

The dynamics of the electron can be then described as follows: initially localized in the vicinity of a particular site \( i \), it may quantum-mechanically tunnel to neighboring site \( j \). In \( \mathcal{H} \) it corresponds simply to the transition from basis state \( |i\rangle \) to state \( |j\rangle \). If we include only the so-called single-band dynamics and neglect other possible degrees of freedom (like spin, orbital, etc.) of the electron, the resulting Hamilton operator (Hamiltonian) reads

\[ \hat{H} = \sum_{i,j \in \Xi} t(i,j)c_i^\dagger c_j = \sum_{i \in \Xi, q \in S} t(q)c_i^\dagger c_{i+q}. \]

Here the summation over \( i \) runs through the whole lattice \( \Xi \). We assume that the complex numbers \( t(i,j) \) (hopping integrals) fulfill the following conditions,

\[ \forall i,j \in \Xi : \quad t(i,j) = t(j,i)^* = t(j-i) \equiv t(q), \quad q \equiv j-i, \]

due to the fact that Hamiltonian is a hermitian operator, and because all lattice sites of a given sub-lattice are assumed to be equivalent (translational invariance). We also put \( t(i,i) = 0 \) for all \( i \). By \( S \) we denote a set of vectors \( q \), for which \( t(q) \neq 0 \). We assume the maximal number of independent hopping integrals \( t(q) \equiv t_s \in \{ t_1, t_2, \ldots, t_C \} \), namely \( C \equiv \frac{1}{2}|S| \), the factor \( \frac{1}{2} \) appears due to (8). Consequently, in general, the Hamiltonian does not possess all symmetry properties of the lattice - the discrete rotational symmetry may be lost unless we impose specific conditions on parameters \( t_s \).

Due to translational invariance of the Hamiltonian (7), it is advisable to express it in Bloch basis, labeled by the values of quasimomentum \( k \), and related to the Wannier basis by the unitary transformation,

\[ c_k^\dagger |0\rangle \equiv |k\rangle = \frac{1}{\sqrt{\Lambda}} \sum_{i \in \Xi} \exp \left( -i k \cdot R(i) \right) |i\rangle \]

with the inverse given by

\[ c_i^\dagger |0\rangle \equiv |i\rangle = \frac{1}{\sqrt{\Lambda}} \sum_{k \in FBZ} \exp(i k \cdot R(i)) |k\rangle. \]
The above formulas refer only to the case of finite \( \Lambda < \infty \), Bravais lattice \( (M = 1) \). The formalism for non-Bravais lattices is not presented here, the limit \( \Lambda \to \infty \) will be considered later.

The vectors \( \mathbf{k} \) in \( (9,10) \), determined by the lattice geometry and PBC imposed, belong to the first Brillouin zone (FBZ), which is the Wigner-Seitz unit cell of the reciprocal lattice centered at \( \mathbf{K} = 0 \) (compare \( [3] \), chapter 9).

Formulas \( (6), (9) \) and \( (10) \) give us also the transformation properties of the creation (annihilation) operators themselves, and can easily find the form of the Hamiltonian \( (7) \) in the Bloch basis\(^2\), in which it is diagonal, \( \hat{H}|\mathbf{k}\rangle = \epsilon(\mathbf{k})|\mathbf{k}\rangle \). Explicitly, we have

\[
\hat{H} = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) c_{\mathbf{k}}^\dagger c_{\mathbf{k}} = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) \hat{n}_{\mathbf{k}}. \tag{11}
\]

The functional dependence of its eigenvalues \( \epsilon(\mathbf{k}) \) on \( \mathbf{k} \), the dispersion relation, results from the lattice geometry, but is also a function of the hopping integrals \( t_s \), \( \epsilon = \epsilon(\mathbf{k}; t_1, \ldots, t_C) \). For \( M = 1 \) it has the following general form

\[
\epsilon(\mathbf{k}; t_1, \ldots, t_C) = t_1 \epsilon_1(\mathbf{k}) + \ldots + t_C \epsilon_C(\mathbf{k}). \tag{12}
\]

We assume, that \( \epsilon(\mathbf{k}; t_1, \ldots, t_C) \) is at least a piecewise continuous, and then integrable, function of \( \mathbf{k} \).

Consider now a limit \( \Lambda \to \infty \). Due to the periodic boundary conditions (PBC), for any finite \( \Lambda \) the number of \( \mathbf{k} \) vectors in FBZ is equal that of lattice vectors \( \mathbf{R} \), \( \mathbf{R} \in \Lambda \). As a consequence, in the limit in question, some physical quantities, expressed as sums over \( \mathbf{k} \in \text{FBZ} \), may be divergent. To keep the values of those quantities finite, we rescale them by the factor \( \Lambda \),

\[
\sum_{\mathbf{k} \in \text{FBZ}} f(\mathbf{k}) \longrightarrow \frac{1}{\Lambda} \sum_{\mathbf{k} \in \text{FBZ}} f(\mathbf{k}). \tag{13}
\]

The sum on the r.h.s of \( (13) \), for a given value of \( \Lambda \), may be regarded as the Riemann sum of a function \( f(\mathbf{k}) \). The important fact is that a mesh of any partition of FBZ given by the values of \( \mathbf{k} \) goes to zero in the limit \( \Lambda \to \infty \), regardless of the particular choice of PBC. Consequently, in that limit, \( (13) \) approaches the value of the Riemann integral over a FBZ of \( f(\mathbf{k}) \), here understood as a function of continuous variable \( \mathbf{k} \). We can then replace the summation in \( (13) \) by the integration over FBZ, according to

\[
\frac{1}{\Lambda} \sum_{\mathbf{k} \in \text{FBZ}} f(\mathbf{k}) \xrightarrow{\Lambda \to \infty} \frac{1}{V} \int_{\text{FBZ}} f(\mathbf{k}) d\mathbf{k}, \tag{14}
\]

where \( V \) is a Jordan measure of the first Brillouin zone.

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\(^2\)Referred to also as the quasimomentum representation or \( \mathbf{k} \)-representation.
1.2 The partition function

1.2.1 General formalism and quasimomentum representation.

According to quantum statistical mechanics (see e.g. [5], p. 245), the partition function, \( Z \), is given by the formula

\[
Z = Z(\beta) = \text{Tr}(\exp(-\beta \hat{H})),
\]

where \( \text{Tr} \) denotes trace of an operator, \( \beta = 1/T \) is an inverse temperature and \( \hat{H} \) is the Hamiltonian of a system considered. We evaluate \( Z \) first in Bloch basis, which is rather simple, due to the fact that one-electron Bloch states \( c_k^-|0\rangle \) are eigenstates of the Hamiltonian \( \hat{H} \). In that case the partition function reads

\[
Z = \frac{1}{\Lambda} \sum_{F BZ} \exp(-\beta \epsilon(k)), \quad \Lambda < \infty,
\]

for finite number of lattice vectors, and

\[
Z = \frac{1}{V} \int_{FBZ} \exp(-\beta \epsilon(k)) \, dk
\]

for the \( \Lambda \to \infty \) limit. To avoid infinite value of \( Z \) in (16) we have applied normalization described in a previous paragraph by formula (13). Introducing for convenience \( C \) new variables \( \xi_s \), defined as follows

\[
\xi_s = -\beta t_s, \quad s \in \{1, 2, \ldots, C\},
\]

and having in mind (12), we can rewrite both (16) and (17) as

\[
Z = Z(\xi_1, \xi_2, \ldots, \xi_C) = \frac{1}{\Lambda} \sum_{FBZ} \exp \left( \sum_{s=1}^{C} \xi_s \epsilon_s(k) \right)
\]

and

\[
Z = Z(\xi_1, \xi_2, \ldots, \xi_C) = \frac{1}{V} \int_{FBZ} \exp \left( \sum_{s=1}^{C} \xi_s \epsilon_s(k) \right) \, dk.
\]

Let us point out, that for most lattice geometries considered, the sum (19) or the integral (20) cannot be easily evaluated, and the explicit form of the functional dependence of \( Z(\xi_1, \xi_2, \ldots, \xi_C) \) on its arguments cannot be evaluated either in terms of elementary functions or in terms of standard special functions.
1.2.2 Coordinate representation

The general formula for the partition function of our one-electron system, evaluated with the help of Bloch basis states (19), (20), has a form of a complicated sum or integral, which usually cannot be handled analytically. However, the trace of an operator does not depend on the basis one uses, and in order to obtain an alternative expression for \( Z(\xi_1, \xi_2, \ldots, \xi_C) \) we compute it now using Wannier basis.

Evaluation of the partition function in the present case requires some effort, below we describe a method used for this purpose. First, assuming \( \Lambda < \infty \), we rescale \( Z \) by \( \Lambda \), in correspondence with the formula (13),

\[
Z = \frac{1}{\Lambda} \sum_{i \in \Xi} \langle i | \exp(-\beta \hat{H}) | i \rangle = \frac{1}{\Lambda} \sum_{i \in \Xi} \sum_{n} \langle i | (\frac{(-\beta \hat{H})^n}{n!}) | i \rangle. \tag{21}
\]

The problem in question is solved, once we know how to evaluate the quantity \( g(n) \) defined as

\[
\frac{1}{\Lambda} \sum_{i \in \Xi} \langle i | (\frac{(-\beta \hat{H})^n}{n!}) | i \rangle \equiv g(n), \tag{22}
\]

for the Hamiltonian (7). Explicitly, in this particular case we have

\[
g(n) = \frac{1}{\Lambda} \sum_{l \in \Xi} \langle l | (\sum_{i,j \in \Xi} -\beta t_{ij} A_{ij})^n | l \rangle, \tag{23}
\]

where we put \( t(ij) \equiv t_{ij} \) and introduce a shorthand \( A_{ij} \equiv c_i^d c_j \) to make the following formulas more compact and transparent. One can easily examine some obvious properties of just introduced operators \( A_{ij} \), below we invoke only two of them,

\[
A_{ij}^\dagger = A_{ji}, \quad A_{ij}A_{ji} = \hat{n}_i(1 - \hat{n}_j). \tag{24}
\]

When calculating \( g(n) \) we have to deal with the terms of the general form

\[
(-\beta)^n t_{12n-12n-1} t_{12n-22n-2} \cdots t_{143} t_{321} A_{12n-1} A_{12n-2} \cdots A_{143} A_{321}, \tag{25}
\]

where \( l_m \in \Xi \). In what follows we concentrate on the operator part of (25),

\[
A_{12n-1} A_{12n-2} \cdots A_{143} A_{321}, \tag{26}
\]

\( ^3 \)We postpone for a moment a question if it is legitimate to interchange the summation over the order of the expansion \( n \) and that over the states \( |i\rangle \).
Most of such terms do not contribute to $g(n)$. This is, firstly, due to the fermion anticommutation relations and properties of the occupation number operator\(^4\) that all sequences of the type
\[
\cdots A_{ii} A_{jj} \cdots, \quad \cdots A_{ii} A_{jj} \cdots \text{ or } \cdots \hat{n}_i (1 - \hat{n}_i) \cdots,
\]
identically vanish. Secondly, because we compute trace in basis of one-electron states, all terms where the product of two or more occupation electron number operators for different sites, $i,j$ appear,
\[
\cdots A_{ii} A_{jm} A_{mj} \cdots = \cdots \hat{n}_i (1 - \hat{n}_j) \hat{n}_j (1 - \hat{n}_m) \cdots,
\]
must vanish, too. This restricts the form of the terms in question to
\[
A_{i_{n+1}i_n} A_{i_{m}i_{m-1}} \cdots A_{i_{s+1}i_s} A_{i_{2i_1}} = \hat{c}_{i_{n+1}}^\dagger (1 - \hat{n}_{i_n}) (1 - \hat{n}_{i_{n-1}}) \cdots (1 - \hat{n}_{i_2}) c_{i_1}. \tag{29}
\]
However, due to the trace operation we have to consider only diagonal terms, i.e. those with the first and the last index in any product of $n A_{ii}$ operators being identical. Consequently, the only allowed terms in an expansion giving nonzero contribution to $g(n)$ must be of the following form
\[
A_{i_{1i_n}} A_{i_{i_{n-1}}} \cdots A_{i_{s+1}i_s} A_{i_{2i_1}} = \hat{c}_{i_1}^\dagger (1 - \hat{n}_{i_n}) (1 - \hat{n}_{i_{n-1}}) \cdots (1 - \hat{n}_{i_2}) c_{i_1}. \tag{30}
\]
Notice that the above expression is a product of $n - 1$ hole number operators sandwiched in between $c_{i_1}^\dagger$ and $c_{i_1}$ operators, and has trace equal unity.

Now let us now return to the full form of the terms \((30)\),
\[
(-\beta)^n t_{i_{1i_n}} t_{i_{i_{n-1}}} \cdots t_{i_{s+1}i_s} A_{i_{i_{i_{n-1}}} A_{i_{i_{n-2}}} \cdots A_{i_{i_2}}} A_{i_{1i_n}} A_{i_{1i_{n-1}}} \cdots A_{i_{i_2}i_1}, \tag{31}
\]
and assume for a moment that among $n$ hopping integrals in \((31)\), $t_s$ appears $n_s$ times, $s = 1,2,\ldots,C$. Having in mind variables $\xi_s$ introduced in \((18)\), we see, that \((31)\) contributes to $g(n)$ given by \((22)\) through the term
\[
\xi_1^{n_1} \xi_2^{n_2} \cdots \xi_C^{n_C}, \quad \sum_{1}^{C} n_s = n. \tag{32}
\]
We denote the total number of terms contributing in the same way to $g(n)$ by $\Gamma(n_1, n_2, \ldots, n_C)$. To obtain $g(n)$ we must sum up the terms \((32)\) for all permitted values $n_1, n_2, \ldots, n_C$,
\[
g(n; \xi_1, \xi_2, \ldots, \xi_C) = \sum_{n_1, n_2, \ldots, n_C}^{\text{constr}} \Gamma(n_1, n_2, \ldots, n_C) \cdot \xi_1^{n_1} \xi_2^{n_2} \cdots \xi_C^{n_C}, \tag{33}
\]
where we have explicitly denoted the dependence of $g(n)$ on $\xi_1, \xi_2, \ldots, \xi_C$, and the fact that summation in (33) obeys the constraint appearing in (32). Comparing (21), (22) and (33), we have

$$Z(\xi_1, \xi_2, \ldots, \xi_C) = \sum_{n_1, n_2, \ldots, n_C} \sum_{n_1, n_2, \ldots, n_C} \frac{\Gamma(n_1, n_2, \ldots, n_C)}{n!} \cdot \xi_1^{n_1} \xi_2^{n_2} \cdots \xi_C^{n_C}. \quad (34)$$

Obviously, from the above formula it follows that the $\Gamma(n_1, n_2, \ldots, n_C)$ coefficients are related to the respective coefficients $\Gamma(n_1, n_2, \ldots, n_C)$ of the Taylor series expansion of $Z(\xi_1, \xi_2, \ldots, \xi_C)$,

$$\Gamma(n_1, n_2, \ldots, n_C) = \frac{n!}{n_1! \cdots n_C!} \cdot Z(n_1 n_2 \cdots n_C), \quad (35)$$

defined as

$$Z(n_1 n_2 \cdots n_C) = \frac{\partial^n}{\partial \xi_1^{n_1} \partial \xi_2^{n_2} \cdots \partial \xi_C^{n_C}} Z(\xi_1, \ldots, \xi_C) \bigg|_{\xi_1=\xi_2=\ldots=\xi_C=0}. \quad (36)$$

However, according to the remark in section 2.1, in most cases (19), (20) and their derivatives with respect to $\xi_s$ cannot be evaluated analytically. In order to find an explicit formula for the Taylor series of the partition function, we have to develop an alternative method of computing coefficients $\Gamma(n_1, n_2, \ldots, n_C)$ or $\Gamma(n_1 n_2 \cdots n_C)$. This problem is solved in the next chapter.

1.2.3 The method of evaluating $\Gamma(n_1, n_2, \ldots, n_C)$.

There exist a method of combinatorial character, which allows us to find $\Gamma(n_1, n_2, \ldots, n_C)$ coefficients. It is based on the following observation: the dynamics of our system, governed by the Hamiltonian (7) may be described by an intuitive picture of an electron tunneling - or ’taking a step’ form one site to the other. More precisely, such a step is generated by $A_{ij}$ operator, and may be visualized by an arrow, pointing from site $j$ to site $i$. Each such arrow is labeled by a complex number - a hopping integral $t_{ij} = t_s$. Consequently, the product of operators given by (30) can be visualized, using terms of graph theory, as a closed path or a cycle, with the respective lattice sites being its vertices, and with the complex number $t_s$ ascribed to each edge. The crucial fact is the one-to-one correspondence between terms (30) and the resulting closed paths, for details see appendix 3.1. For our purposes it is important which vertex of our graph is a terminal one, (i.e. this from which our path starts and where it ends), the graphs differing by a terminal vertex are different from our point of view. Notice also, that any vertex, including a terminal one, may be ’visited’ by an electron more then once, i.e. there may
be more than one edge connecting two vertices, and thus our closed paths does not have to be simple.

The set of all vertices that can be connected by a directed edge with a particular initial site are given by vectors \( q \in \mathcal{S} \). In other words, electron can move in direction and at the distances determined by those vectors, or equivalently, by the hopping integrals \( t(q) \). (This is the reason why it is convenient to assume the maximal number of distinct hopping integrals, i.e. one \( t \) for every pair \((q, -q), \pm q \in \mathcal{S}\)). The above described crystal directions should not be confused with \( D \) mutually orthogonal spacial directions, which, in principle can be chosen at will. Obviously, for the closed path we have to fulfill the condition that a \( D \)-dimensional vector of the total displacement must be equal zero.

At first glance it seems than in order to find \( \Gamma(n_1, n_2, \ldots, n_C) \) for a given lattice geometry, we have to compute the total number of the closed paths of length \( n \), with exactly \( n_s \) edges labeled by the respective hopping integral \( t_s \). However, due to the translational invariance of the Hamiltonian and our normalization procedure, the summation over terminal sites in trace operation just cancel the normalization factor \( 1/\Lambda \). What remains then is to compute the number of such paths with one particular site chosen as a terminal one, numbered closed paths of length \( n \), with \( n_s \) edges

\[
\Gamma(n_1, n_2, \ldots, n_C) = \text{Number of closed paths of length } n, \text{ with } n_s \text{ edges labeled by } t_s, \text{ and with one particular site } i \text{ chosen as the terminal vertex.} \tag{37}
\]

This allows us to compute \( Z(\xi_1, \xi_2, \ldots, \xi_C) \) also in the \( \Lambda \to \infty \) limit, the difference with the case of finite lattice is that in the latter, when computing \( \Gamma(n_1, n_2, \ldots, n_C) \), periodic boundary conditions must be taken into account.

The number of independent variables in \( Z(\xi_1, \xi_2, \ldots, \xi_C) \) can be reduced from its maximal value \( C \) by putting \( \xi_s = \xi_w \) for some \( s, w \), after all coefficients \( \Gamma(n_1, n_2, \ldots, n_C) \) are found. In the extreme case, partition function becomes function of one variable \( \xi \) only, and the total number of all closed paths of the total length \( n \), starting from a particular lattice site, denoted by \( \hat{\Gamma}(n) \), is equal

\[
\hat{\Gamma}(n) \equiv \sum_{n_1, n_2, \ldots, n_C}^{\text{constr}} \Gamma(n_1, n_2, \ldots, n_C) = g(n; 1, 1, \ldots, 1). \tag{38}
\]

To summarize the above discussion, we make the following observation. Define a graph \( \gamma(\hat{H}) \), such that its vertices are lattice sites of the lattice

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5By length we mean, according to the terminology of graph theory, the number of edges, i.e. the order of the expansion of \( \exp(-\beta \hat{H}) \) and not the distance in a real space.
considered, and that vertices \( j \) and \( i \) are connected by an edge if and only if \( t_{ij} \neq 0 \). In the case of finite lattice and for all hopping integrals equal unity, \( t_{ij} = t = 1 \), the matrix of the Hamiltonian in the Wannier representation is simply the adjacency matrix of the graph \( \gamma(\hat{H}) \). This observation immediately shows the essence of our method, the \( n \)-th power of adjacency matrix contains information about the number of all paths of length \( n \), its trace gives the total number of all closed paths. Generalization to the case of complex \( t_s \) requires some kind of weighted graphs.

For infinite lattices such a simple picture is no longer available.

1.2.4 The main formula

I the previous section we have presented the method of finding the coefficients \( \Gamma(n_1, n_2, \ldots, n_C) \), which does not require explicit evaluation of the sum (19) or integral (20) nor the respective partial derivatives. Equating two alternative expressions for \( Z \), formulas (19) or (20) and (34), we obtain

\[
\frac{1}{\Lambda} \sum_{FBZ} \exp \left( \sum_{1}^{C} \xi_{s} \varepsilon_{s}(k) \right) = \sum_{n} \sum_{n_1,n_2,\ldots,n_C}^{\text{const}} \frac{\Gamma_f(n_1, n_2, \ldots, n_C)}{n!} \xi_1^{n_1} \xi_2^{n_2} \cdots \xi_C^{n_C},
\]

(39)

or, for the case of infinite lattice\(^\text{6}\),

\[
\frac{1}{V} \int_{FBZ} \exp \left( \sum_{1}^{C} \xi_{s} \varepsilon_{s}(k) \right) dk = \sum_{n} \sum_{n_1,n_2,\ldots,n_C}^{\text{const}} \frac{\Gamma_i(n_1, n_2, \ldots, n_C)}{n!} \xi_1^{n_1} \xi_2^{n_2} \cdots \xi_C^{n_C}.
\]

(40)

This is the main result of the present paper. Above formulas, for particular cases of lattice geometries, generate mathematical identities that may be even yet unknown.

There are two points of view one can have on (39), (40). Firstly, its r.h.s is an explicit expression for the series expansion of \( Z(\xi_1, \xi_2, \ldots, \xi_C) \) given by the nontrivial sum or integral appearing on the l.h.s. Thus, it could be regarded as some kind of generalization of the well-known formula \( I_0(2\xi) \) giving a modified Bessel function \( I_0(2\xi) \). Although the occurring series are rather complicated and may be found inconvenient for practical computational purposes, they may be interesting from the point of view of the mathematical analysis.

On the other hand, quasimomentum representation of \( Z(\xi_1, \xi_2, \ldots, \xi_C) \) may be used to obtain a coefficients \( \Gamma(n_1, n_2, \ldots, n_C) \) - numbers of closed

\(^{6}\)Throughout the text we keep the same symbol \( \Gamma \) for both \( \Lambda < \infty \) and \( \Lambda \to \infty \), only here we distinguish both cases by respective superscript to avoid misunderstanding.
paths of some specific kind, for a given lattice geometry. Namely, let us remind the Reader, that according to (34), (35) and (40), (39) we have

$$\Gamma_f(n_1, n_2, \ldots, n_C) = \frac{n!}{n_1!n_2! \cdots n_C!} \cdot \frac{\partial^n \left( \frac{1}{V} \sum_{FBZ} \exp \left( \sum_{s} \xi_s \epsilon_s(k) \right) \right)}{\partial \xi_1^{n_1} \partial \xi_2^{n_2} \cdots \partial \xi_C^{n_C}}, \quad (41)$$

$$\Gamma_i(n_1, n_2, \ldots, n_C) = \frac{n!}{n_1!n_2! \cdots n_C!} \cdot \frac{\partial^n \left( \frac{1}{V} \int_{FBZ} \exp \left( \sum_{s} \xi_s \epsilon_s(k) \right) d\mathbf{k} \right)}{\partial \xi_1^{n_1} \partial \xi_2^{n_2} \cdots \partial \xi_C^{n_C}}, \quad (42)$$

for finite and infinite lattice, respectively. The r.h.s of the above formulas can be easily computed numerically, and therefore our results may be interesting from the point of view of graph theory or combinatorics.

Finally, in the case of all $\xi_s$ equal, due to (38) formula (40) reads

$$Z(\xi) = \frac{1}{V} \int_{FBZ} \exp \left( \xi \sum_{s} \epsilon_s(k) \right) d\mathbf{k} = \sum_n \frac{\tilde{\Gamma}(n)}{n!} \xi^n. \quad (43)$$

In the next section the above equality is utilized frequently instead of the most general case (40).

## 2 The results

In this part we present our results. For each case we begin with the brief description of the geometry of the direct as well as the reciprocal lattice. Then, the set $\mathcal{S}$, as well as $C$- the number of independent hopping integrals in the Hamiltonian (7), the dispersion relation and the partition function in quasimomentum representation are given. Next, we explain in detail how to compute the partition function in Wannier representation, for each particular lattice geometry. Finally, we compute explicitly first few terms of the Taylor series expansion of $Z$, both by combinatorial techniques as well as by numerical integration of the partition function in $\mathbf{k}$-representation.

Except for the linear chain lattice (see 2.1.1), we consider infinite lattices only, and most analyzed cases are Bravais lattices, except for paragraph 2.4 where we deal with the non-Bravais honeycomb and diamond lattices. Real hopping integrals are assumed throughout the main text, the case of complex integral for particular lattice geometry is analyzed in appendix 3.2.
2.1 Linear chain with nearest neighbor hopping

In the present paragraph we consider the linear chain of atoms, with the Hamiltonian \((7)\) given by

\[
\hat{H}_L = t \sum_i \sum_{q=-1,1} c_i^\dagger c_{i+q},
\]

\((44)\)

i.e. with the only nonzero \(t_s\) between nearest neighboring sites.

2.1.1 The case of a finite lattice

We begin from the case of finite number of sites, consequently, we have to impose the periodic boundary conditions (PBC). Diagonalization of the Hamiltonian \((44)\) by Fourier transform yields a dispersion relation

\[
\epsilon_k = 2t \cos (k),
\]

\((45)\)

where due to the PBC quasimomentum \(k\) is given by

\[
k = \frac{2m\pi}{\Lambda}, \quad m \in \mathbb{Z}.
\]

\((46)\)

To find \(\Lambda\) allowed values of \(m\) (or, equivalently, \(k\)), i.e. the first Brillouin zone (FBZ), we consider separately the case of even and odd \(\Lambda\). We obtain, respectively

\[
m \in \left\{-\frac{\Lambda}{2} + 1, \ldots, \frac{\Lambda}{2} - 1, \frac{\Lambda}{2}\right\}, \quad \Lambda \text{ even},
\]

\((47)\)

\[
m \in \left\{-\frac{(\Lambda - 1)}{2}, -\frac{(\Lambda - 1)}{2} + 1, \ldots, \frac{(\Lambda - 1)}{2}\right\}, \quad \Lambda \text{ odd}.
\]

\((48)\)

The resulting values of \(k\) are then

\[
k \in \left\{-\frac{\pi(\Lambda - 2)}{\Lambda}, \ldots, \frac{\pi(\Lambda - 2)}{\Lambda}, \pi\right\}, \quad \Lambda \text{ even}
\]

\((49)\)

\[
k \in \left\{-\frac{\pi(\Lambda - 1)}{\Lambda}, \ldots, \frac{\pi(\Lambda - 3)}{\Lambda}, \frac{\pi(\Lambda - 1)}{\Lambda}\right\}, \quad \Lambda \text{ odd}.
\]

\((50)\)

Obviously, the permitted values of \(k\) are related to the \(\Lambda\) roots of equation

\[
z^\Lambda = 1, \quad z \in \mathbb{C}
\]

\((51)\)

in the following way

\[
k = \text{arg}z.
\]

\((52)\)
The partition function depends now on one variable, \( Z_L \equiv Z_L(\xi), \xi = -\beta t \), expressed in quasimomentum representation (17) it reads

\[
Z_L(\xi, \Lambda) = \frac{1}{\Lambda} \sum_{k \in \text{FBZ}} e^{2\xi \cos(k)}.
\]

(53)

with the FBZ given by (49, 50). We denoted explicitly the dependence of \( Z_L \) on both its natural argument \( \xi \) as well as on the number of lattice sites \( \Lambda \).

In order to evaluate \( Z_L(\xi, \Lambda) \) in the Wannier representation, notice, that from any site electron can move to the nearest neighboring site either in positive (clockwise) or negative (anti clockwise) direction along the chain. Denote number of such steps by \( n^+ \) and \( n^- \), respectively. Obviously, \( n = n^+ + n^- \), we also define

\[
d = d(n, \Lambda) = n^+ - n^-.
\]

(54)

For a closed path of length \( n \) on the lattice with \( \Lambda \) sites, the following condition has to be fulfilled

\[
d(n, \Lambda) = c\Lambda, \quad c \in \mathbb{Z}.
\]

(55)

In order to find the permitted values of \( c \), let us note, that for any \( n \) and \( \Lambda \) we have

\[
n = w\Lambda + r, \quad r < \Lambda.
\]

(56)

or, equivalently,

\[
w\Lambda = n - n(\text{mod}\Lambda) = \Lambda\lfloor n/\Lambda \rfloor.
\]

(57)

Formula (56) shows, that the electron can wind at most \( w \) times around the chain, and then have still \( r \) steps to make to complete the path. Consequently, \( c \) can take any value between \(-w\) and \( w \),

\[
c \in \{-w, -w + 1, \ldots, w - 1, w\} \equiv C_L,
\]

(58)

but \( r \) must be an even number, and for even \( \Lambda \) only the even powers of \( \xi \) are present in the expansion of \( Z_L(\xi) \).

The number of closed paths of length \( n \) with exactly \( n^+ \) steps in the positive direction is \( \binom{n}{n^+} = n!/(n^+!n^-!) \), the summation over all allowed values of \( n^+ \) yields their total,

\[
\Gamma_L(n; \Lambda) \equiv \sum_{n^+} \frac{n!}{n^+!n^-!} = \sum_{d(n)} \frac{n!}{\lfloor \frac{1}{2}(n + d(n)) \rfloor ! \lfloor \frac{1}{2}(n - d(n)) \rfloor !}
\]

(59)
due to (54) and where values of \(d\) (or \(n^+\)) are given by (55, 58). Finally, the partition function reads

\[
Z_L(\xi, \Lambda) = \sum_{n=0}^{\infty} \Gamma_L(n, \Lambda) \xi^n = \sum_{n=0}^{\infty} \xi^n \sum_{d(n)} \frac{n!}{\left[\frac{1}{2}(n + d)!\right]\left[\frac{1}{2}(n - d)!\right]!}
\]

\[
= \sum_{n=0}^{\infty} \sum_{d(n)} \frac{\xi^n}{\left[\frac{1}{2}(n + d)!\right]\left[\frac{1}{2}(n - d)!\right]!} \equiv \sum_{n=0}^{\infty} L_n(\Lambda) \xi^n. \tag{60}
\]

Equating (60) and (53), having in mind (46), we obtain

\[
Z_L(\xi, \Lambda) = \frac{1}{\Lambda} \sum_{m(\Lambda)} \exp \left(2\xi \cos \left(\frac{2m\pi}{\Lambda}\right)\right) = \sum_{n=0}^{\infty} L_n(\Lambda) \xi^n, \tag{61}
\]

the values of \(m(\Lambda)\) are given by (47) and (48).

### 2.1.2 The case of infinite lattice

Consider now the limit \(\Lambda \to \infty\). Then no path can be closed by moving around the chain. Consequently, only terms with \(d = 0\) contribute to (59), (60) and \(n\) must be even. Defining: \(\nu = n/2\), we can write (60) as

\[
Z_L(\xi, \infty) \equiv Z_L(\xi) = \sum_{n=0,\text{even}}^{\infty} \frac{\xi^n}{(n/2)!(n/2)!} = \sum_{\nu=0}^{\infty} \frac{\xi^{2\nu}}{\nu!\nu!}. \tag{62}
\]

In the limit considered \(\text{FBZ} = [-\pi, \pi]\) and we replace the summation over \(\text{FBZ}\) by an integration (compare formula (14)). Equating two formulas for \(Z_L(\xi)\), analogously to (61) we find

\[
\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{2\xi \cos(k)} dk = \sum_{\nu=0}^{\infty} \frac{\xi^{2\nu}}{\nu!\nu!}. \tag{63}
\]

This is the equality (1) quoted in the introduction, and \(Z_L(\xi) = I_0(2\xi)\).

### 2.2 Linear chain with nearest and next-nearest neighbor hopping

Also in this paragraph we analyze the case of an infinite linear chain, so the direct and reciprocal lattice geometry are the same as in section 3.2. However, now we assume slightly more general form of the Hamiltonian, with
the nonzero values of the nearest- as well as next-nearest-neighbor hopping integrals,
\[ \hat{H}_L = \sum_i \sum_{q=-1,1} \left( t_1 c_i^\dagger c_{i+q} + t_2 c_i^\dagger c_{i+2q} \right). \] (64)

This difference results in a change in dispersion relation,
\[ \epsilon_L(k) = 2t_1 \cos(k) + 2t_2 \cos(2k), \quad k \in [-\pi, \pi] \equiv \text{FBZ}. \] (65)

In the present case the partition function depends on two variables \( \xi_1 = -\beta t_1, \) \( \xi_2 = -\beta t_2. \) Written in the quasimomentum representation it reads
\[ Z_L(\xi_1, \xi_2) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{2\xi_1 \cos(k) + 2\xi_2 \cos(2k)} dk \equiv \sum_{n_1, n_2} L_{n_1, n_2} \epsilon_1^{n_1} \epsilon_2^{n_2}. \] (66)

Let us now turn to the problem of evaluating \( Z_L(\xi_1, \xi_2) \) in coordinate representation. We start with the simple observation that there are two types of 'steps', related to hopping integrals \( t_1 \) and \( t_2. \) Their length in the real space, measured in lattice constants, is equal 1 and 2, respectively.\(^7\) Let \( n_1 \) and \( n_2 \) be the numbers of corresponding steps, with \( n = n_1 + n_2 \) being their total. In contrary to the situation in paragraph 3.2, in the present case \( n \) can be odd, but \( n_1 \) cannot, as it is impossible to close a path in such a case. Consequently, \( n_1 \) and \( n_2 \) must have the same parity, however for \( n_1 = 0, \) \( n_2 = n \) must be even.

We denote the number of steps of the real-space length \( \lambda \) in positive (negative) direction along the chain by \( n_\lambda^+ (n_\lambda^-) \) respectively. Obviously,
\[ n_\lambda = n_\lambda^+ + n_\lambda^-, \] (67)
and we also define
\[ d_\lambda = n_\lambda^+ - n_\lambda^-, \quad \lambda = 1, 2. \] (68)

In the case considered, closed paths are those, for which
\[ d_1 + 2d_2 = 0. \] (69)

To find \( \Gamma(n_1, n_2), \) let us first fix \( n_1^+, n_2^+ \) on some values permitted by (69). The number of closed paths with exactly \( n_1^+, n_2^+ \) 'positive' steps is
\[ \left( \begin{array}{l} n \\ n_1 \end{array} \right) \left( \begin{array}{l} n_1^+ \\ n_1^+ \end{array} \right) \left( \begin{array}{l} n_2^+ \\ n_2^+ \end{array} \right) = \frac{n!}{n_1^+! n_1^-! n_2^+! n_2^-!}. \] (70)

\(^7\)The Reader is warned to not confuse the length of the 'step', \( \lambda, \) with length of the path, \( n, \) being the total number of steps.
This is because we have to choose the order in which $n_1$ 'short' ($\lambda = 1$), and $n-n_1$ 'long' ($\lambda = 2$) steps appear in the path, and then choose those $n_1^+$ ($n_2^+$) of the $n_1$ ($n_2$) steps of each type, that are taken in the respective positive direction. To obtain the $\Gamma_L(n_1, n_2)$ we have to sum (70) over allowed values of $n_1^+, n_2^+$. 

Before we do that, it is convenient to express first $n_1^+, n_2^-$ through $n_\lambda, d_\lambda$ with the help of the equations (67, 68), and utilize the constraint (69) to eliminate $d_1$. The only difficulty is that permitted values of $d_2$ depend in a nontrivial way on $n_1, n_2$. To find the explicit form of this dependence, we have to consider two cases, $n_1 \geq 2n_2$ and $n_1 \leq 2n_2$. In the first case, for any value of $d_2$ ($|d_2| \leq n_2$), we are able to find such a corresponding $d_1$ that the condition (69) holds. In the case $n_1 \leq 2n_2$, value $d_{2}^{\text{max}}$ depends on $n_1$, and also on the parity, $P$, of both $\frac{1}{2}n_1$ and $n_2$, in the following way 

$$d_{2}^{\text{max}} = \frac{1}{2}n_1 \text{ if } P(\frac{n_1}{2}) = P(n_2), \quad \frac{1}{2}(n_1 - 2) \text{ otherwise.}$$

Note, that for $n_1 = 2n_2$ results for both cases coincide. Finally, we obtain the following formula for $\Gamma_L(n_1, n_2)$,

$$\Gamma(n_1, n_2) = \frac{(n_1 + n_2)!}{n_1!n_2!} \sum_{d_2} \left( \frac{n_1}{2}(n_1 - 2d_2) \right) \left( \frac{n_2}{2}(n_2 - d_2) \right), \quad (71)$$

and after simple algebra, for the coefficients of the expansion (66),

$$L_{n_1, n_2} = \sum_{d_2} \frac{1}{(\frac{1}{2}(n_1 + 2d_2))!(\frac{1}{2}(n_1 - 2d_2))!(\frac{1}{2}(n_2 + d_2))!(\frac{1}{2}(n_2 - d_2))!}. \quad (72)$$

Summation in (72) is over the elements of the set $D_2$,

$$D_2 = \{-d_{2}^{\text{max}}, -d_{2}^{\text{max}} + 2, \ldots, d_{2}^{\text{max}} - 2, d_{2}^{\text{max}}\},$$

and we recall once more the dependence of $d_{2}^{\text{max}}$ on $n_1, n_2$:

- for $n_1 \leq 2n_2$ 
  $$d_{2}^{\text{max}} = \frac{1}{2}n_1 \text{ if } P(\frac{n_1}{2}) = P(n_2), \quad \frac{1}{2}(n_1 - 2) \text{ otherwise,}$$

- for $n_1 \geq 2n_2$ 
  $$d_{2}^{\text{max}} = n_2.$$

Equation (66), combined with the explicit form of $L_{n_1, n_2}$, (72), is a central result of this section, and may be regarded as generalization of (63).

The coefficients $L_{n_1, n_2}$ have a quite complicated structure, however, there exist some relations between them. This is because, due to identity

$$\cos(2k) = 2\cos^2(k) - 1, \quad (73)$$
\( Z_L(\xi_1, \xi_2) \) obeys the following partial differential equation

\[
- \frac{\partial Z_L}{\partial \xi_2} + \frac{\partial^2 Z_L}{\partial \xi_1^2} - 2Z_L = 0. \tag{74}
\]

This implies the relations between the coefficients \( \text{(72)} \),

\[
(n_1 + 2)(n_1 + 1)L_{n_1+2,n_2} - (n_2 + 1)L_{n_1,n_2+1} - 2L_{n_1,n_2} = 0. \tag{75}
\]

### 2.3 Triangular and bcc lattices

In this section we examine two-dimensional triangular, as well as three-dimensional bcc lattices. The reason why we consider those two cases together is that the formulas giving the number of closed paths have a very similar form for both lattices. This is due to the similar geometry of triangular and bcc lattices, with the nearest neighbors of a given site forming two interpenetrating simplices in two (three) dimensions, respectively.

#### 2.3.1 Triangular lattice

Each site of an infinite triangular lattice has six nearest neighbors grouped in pairs along three lattice directions, their positions are given by \( \pm \mathbf{e}_i \),

\[
\mathbf{e}_1 = (1, 0), \quad \mathbf{e}_2 = \frac{1}{2}(-1, \sqrt{3}), \quad \mathbf{e}_3 = -\frac{1}{2}(1, \sqrt{3}). \tag{76}
\]

The reciprocal lattice of a triangular lattice is also a triangular one. The first Brillouin zone is a hexagon centered in the origin, with the vertices

\[
\pm (2\pi, -\frac{2\pi \sqrt{3}}{3}), \quad \pm (2\pi, \frac{2\pi \sqrt{3}}{3}), \quad \pm (4\pi \sqrt{3}/3, 0), \tag{77}
\]

and area equal \( 8\sqrt{3}\pi^2 \). In the Hamiltonian \( \text{(7)} \) we assume nonzero hopping integrals only between the nearest neighbors of a given site \( \mathbf{i} \). In general, we can relate a different hopping integral to each of the three lattice directions. Instead, we concentrate on the symmetric case \( t_1 = t_2 = t_3 \equiv t \), there is however no conceptual difficulty to extend the following results to the most general one. The dispersion relation reads now

\[
\epsilon_T(k_x, k_y) = 2t \cos(k_x) + 4t \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right). \tag{78}
\]

and, consequently,

\[
Z_T(\xi) = \frac{1}{8\sqrt{3}\pi^2} \int e^{\xi(2\cos(k_x) + 4\cos\left(\frac{k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right))} dk_x dk_y = \sum_n T_n \xi^n. \tag{79}
\]
Now we pass to the problem of finding $Z_T(\xi)$ in coordinate representation. We denote the number of steps in the direction given by $\pm \mathbf{e}_i$ as $\pm n_i$, with $n_i^+ + n_i^- \equiv n_i$, and define

$$d_i = n_i^+ - n_i^-,$$

(80)

Let $\Delta_x (\Delta_y)$ be the total displacement along $x$ ($y$) coordinate. We have then

$$\Delta_x = d_1 - \frac{1}{2}(d_2 + d_3), \quad \Delta_y = \frac{\sqrt{3}}{2}(d_2 - d_3),$$

(81)

and, as for a closed paths we require $\Delta_x = \Delta_y = 0$, we obtain the condition

$$d_1 = d_2 = d_3 \equiv d.$$

(82)

One can easily convince himself that maximal allowed value of $d$ is

$$d_{\text{max}} = \min(n_1, n_2, n_3).$$

(83)

The number of closed paths with exactly $n_i^+$, $n_i^-$ ‘positive’ and ‘negative’ steps in each direction is equal

$$\frac{n!}{n_1! n_2! n_3!} \left( \begin{array}{c} n_1 \\ n_1^+ \end{array} \right) \left( \begin{array}{c} n_2 \\ n_2^+ \end{array} \right) \left( \begin{array}{c} n_3 \\ n_3^+ \end{array} \right),$$

(84)

and the total number of all paths of length $n$ is then obtained by summing first over all permitted values of $n_i^+$, and then over all values $n_i = n_i^+ + n_i^-$ obeying

$$n_1 + n_2 + n_3 = n.$$

(85)

It is, however, convenient to eliminate first $n_i^+(n_i^-)$ with the help of (80), and apply the conditions (82), (83). As the result, the coefficients $T_n \equiv \tilde{\Gamma}(n)/n!$ are given by

$$T_n = \frac{1}{n!} \sum_{n_1,n_2,n_3} \frac{n!}{n_1! n_2! n_3!} \sum_d \left( \frac{1}{2}(n_1 + d) \right) \left( \frac{1}{2}(n_2 + d) \right) \left( \frac{1}{2}(n_3 + d) \right).$$

(86)

The first summation in (86) is taken over those $n_1, n_2$ and $n_3$ which satisfy condition (85). What is more, $n_1, n_2$ and $n_3$ must have the same parity, for even $n$ all $n_i$ are even, whereas for odd $n$ all $n_i$ must be odd, too. This reflects the fact, that any closed path can be regarded as combination of a number of elementary paths of the two kinds: first, with $n = 2$, is a step forward and step backward in some direction, the second, with $n = 3$, consists of one step in each direction. The second summation runs over
\[ d \in \{-d_{\text{max}}, -d_{\text{max}} + 2, \ldots, d_{\text{max}} - 2, d_{\text{max}}\}. \]  

In formula (86) some factorials cancel, and we finally obtain

\[
T_n = \sum_{n_1,n_2,n_3} \sum_d \prod_{i=1}^3 \frac{1}{\frac{1}{2}(n_i + d)! \left( \frac{1}{2}(n_i - d)! \right)!}. \tag{87}
\]

Explicitly computing \( Z_T(\xi) \) up to sixth order using the above formula, we obtain

\[
Z_T(\xi) = 1 + 3\xi^2 + 2\xi^3 + \frac{15}{4}\xi^4 + 3\xi^5 + \frac{17}{6}\xi^6 + \mathcal{O}(\xi^7). \tag{88}
\]

This coincides with the result obtained by integration of the expansion of the exponent in (79) to the same order in \( \xi \).

### 2.3.2 Bcc (body centered cubic) lattice

This case is in many respects very similar to the just examined triangular lattice, with the main difference being higher dimensionality of the bcc lattice. Each lattice site has now eight, instead of six, nearest neighbors, given by vectors \( \pm \mathbf{e}_i \),

\[
\begin{align*}
\mathbf{e}_1 &= \frac{1}{2}(1,1,1), & \mathbf{e}_2 &= \frac{1}{2}(-1,-1,1), \\
\mathbf{e}_2 &= \frac{1}{2}(-1,1,-1), & \mathbf{e}_4 &= \frac{1}{2}(1,-1,-1). \tag{89}
\end{align*}
\]

Similarly to the case of triangular lattice, non-zero hopping integrals are assumed only between nearest neighbors, and we put all of them equal, \( t_1 = t_2 = t_3 = t_4 \equiv t \) (consequently, \( \xi_1 = \xi_2 = \xi_3 = \xi_4 \equiv \xi \)). Reciprocal lattice of the bcc lattice is the fcc lattice (see [3], p. 74), the first Brillouin zone is regular rhombic dodecahedron with the volume \( V = 16\pi^3 \). The dispersion relation is

\[
\epsilon_{\text{bcc}}(k_x, k_y, k_z) = 8t \cos(\frac{k_x}{2}) \cos(\frac{k_y}{2}) \cos(\frac{k_z}{2}), \tag{90}
\]

and the partition function in \( \mathbf{k} \)-representation reads

\[
Z_{\text{bcc}}(\xi) = \frac{1}{16\pi^3} \int e^{8\xi \cos(\frac{k_x}{2}) \cos(\frac{k_y}{2}) \cos(\frac{k_z}{2})} dk_x dk_y dk_z \equiv \sum_n \mathcal{B}_n \xi^n. \tag{91}
\]

The coefficients \( \mathcal{B}_n \) are obtained in a way very similar to those for the triangular lattice, also the notation is analogous and self-explanatory, we skip the derivation then and present only final results. \( \mathcal{B}_n \) are given by

\[
\mathcal{B}_n = \frac{1}{n!} \sum_{n_1,n_2,n_3,n_4} \frac{n!}{n_1!n_2!n_3!n_4!} \sum_d \prod_{i=1}^4 \left( \frac{n_i}{\frac{1}{2}(n_i + d)} \right). \tag{92}
\]
The first summation in (92) is taken over those $n_1, n_2, n_3, n_4$ which satisfy the condition $n_1 + n_2 + n_3 + n_4 = n$, where $n_i$ is a number of steps in the direction given by $\pm \mathbf{e}_i$. Likewise in the previous section, all $n_i$ must have the same parity, which implies that $n$ must be even in the present case. The second summation runs over the elements of the set

$$\mathcal{D}_{b cc} = \{-d_{\text{max}}, -d_{\text{max}} + 2, \ldots, d_{\text{max}} - 2, d_{\text{max}}\}$$

(93)

where

$$d_{\text{max}} = \min(n_1, n_2, n_3, n_4).$$

(94)

After obvious simplifications, we finally obtain

$$B_n = \sum_{n_1, n_2, n_3, n_4} \sum_{d} \prod_{i=1}^{4} \frac{1}{(\frac{1}{2}(n_i + d))!((\frac{1}{2}(n_i - d))!}}.$$  

(95)

Explicit evaluation of $Z_{b cc}(\xi)$ up to twelfth order in $\xi$, either using the formula (95) or by numerical integration of (91), gives the expansion

$$B(\xi) = 1 + 4\xi^2 + 9\xi^4 + \frac{100}{9}\xi^6 + \frac{1225}{144}\xi^8 + \frac{441}{100}\xi^{10} + \frac{5929}{3600}\xi^{12} + \mathcal{O}(\xi^{14}).$$

(96)

Interestingly, for $n \leq 30$ all $B_n$ are squares of rational numbers. The question arises, is this true for all values of $n$? However, at the moment we are not able to prove this conjecture or to find counterexample.

### 2.4 Honeycomb and diamond lattices

Likewise in the previous section, here we also analyze together two lattices, namely the two-dimensional honeycomb (graphene) lattice and three-dimensional diamond lattice. Once again, the reason is the similar geometry of both lattices, in the present case three (four) nearest-neighbors of a given site form a two (three) dimensional simplex, respectively. This results in a very similar form of the Taylor series expansion for the partition function in this two cases. Both honeycomb and diamond are non-Bravais lattices, with the basis consisting of $M = 2$ atoms, we denote the resulting two sublattices $A$ and $B$, respectively. As a consequence, evaluation of the partition function in quasimomentum representation is not that straightforward as in the Bravais ($M = 1$) case. However, this is a standard textbook problem, so we omit the detailed explanations. What is important, our method applies here without any serious modification.
2.4.1 Honeycomb lattice

The nearest neighbors of any lattice site $j \in A$ of an infinite honeycomb lattice are given by vectors

$$e_1 = (0, -\frac{\sqrt{3}}{3}), \quad e_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{6}\right), \quad e_3 = \left(-\frac{1}{2}, \frac{\sqrt{3}}{6}\right).$$

(97)

whereas the neighbors of site $i \in B$ by $-e_1, -e_2, -e_3$. Because honeycomb lattice is, in fact, a triangular Bravais lattice with two-site atomic basis, its reciprocal lattice is also a triangular lattice, identical to that considered in section 5.1, due to the particular choice of vectors (97). Consequently, also the first Brillouin zone is the same, i.e. it is a hexagon given by (77).

In the Hamiltonian (7) the non-zero values of the hopping integrals are assumed only to three nearest neighbors of a given site, and we put them equal. In the present case the dispersion relation consist of $M = 2$ subbands,

$$\epsilon_{G,\sigma}(k_x, k_y) = \sigma t \sqrt{3 + 2 \cos(k_x) + 4 \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right)},$$

(98)

where $\sigma = -1$ ($\sigma = 1$) refers to lower (higher) subband, respectively. To evaluate the partition function we have to integrate states within each subband, and than to add contributions from both of them. Then

$$Z_G(\xi) = \frac{1}{8}\sqrt{3} \pi^2 \int_{FBZ} \sum_{\sigma = -1, 1} e^{\xi \sqrt{3 + 2 \cos(k_x) + 4 \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{\sqrt{3}k_y}{2}\right)}} dk_x dk_y = \frac{1}{4}\sqrt{3} \pi^2 \int_{FBZ} \cosh \left(\xi \epsilon_{G,1}(k_x, k_y)\right) dk_x dk_y \equiv \sum_n G_n \xi^n. \quad (99)$$

Now let us evaluate $Z_G(\xi)$ in Wannier basis. We have $\Xi = M\Lambda = 2\Lambda$, terminal vertex $j$ of any closed path may belong either to sublattice $A$ or $B$. Those two cases are equivalent with respect to the way we compute the number of closed paths, the only consequence is an additional factor 2.

In order to close the path, the number of steps in each of three lattice directions, taken form $A$ to $B$ must be equal to that of steps form $B$ to $A$, consequently a path must be of the form $A \to B \to A \to \ldots \to B \to A$. Denote the number of steps, taken from $j \in A$ in the $i$-th direction (i.e. given by $\pm e_i$) as $p_i$. To find $\Gamma(n)$ we have to choose those $p_i$ of the total $p$ steps $A \to B$ that are taken in $i$-th direction, and then independently do the same for steps $B \to A$. The resulting number is equal $\left(p!/\left(p_1!p_2!p_3!\right)\right)^2$. Summing
over all values of $p_1, p_2, p_3$, which in the present case are of arbitrary parity, but obey the constraint $p_1 + p_2 + p_3 = p \equiv n/2$, we obtain
\begin{equation}
\tilde{\Gamma}_G(n) = 2 \sum_{p_1, p_2, p_3} \left( \frac{p!}{p_1!p_2!p_3!} \right)^2 = n!G_n \tag{100}
\end{equation}
where the factor 2 was included according to the previous discussion. Using formula (100) we find the coefficients $G_n$ for $n \leq 6$. This gives us
\begin{equation}
G(\xi) = 2 + 3\xi^2 + \frac{5}{4}\xi^4 + \frac{31}{120}\xi^6 + \mathcal{O}(\xi^8). \tag{101}
\end{equation}
This is precisely what one gets expanding (99) up to sixth order in $\xi$ and doing the remaining integrations.

### 2.4.2 Diamond lattice

Diamond lattice is related to the honeycomb lattice in very much the same way as bcc to the triangular one. It can be regarded as a fcc (face centered cubic) lattice with two-atom basis, and thus two sublattices, $A$ and $B$. Consequently, the first Brillouin zone is that of fcc lattice, namely truncated octahedron, its volume is $V = 32\pi^3$ (see [3], p. 76, with $a = 1$). Each site of sublattice $A$ ($B$) has four neighbors, their positions are given by $e_i$ ($-e_i$), respectively, where $e_i$ vectors are the following
\begin{equation}
e_1 = \frac{1}{4}(1, 1, 1), \quad e_2 = \frac{1}{4}(-1, -1, 1), \quad e_2 = \frac{1}{4}(-1, 1, -1), \quad e_4 = \frac{1}{4}(1, -1, -1). \tag{102}
\end{equation}
Likewise in the honeycomb lattice case, the dispersion relation consist of two subbands labeled by $\sigma = -1, 1$; it is related to the dispersion relation of the fcc lattice as follows,
\begin{equation}
\epsilon_D(\kappa_x, \kappa_y, \kappa_z) = \sigma t \sqrt{4 + 4\epsilon_{\text{fcc}}(\kappa_x, \kappa_y, \kappa_z)} \tag{103}
\end{equation}
where
\begin{equation}
\epsilon_{\text{fcc}}(\kappa_x, \kappa_y, \kappa_z) = 4t \left( \cos \frac{k_x}{2} \cos \frac{k_y}{2} + \cos \frac{k_x}{2} \cos \frac{k_z}{2} + \cos \frac{k_y}{2} \cos \frac{k_z}{2} \right). \tag{104}
\end{equation}
The resulting partition function is then
\begin{align}
Z_D(\xi) &= \frac{1}{32\pi^3} \int_{FBZ} \sum_{\sigma = -1} e^{\sigma\xi\sqrt{4 + 4\epsilon_{\text{fcc}}(\kappa_x, \kappa_y, \kappa_z)}} d\kappa_x d\kappa_y d\kappa_z \equiv \sum_n D_n \xi^n \\
&= \frac{1}{16\pi^3} \int_{FBZ} \cosh(\xi\sqrt{4 + 4\epsilon_{\text{fcc}}(\kappa_x, \kappa_y, \kappa_z)}) d\kappa_x d\kappa_y d\kappa_z. \tag{105}
\end{align}
The way we compute the number of closed paths in the present case directly follows the case of honeycomb lattice, with the only difference that now we have three, instead of two, spatial dimensions. We have then

$$\tilde{\Gamma}_D(n) = 2 \sum_{p_1, p_2, p_3, p_4} \left(\frac{p_1!}{p_1!p_2!p_3!p_4!}\right)^2 = n!G_n,$$  \hspace{1cm} (106)

where \( n_i = 2p_i \), \( i = 1, \ldots, 4 \), \( n = 2p \), and \( p \) is constrained by \( \sum_{i=1}^{4} p_i = p \), but again each \( p_i \) may be of arbitrary parity, and the factor 2 appears due to the number of equivalent sublattices. \( Z_D(\xi) \) expanded up to eighth order in \( \xi \), reads explicitly

$$2 + 4\xi^2 + \frac{7}{3}\xi^4 + \frac{32}{45}\xi^6 + \frac{97}{720}\xi^8 + \mathcal{O}(\xi^{10}).$$  \hspace{1cm} (107)

3 Appendices

3.1 Appendix A. One to one correspondence between the terms given by the formula (30) and respective closed paths

In this paragraph we give a simple justification of the fact, that there is a one to one correspondence between terms (30) and closed paths they generate.

Clearly, any term (30) leads to some path. We have to show that different such terms correspond to different paths. Let us consider some term in question,

$$A_{i_1i_n} A_{i_ni_{n-1}} \cdots A_{i_{k+1}i_k} A_{i_ki_{k-1}} A_{i_{k-1}i_{k-2}} \cdots A_{i_{j+1}i_j} A_{i_ji_{j-1}} A_{i_{j-1}i_{j-2}} \cdots A_{i_{2i_1}},$$  \hspace{1cm} (108)

and assume, that apart from the above, there exist some other ordering of its \( n \) \( A_{ij} \) operators, which gives the same closed path. Any such ordering may be obtained by some permutation of \( A_{ij} \) operators in formula (108), it is enough then to examine the case of a transposition. Let us swap \( A_{ik_{k-1}} \) and \( A_{ij_{j-1}} \), assuming first that \( A_{ij_{j-1}} \neq A_{i_{2i_1}} \) and \( A_{ik_{k-1}} \neq A_{i_{i_n}} \),

$$A_{ii_{i_n}} A_{i_{i_n}i_{n-1}} \cdots A_{i_{k+1}i_k} A_{i_{j-1}i_{j-1}} A_{i_{k-1}i_{k-2}} \cdots A_{i_{j+1}i_j} A_{i_{k_{k-1}}i_{k_{k-1}}} A_{i_{j-1}i_{j-2}} \cdots A_{i_{2i_1}}.$$  \hspace{1cm} (109)

Obviously if \( A_{ik_{k-1}} = A_{ij_{j-1}} \), this transposition does not affect (108), yielding identical term. In the opposite case, after writing some \( A_{ij} \) operators in terms of creation and annihilation operators, (109) reads

$$A_{ii_{i_n}} A_{i_{i_n}i_{n-1}} \cdots A_{k+i_{k}} c^+_i c_{j-1} A_{i_{k-1}i_{k-2}} \cdots c^+_i c_{j+1} A_{ik_{k-1}} A_{i_{j-1}i_{j-2}} \cdots A_{i_{2i_1}}.$$  \hspace{1cm} (110)
There are two possibilities now: either some operators in between $c_{ij}^\dagger$ and $c_{ij}$ carry site index $i$ or this index does not appear there. In the former case, after commuting some operators, a part of the term (109) has the form

\[
\cdots \cdot c_{ij}^\dagger (1-n_{ij})c_{ij} \cdots = \cdots c_{ij}^\dagger c_{ij} \cdots = \cdots n_{ij} \cdots ,
\]

in the latter case that part also reduces to $\cdots c_{ij}^\dagger c_{ij} \cdots = \cdots n_{ij} \cdots$. Consequently, in both cases the whole term (109) vanishes, due to the fact that we compute trace using one-particle states only. The same reasoning applies to the reversal of order in which $c_{ik}^\dagger$ and $c_{ik}$ appear in (109).

If one, but not both, of the permuted operators is $A_{i_2i_1}$ or $A_{i_1i_n}$ the above reasoning applies without a modification. Finally, if we interchange $A_{i_2i_1}$ with $A_{i_1i_n}$, in order to obtain the non-zero term, $i_2 = i_n$ must hold. But then we obtain the path with terminal vertex $i_2 \neq i_1$, so different from our point of view.

### 3.2 Appendix B. Linear chain of atoms with complex nearest-neighbor hopping integrals

Consider the case analyzed in section 2.1 but let the hopping integral be an arbitrary complex number, $t = |t|e^{i\phi}$. This leads to a modified dispersion relation,

\[
\epsilon_L(k, \phi) = 2|t| \cos (k + \phi).
\] (111)

Consequently, the partition function is given by

\[
Z_L(\rho, \phi, \Lambda) = \frac{1}{\Lambda} \sum_{k \in FBZ} \exp \left( -2\rho \cos (k + \phi) \right),
\] (112)

where $\xi = -\beta t = -\rho e^{i\phi}$ and $\rho = |\xi|$. $Z_L(\rho, \phi, \Lambda)$ is obviously real, periodic function of $\phi$ with a period $2\pi$. Expanded in a Fourier series it reads

\[
Z_L(\rho, \phi, \Lambda) = \sum_{p=-\infty}^{\infty} C_p(\rho) e^{ip\phi}, \quad C_p^*(\rho) = C_{-p}(\rho).
\] (113)

On the other hand, from the way we compute $Z_L$ in coordination representation, it is clear that each step in a positive (negative) direction brings a factor $e^{i\phi}$ ($e^{-i\phi}$), respectively, and that each path is characterized by a total phase $\phi d$,

\[
Z_L(\rho, \phi, \Lambda) = \sum_{n=0}^{\infty} \sum_{d(n)} (-\rho)^n (e^{i\phi})^d \frac{1}{n!} \frac{1}{(n-d)!}.
\] (114)

This shows, that in the expansion (113) the only nonzero terms are those with $p = d = c\Lambda$, and $d$ given by (55, 58). Comparing (114) and (113), we
see that $C_d(\rho) = C_{-d}(\rho)$, and that (113) can be rewritten as

$$Z_L(\rho, \varphi, \Lambda) = a_0(\rho) + \sum_{d(n)>0} a_d(\rho) \cos(\varphi d),$$

where

$$a_0(\rho) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \sum_{k \in \text{FBZ}} e^{-2\rho \cos(k+\varphi)} d\varphi = \sum_{n=0}^{\infty} \frac{(-\rho)^n}{\left(\frac{1}{2}n\right)!^2},$$

$$a_d(\rho) = \frac{1}{\pi \Lambda} \int_{-\pi}^{\pi} \sum_{k \in \text{FBZ}} e^{-2\rho \cos(k+\varphi)} \cos(\varphi d) d\varphi = \sum_{n=0}^{\infty} \frac{2(-\rho)^n}{\left[\frac{1}{2}(n+d)\right]! \left[\frac{1}{2}(n-d)\right]!}.$$

Assume now even $\Lambda$, then $n = 2\nu$, $d = 2\delta$. Equating (114) to (115) and having in mind (116, 117) we obtain the following generalization of (61),

$$\sum_{k \in \text{FBZ}} \frac{\exp(-2\rho \cos(k+\varphi))}{\Lambda} = \sum_{\nu=0}^{\infty} \left(\frac{1}{\nu!^2} + 2 \sum_{\delta(\nu)>0} \frac{\cos(2\delta \varphi)}{[(\nu+\delta)]! [(\nu-\delta)]!}\rho^{2\nu}\right) = \sum_{\nu=0}^{\infty} \left(\sum_{\delta(\nu)} \frac{\cos(2\delta \varphi)}{[(\nu+\delta)]! [(\nu-\delta)]!}\rho^{2\nu}\right).$$

If we put $\varphi = \pi$ in the above formula we obtain the results given by (60, 61). On the other hand, for $\varphi = \frac{\pi}{2}$ we have $\cos(2\delta \varphi) = \cos(\delta \pi) = (-1)^\delta$ and then

$$\frac{1}{\Lambda} \sum_{k \in \text{FBZ}} \exp(2\rho \sin(k)) = \sum_{\nu=0}^{\infty} \left(\sum_{\delta(\nu)} \frac{(-1)^\delta}{[(\nu+\delta)]! [(\nu-\delta)]!}\rho^{2\nu}\right).$$

Summary and conclusions

In this paper we have presented the method of evaluating the partition function of a single-electron, periodic system, using specific basis, in which the system Hamiltonian is not diagonal. Utilizing the symmetry properties of the system and its Hamiltonian, as well as invariance of trace operation with respect to change of the basis in the Hilbert space, we are able to establish several mathematical identities. They could be found important from the point of view of both pure and computational mathematics.

The possible extensions of the present works include first analysis of infinite lattices not examined yet, like fcc or kagome lattice, as well as detailed investigation of finite lattices for geometries more complicated than that of linear chain, and also for various PBC. The extension of the method to many-electron systems or systems without translational invariance is also possible in principle, but the technical difficulties that arise make the application of combinatorial techniques very problematic in these cases.
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