

The conductivity of superimposed key-graphs with a common one-dimensional adjacency nullspace

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Abstract

Two connected labelled graphs H_1 and H_2 of nullity one, with identical one-vertex deleted subgraphs $H_1 - z_1$ and $H_2 - z_2$ and having a common eigenvector in the nullspace of their 0-1 adjacency matrix, can be overlaid to produce the superimposition Z . The graph Z is $H_1 + z_2$ and also $H_2 + z_1$ whereas $Z + e$ is obtained from Z by adding the edge $\{z_1, z_2\}$. We show that the nullity of Z cannot take all the values allowed by interlacing. We propose to classify graphs with two chosen vertices according to the type of the vertices occurring by using a 3-type-code. Out of the 27 values it can take, only 9 are hypothetically possible for Z , 8 of which are known to exist. Moreover, the SSP molecular model predicts conduction or insulation at the Fermi level of energy for 11 possible types of devices consisting of a molecule and two prescribed connecting atoms over a small bias voltage. All 11 molecular device types are realizable for general molecules, but the structure of Z and of $Z + e$ restricts the number to just 5.

Keywords: Nullity, core vertices, key-graphs, superimposition, circuit.

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Prevodnost prekrivajočih se ključnih grafov s skupnim enodimenzionalnim sosednostnim jedrom

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Povzetek

Dva povezana označena grafa H_1 in H_2 ničnosti ena, z identičnima podgrafoma $H_1 - z_1$ in $H_2 - z_2$, dobljenima iz njiju z izbrisom po enega vozlišča, in s skupnim lastnim vektorjem v jedru njune 0-1 matrike sosednosti, lahko sopolstavimo tako, da dobimo prekrivanje Z . Graf Z je tako $H_1 + z_2$ kot $H_2 + z_1$, medtem ko je graf $Z + e$ dobljen iz Z z dodajanjem povezave $\{z_1, z_2\}$. Pokažemo, da ničnost grafa Z ne more zavzeti vseh vrednosti, ki jih dovoljuje prepletanje. Predlagamo klasifikacijo grafov z dvema izbranimi vozliščema glede na vrsto dobljenih vozlišč z uporabo 3-znakovne kode. Izmed 27 vrednosti, ki jih lahko zavzame, jih je samo 9 hipotetično mogočih za Z , in za 8 od njih vemo, da obstajajo. Poleg tega, molekularni model SSP napoveduje prevodnost ali izolacijo na Fermijevi ravni energije za 11 možnih tipov sestavov, zgrajenih iz molekule in dveh predpisanih veznih atomov nad majhno pristransko napetostjo. Vseh 11 tipov molekularskih sestavov se da realizirati za splošne molekule, vendar strukturi grafov Z in $Z + e$ omejujeta to število na samo 5.

Ključne besede: Ničnost, vozlišča sredice, ključni grafi, prekrivanje, vezje.

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