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BRIEF COMMUNICATION

Another form of the transmission function

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Abstract The transmission function describes the passage of the electric current from one point of an electric circuit to another. By now, this is also applied to molecules which are potential candidates for uses in the molecular electronics. We mean the modern branch of electronics which has a goal of reducing the sizes of its devices down to molecular ones and planning indeed to apply single molecules as conducting wires and functional components of microcircuits. For calculating the transmission function, some authors utilize the well-known idea of representing a molecule by a (molecular) graph, which allows them to apply for treating the latter also powerful methods of spectral graph theory. For instance, we refer to the paper by Fowler et al. (Chem Phys Lett. 465 2008) 142–146, where one such expression for this function is given. Our objective is to demonstrate that the same calculational result can be obtained using a different set of characteristic polynomials of graphs (which also slightly reduces a mathematical notation). Specifically, we apply one theorem of Kolmykov to the basic formula derived by these authors.

Keywords Molecular electronics · Transmission function · Molecular graph · Characteristic polynomial · Spectral theory of graphs · Theorem of Kolmykov

1 Introduction

In the theory of electric circuits, the *transmission function* describes the passage of electric current between two selected points of a circuit. By now, this has also been applied to molecules. The governing idea for the microminiaturization of electronic

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devices is to reduce sizes of these devices down to molecular ones. To this end, many molecules are now viewed as potential candidates to become microwires, microresistors, and other functional components of microcircuitry.

This process also touches upon mathematical tools which may better serve for such goals. Our attention is first of all attracted by formulae which utilize spectral theory of graphs. Herein, we modify one already known formula using a theorem by Kolmykov and some other technics.

Let $G = (V; E)$ be a finite connected graph with vertex set V and edge set E; $|V| = n$; $|E| = m$. Specifically, in a molecular graph $G(M)$, the set V represents atoms, and E does chemical bonds of a respective molecule M. In general, molecular graphs admit multiple edges and also selfloops depicting valence electrons. The *adjacency matrix* $A = [a_{jk}]_{j,k=1}^{n}$ of a simple molecular graph has an entry

$$a_{jk} = \begin{cases} 0, & \text{if } j \text{ and } k \text{ are not connected by a chemical bond;} \\ 1, & \text{if } j \neq k \text{ and atoms } j \text{ and } k\text{are connected with a chemical bond.} \end{cases} \tag{1}$$

Below, we consider also graphs with weighted selfloops, which demands to introduce nonzero quantities for diagonal entries of the adjacency matrix. (Notice that the formalism of weighted selfloops can be reduced here to considering just weighted vertices, since both approaches produce the same adjacency matrix.)

To us, of great importance is the characteristic polynomial $P(A; x) = \det(xI - A)$ of the adjacency matrix A (having here only 0s and 1s as nondiagonal entries), where I is a diagonal unit matrix. In spectral theory of graphs [1], the characteristic polynomial $P(G; x)$ of a graph G is defined as $P(A; x)$.

Now, introduce the following (standard) notation [1]: $G_{-\alpha}$, $G_{-\alpha\beta}$, $G_{-\alpha-\beta}$, $G_{+\alpha\beta}$ which consecutively denote a graph G less its vertex α, less its edge $\alpha\beta$ (but not the endpoints, if G has and edge $\alpha\beta$), less endpoints α and β with all incident edges, and the graph G with added edge $\alpha\beta$ if this had not earlier been in G; $1 \le \alpha, \beta \le n$.

The conductance $g_{\alpha\beta} = \frac{2e^2}{\hbar} T_{\alpha\beta}(\varepsilon)$ between two sites α and β in a molecular network [2] depends on the *transmission function*, or *transmission coefficient* $T_{\alpha\beta}(\varepsilon)$ [3,4]. According to expression (1) in [5], the transmission function $T_{\alpha\beta}(\varepsilon)$ between two atoms of a molecule without a bond connecting them (or between two disconnected vertices α and β of the respective molecular graph) is written down as

$$T_{\alpha\beta}(\varepsilon) = \frac{\sin q_\alpha \sin q_\beta \, (\tilde{u}\tilde{t} - \tilde{s}\tilde{v})}{|e^{i(q_\alpha + q_\beta)}\tilde{s} - e^{iq_\beta}\tilde{t} - e^{iq_\alpha}\tilde{u} + \tilde{v}|^2}, \tag{2}$$

where q_α and q_β are the wavevectors of the electron orbitals (with energy ε) in left and right contacts, respectively, while $\tilde{s} := P(G; x)$, $\tilde{t} := P(G_{-\alpha}; x)$, $\tilde{u} := P(G_{-\beta}; x)$, and $\tilde{v} = P(G_{-\alpha-\beta}; x)$.

In this paper, we deal first with a fragment of the last formula, *viz.:*

$$\Omega := \tilde{u}\tilde{t} - \tilde{s}\tilde{v} \equiv P(G_{-\alpha}; x)P(G_{-\beta}; x) - P(G; x)P(G_{-\alpha-\beta}; x). \tag{3}$$

Here, we turn to the next section, where the expression Ω will be given in a modified, slightly reduced form.

2 The main part

Kolmykov proved the following [6,7]:

Theorem 1 *Let* $G,\ G_{+\alpha\beta},\ G_{\alpha\beta},\ G_{\alpha},\ G_{\beta},\ G_{-\alpha-\beta}$ *be as explained. Then,*

$$P(G_{+\alpha\beta}; x) = P(G; x) - P(G_{-\alpha-\beta}; x) - 2\sqrt{P(G_{-\alpha}; x)P(G_{-\beta}; x) - P(G; x)P(G_{-\alpha-\beta}; x)}. \quad (4)$$

The reader can immediately see that the selected fragment Ω of (2) is just the entire expression under the square root in (4). Hence, making elementary transformations of (4), we can resolve it for Ω, which gives

$$\Omega = \frac{1}{4}[P(G_{+\alpha\beta}; x) + P(G_{-\alpha-\beta}; x) - P(G; x)]^2. \quad (5)$$

Now, we come to:

Proposition 2 *Let* $\tilde{w} := P(G_{-\alpha\beta}; x)$ *and* $T_{\alpha\beta}(\varepsilon)$ *be as in (2). Then*

$$T_{\alpha\beta}(\varepsilon) = \frac{\sin q_\alpha \sin q_\beta\, (\tilde{v} + \tilde{w} - \tilde{s})^2}{4 \cdot |e^{i(q_\alpha+q_\beta)}\tilde{s} - e^{iq_\beta}\tilde{t} - e^{iq_\alpha}\tilde{u} + \tilde{v}|^2}, \quad (6)$$

which involves one new polynomial $\tilde{w}$ *but drops two polynomials* $\tilde{t}$ *and* $\tilde{u}$ *in the enumerator, used earlier in (2).*

We further modify the denominator of (2). To this end, we introduce here another auxiliary graph $G_{\circ\circ}$ which is the above graph G with two weighted selfloops now attached to vertices α and β: the former has the weight $\xi_\alpha = e^{-iq_\alpha}$ and the latter $\xi_\beta = e^{-iq_\beta}$. Note that now adjacency matrix $A(G_{\circ\circ})$ of the graph $G_{\circ\circ}$ has two nonzero diagonal entries $a_{\alpha\alpha} = \xi_\alpha$ and $a_{\beta\beta} = \xi_\beta$.

Further, let Δ_α be obtained by substituting zeros (0s) for all entries of the αth column of the secular determinant $\Delta_0 := \det[xI - A(G)]$ except for its only on-diagonal entry which is now set to $-e^{-iq_\alpha}$ (but was originally 0, in Δ_0). That is, $-e^{-iq_\alpha}$ is the only nonzero entry in the αth column of Δ_α. Moreover, let Δ_β denote the determinant obtained in a similar way, involving the on-diagonal entry $-e^{-iq_\beta}$ in the βth column. Lastly, denote by $\Delta_{\alpha\beta}$ the determinant resulted from both operations performed at once (on both αth and βth columns and respective on-diagonal entries of Δ_0).

Any determinant of an $n \times n$ matrix ($n > 1$) with only one nonzero entry in some column(s) can be reduced to a determinant of a smaller size. Employing such reduction here allows to compile the following set of equalities (needed for the proof of the forthcoming Lemma 3):

$$\begin{cases} \Delta_0 = \det[xI - A(G)], \\ \Delta_\alpha = -e^{-iq_\alpha} \det[xI - A(G_\alpha)], \\ \Delta_\beta = -e^{-iq_\beta} \det[xI - A(G_\beta)], \\ \Delta_{\alpha\beta} = +e^{-i(q_\alpha+q_\beta)} \det[xI - A(G_{\alpha\beta})]. \end{cases} \tag{7}$$

The next lemma is here important:

Lemma 3 *Let* Λ *denote the denominator of (2) and* $\tilde{r} = P(G_{\circ\circ}; x)$. *Then*

$$\Lambda = |e^{i(q_\alpha+q_\beta)}(\tilde{s} - e^{-iq_\alpha}\tilde{t} - e^{-iq_\beta}\tilde{u} + e^{-i(q_\alpha+q_\beta)}\tilde{v})|^2 = |e^{i(q_\alpha+q_\beta)}\tilde{r}|^2. \tag{8}$$

Proof First, we partially expand the secular determinant $\Delta := \det[xI - A(G_{\circ\circ})]$ using only two columns (rows) which contain diagonal entries $x - e^{-iq_\alpha}$ and $x - e^{-iq_\beta}$ (involving the weights of selfloops attached to vertices α and β, respectively). This gives

$$\Delta = \Delta_0 - \Delta_\alpha - \Delta_\beta + \Delta_{\alpha\beta}.$$

Using (8), we rewrite this equation in a more explicit form:

$$\Delta = \det[xI - A(G)] - e^{-iq_\alpha}\det[xI - A(G_{-\alpha})] - e^{-iq_\beta}\det[xI - A(G_{-\beta})] \\ +e^{-i(q_\alpha+q_\beta)}\det[xI - A(G_{-\alpha-\beta})].$$

The obtained expansion in determinants can equivalently be rewritten as

$$\Delta = P(G; x) - e^{-iq_\alpha}P(G_\alpha; x) - e^{-iq_\beta}P(G_\beta; x) + e^{-i(q_\alpha+q_\beta)}P(G_{-\alpha-\beta}; x).$$

Hence, using the notation of [5], we get

$$\Delta = \tilde{s} - e^{-iq_\alpha}\tilde{t} - e^{-iq_\beta}\tilde{u} + e^{-i(q_\alpha+q_\beta)}\tilde{v} = \tilde{r},$$

which is the proof. □

Now, by virtue of Lemma 3, we easily derive from Proposition 2 our final result:

Proposition 4 *Let* $T_{\alpha\beta}(\varepsilon)$ *be as above. Then*

$$T_{\alpha\beta}(\varepsilon) = \frac{\sin q_\alpha \sin q_\beta \, (\tilde{v} + \tilde{w} - \tilde{s})^2}{4 \cdot |e^{i(q_\alpha+q_\beta)}\tilde{r}|^2}. \tag{9}$$

Note in passing that the expression $e^{i(q_\alpha+q_\beta)}\tilde{r}$ in (9) may be replaced by its complex conjugate, since (9) uses just the modulus thereof.

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