Theoretical modelling of nanodevices in the frameworks of embedded molecular cluster model

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Abstract

Applicability of cluster embedding method with non-orthogonal wave functions for theoretical study of processes in nanodevices is studied. We demonstrate that our cluster embedding method is compatible with quantum transport theory based on time-dependent DFT. We conclude that quantum transport theory methods may be applied if we use one-electron approaches both with orthogonal and non-orthogonal wave functions. Possibilities to generalise quantum transport theory methods on the many-electron case and theoretical modelling of nanodevices beyond approaches based on one-electron approximation are discussed.

Keywords: embedded molecular cluster model, non-orthogonal wave functions, quantum transport theory, current in nanodevices

1 Introduction

When we theoretically describe nanodevice we have to treat the whole quantum system as two subsystems: small finite fragment of the system containing nanodevice (cluster) and the rest of the system containing electrodes. Problem "cluster in the field of the rest of system" is successfully solved in the frameworks of embedded molecular cluster (EMC) model with *orthogonal* wave functions. We have modified EMC model treating cluster embedding problem in the frameworks of one-electron approximation with *non-orthogonal* wave functions. We have proposed new cluster embedding scheme based on our approach [1].

Our present aim is application of our cluster embedding method for quantum-chemical modelling of processes in nanosystems and calculation of electrical properties of nanodevices.

2 Overview

One of the approaches for theoretical description of nanodevices is quantum transport theory developed by Gross with co-workers [2]. We study possibility to combine our approach with approach of Gross et al [2] based on time-dependent DFT (TDDFT). We demonstrate [3] that our cluster embedding method is compatible with DFT Kohn-Sham method. We conclude that our embedding scheme may be combined with TDDFT if electron transitions are described correctly: occupied and vacant cluster states are localized in the cluster region in the same manner. To get occupied and vacant states of the same localization degree, we use modified form [4] of our initial cluster embedding equations [1]. We demonstrate that our cluster embedding method is compatible with electric current calculation method based on TDDFT [2] and propose approach for calculation of electric parameters of nanodevices.

3 Conclusions

Quantum transport theory methods for electric current calculation may be applied if we use one-electron approaches. In this case we can easily construct one-electron density and get continuity equation for electric current. To treat processes in nanodevices, we should overcome limitations of one-electron approaches using configuration interaction (CI) or perturbation theory (PT) methods. Our cluster embedding scheme is compatible with PT or CI methods. One-electron density may be constructed for these methods, too. But possibility to get continuity equation and expression for electric current in general form requires further investigation.

References

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