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Quantum particles and Gaussian model on graphs

P.F. Buonsante*, R. Burioni, D. Cassi, I. Meccoli,
S. Regina, A. Vezzani

Istituto Nazionale di Fisica della Materia, Dipartimento di Fisica, Università di Parma,
Parco Area delle Scienze 7a, I-43100 Parma, Italy

Abstract

A quantum particle on a general discrete structure with a local external potential is described by a generalized tight-binding Hamiltonian on a graph. Here, we show that this model can be naturally mapped on a classical statistical model (the Gaussian model) on the same graph. This equivalence provides not only a powerful technical tool for model solving, but it also puts into evidence general fundamental properties of quantum inhomogeneous systems. © 2000 Published by Elsevier Science B.V. All rights reserved.

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1. Introduction

The electronic properties of real non-crystalline structures such as glasses and polymers can be dramatically different from the correponding ones on crystals. This is mainly due to the lack of translation invariance and of its mathematical consequences: a reciprocal lattice cannot be defined, Fourier transform becomes unuseful and geometry-induced localization can take place, with a deep effect on transport. The geometry of these systems is no longer described by a lattice, but by a generic network, i.e., a graph, and the usual lattice models have to be replaced with models on graphs. This extension is in general non-trivial and even the simplest Hamiltonian can exhibit exotic behaviours. This is the case for the tight-binding model we will consider in the following [1]. The study of such a simple Hamiltonian, which on a lattice can be easily diagonalized by Fourier transform, on a graph requires alternative techniques. Here, we propose a new approach based on an exact mapping on the Gaussian model, a classical

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* Corresponding author. Fax: +39-0521 905223.

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statistical model whose properties are well known and which can be analytically studied by combinatorial techniques.

2. The generalized tight-binding Hamiltonian on a graph

The tight-binding approximation (see e.g. Ref. [2]) is commonly used to describe a quantum particle on a discrete structure. The generic Hamiltonian can be written as the sum of the kinetic energy and the potentials generated by the atoms of the structure:

$$H^{(I)} = \frac{p^2}{2m} + \sum_i V_i(\boldsymbol{r}) \,. \tag{1}$$

We shall assume that near each site i the potential term can be approximated by the atomic potential V_i of the atom at the same site i. This assumption is appropriate when the distance between two sites is greater than the typical atomic dimensions or when the atomic orbitals contributing to the conduction are very narrow (as the d or f orbitals, in transition metals). In this case, the electronic wave function can be written as a superposition of atomic orbitals, whose coefficients depend on the geometry of the structure:

$$\psi(\boldsymbol{r}) = \sum_i \phi_i(\boldsymbol{r} - \boldsymbol{R}_i) b_i \,, \tag{2}$$

where $\phi_i(\boldsymbol{r} - \boldsymbol{R}_i)$ is the orbital of the atom at site i.

Now, we obtain the tight-binding model assuming the atomic orbitals to overlap only if the corresponding sites are nearest neighbours, or adjacent. The adjacency relation is the only surviving information about the geometry of the original system. It can be algebraically expressed introducing the *adjacency matrix* A_{ij} defined by $A_{ij} = 1$ if i and j are nearest neighbours and $A_{ij} = 0$ otherwise. The adjacency matrix is the starting point of algebraic graph theory and the abstract structure consisting of points i and links connecting them pairwise when $A_{ij} = 1$ is defined to be a *graph* G.

This formalism is particularly useful in deriving the form of the second quantization Hamiltonian for the electron on a discrete structure (see e.g. Ref. [3]). In this case the coefficients of the linear combination of atomic orbitals (2) are replaced by operators of annihilation or creation of a particle on site i:

$$\hat{\psi}(\boldsymbol{r}) = \sum_i \phi_i(\boldsymbol{r} - \boldsymbol{R}_i) \hat{c}_i \,. \tag{3}$$

In this way, we have

$$H^{(II)} = \int \mathrm{d}\boldsymbol{r}\, \hat{\psi}^\dagger(\boldsymbol{r}) H^{(I)} \hat{\psi}((\boldsymbol{r})) = \sum_{i,j} B_{ij} \hat{c}_i^\dagger \hat{c}_j \,. \tag{4}$$

The coefficient B_{ij} in Eq. (4) is to be evaluated in the tight-binding approximation previously described. Assuming again that the superposition between orbitals and atomic potentials is negligible if the corresponding sites are not nearest neighbours, one obtains

$$B_{ij} = a_i \delta_{ij} + t_{ij} A_{ij} \,, \tag{5}$$

where the hopping coefficients $t_{ij} = t_{ji}$ and the diagonal terms a_i are determined by the atomic potentials and by the overlap integrals.

When the structure is homogeneous, all sites are equivalent and both t_{ij} and a_i are constant. This implies in particular that the diagonal term can be dropped so that one recovers the usual form of the tight-binding Hamiltonian. In a more general case, where the structure is inhomogeneous, a local term always appears in the generalized tight-binding Hamiltonian (GTBH), acting as an effective potential generated by the inhomogeneities of the structure. Obviously in this formulation we can also include the case of a local external potential of arbitrary form, simply by changing the expression of the diagonal term a_i.

3. The Gaussian model on a graph

Let us consider a Gaussian model with bounded, positive, nearest-neighbour couplings on a graph G. Its Hamiltonian has the form

$$H = \frac{1}{4} \sum_{i,j \in G} J_{ij}(\phi_i - \phi_j)^2 + \frac{1}{2} \sum_{i \in G} m_i^2 \phi_i^2 , \qquad (6)$$

where $0 < \varepsilon \leqslant J_{ij} \leqslant K < \infty$ if (i,j) is a link of the graph, $J_{ij} = 0$ otherwise, and the m_i^2 are real positive parameters called squared masses of the field ϕ_i, defined on the sites of the graph. If we introduce the matrices $M_{ij} \equiv m_i \delta_{ij}$ and $Z_{ij} \equiv z_i \delta_{ij}$, where $z_i \equiv \sum_j J_{ij}$, we can write Hamiltonian (6) as

$$H = \frac{1}{2} \sum_{i,j \in G} \phi_i (L + M^2)_{ij} \phi_j , \qquad (7)$$

where $L = Z - J$ is the generalized Laplacian matrix. According to the Boltzmann statistical weight $\exp[-H(\phi)]$ the two points correlation function has the form $\langle \phi_i \phi_j \rangle = (L + M^2)^{-1}_{ij}$. Let us prove that such a function may be expanded as a sum over the paths connecting the sites i and j, C_{ij} [4]. This can be done by observing that

$$\langle \phi_i \phi_j \rangle = (Z + M^2 - J)^{-1}_{ij} = \frac{1}{z_j + m_j^2} \sum_{n=0}^{\infty} [(Z + M^2)^{-1} J]^n_{ij} . \qquad (8)$$

Of course, we can write the generic entry of the matrix $[(Z + M^2)^{-1} J]^n$ as a chained product of n entries of $(Z + M^2)^{-1} J$, summed over the intermediate entry indices. Since the entries of the latter matrix are different from zero only if their indices refer to nearest-neighbour sites, the chained product does not vanish only if the intermediate indices refer to sites belonging to the same n-link path joining the sites associated to the external indices. Thus, we can write

$$[(Z + M^2)^{-1} J]^n_{ij} = \sum_{C^n_{ij}} \prod_{(h,k) \in C^n_{ij}} \frac{J_{hk}}{z_h + m_h^2} , \qquad (9)$$

where C^n_{ij} denotes a generic n-link path joining the sites i and j. Inserting Eq. (9) into Eq. (8) we get

$$\langle \phi_i \phi_j \rangle = \frac{1}{z_j + m_j^2} \sum_n \sum_{C^n_{ij}} \prod_{(h,k)\in C^n_{ij}} \frac{J_{hk}}{z_h + m_h^2} \equiv \sum_{C_{ij}} \frac{J_{C_{ij}}}{\mu_{C_{ij}}}\,, \tag{10}$$

where we have introduced

$$J_{C_{ij}} \equiv \prod_{(h,k)\in C_{ij}} J_{hk}, \qquad \mu_{C_{ij}} \equiv \prod_{k\in C_{ij}} \frac{1}{z_k + m_k^2}\,. \tag{11}$$

By expression (10), we can write any two-point correlation function as a sum over the paths joining the associated sites, as we anticipated above. Every term of the sum, corresponding to a single path, is the ratio of the two quantities defined in Eq. (11), which are both path dependent.

4. Walk expansion and equivalence

We now describe a general procedure for calculating the Green's functions for the GTBH:

$$H = \sum_{i,j} A_{ij} t_{ij} c_i^\dagger c_j + \sum_i a_i c_i^\dagger c_i \equiv H_{\mathrm{HOP}} + H_{\mathrm{AT}}\,. \tag{12}$$

The solution of this problem is straightforward when the graph is translationally invariant. However, on a general graph a local term appears which can assume different values on different sites and the transformation diagonalizing the adjacency matrix can be very difficult to determine. On the other hand, the model describes non-interacting particles so that all the vertices can always be written as a product of one-particle Green's functions.

The procedure we present below does not require the explicit form of the diagonalization transform and it exploits the property that the particles described in Eq. (12) are non-interacting. Our technique consists of a complete resummation of the perturbative expansion in the hopping parameter (Fig. 1). One starts by considering the diagonal "atomic Hamiltonian" $H_{\mathrm{AT}} = \sum_i a_i c_i^\dagger c_i$ and the corresponding Green's functions

$$G^{(0)}_{ij}(\omega) = \delta_{ij} A_i(\omega) = \frac{1}{\omega - a_i + i\varepsilon\,\mathrm{sgn}(\omega)}\,. \tag{13}$$

The generic term of order n of the perturbation expansion in the hopping parameter for $G_{ij}(\omega)$ is constructed as follows. One considers a generic n-steps walk joining the sites i and j: it is a sequence of $n+1$ nearest-neighbours sites, the first is i and the last is j. For every link (l,m) in the walk, the corresponding hopping term t_{lm} is inserted; for every visited site l the corresponding atomic Green's function $A_l(\omega)$ is introduced. The complete nth-order term is obtained by summing over the all possible n-steps walks:

$$G^{(n)}_{ij}(\omega) = \sum_{C^n_{ij}} \prod_{(h,k)\in C^n_{ij}} t_{hk} \prod_{h\in C^n_{ij}} A_h(\omega)\,. \tag{14}$$

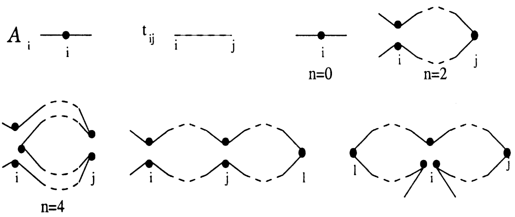

Fig. 1. A diagramatic representation of the perturbative expansion for the Green's function in the hopping parameter.

Obviously, the exact Green's function is obtained summing over all lenghts n of the walks:

$$G_{ij}(\omega) = \sum_{C_{ij}} \prod_{(h,k)\in C_{ij}} t_{hk} \prod_{h\in C_{ij}} A_h(\omega)\,. \tag{15}$$

Comparing Eqs. (10) and (15), it is now clear that the correlation functions of the Gaussian model on a graph and the Green's function for a quantum particle moving on the same structure are deeply related. More explicitly, we identify the quantities relative to the two models. The hopping term t_{ij} of the tight-binding Hamiltonian can be identified with the coupling constant J_{ij} of the Gaussian model, while the factor $1/(z_i + m_i^2)$ in Eq. (10) is naturally identified with the atomic Green function (13).

5. Conclusions

The exact mapping between tight-binding Green's functions and Gaussian model correlation functions provides an interesting parallel between quantum and classical systems and it opens a new perspective for analytic solutions of electron models on general discrete networks. Indeed, analytic expressions for Gaussian correlation functions can be determined on a large class of graphs by combinatorial and random walks techniques. As a first step, this mapping has provided a complete exact solution for tight-binding models on some simple but very interesting tree graphs (comb graphs) [1] whose non-trivial geometry has strong effects on spectral and eigenstates properties. Comb graphs are a particular case of a larger class of bundled structures where closed expressions for the Green's functions have been obtained by the Gaussian approach and this technique appears to be very useful for future developement in the study of quantum particles properties on inhomogeneous networks.

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