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

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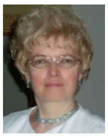

Abstract

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 case of temperature-dependent electron transitions and theoretical modelling of temperature-dependent processes in nanodevices 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 this 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 Cluster embedding equations

Our cluster embedding scheme [1] is based on Hartree-Fock (HF) method. In the last years HF one-electron equations are rarely used. Calculations usually are carried out in the frameworks of density functional theory (DFT) with one-electron Kohn-Sham equations. Besides that, for theoretical modeling of nanodevices we want to apply quantum transport theory based on DFT. Therefore, we should find cluster embedding equations our variation procedure gives when we use DFT Kohn-Sham approach.

Total energy of many-electron system described by non-orthogonal one-electron wave functions on the both HF and DFT Kohn-Sham levels may be written in the same way. Varying expression for the total energy and analyzing our variation procedure we demonstrate [2] that our cluster embedding method based on HF calculation scheme is compatible with DFT Kohn-Sham calculation scheme. Cluster embedding equations remain the same if instead of Fock operator we use Kohn-Sham Hamiltonian. Therefore, there exists possibility to combine our cluster model (with non-orthogonal one-electron wave functions) and quantum transport theory based on time-dependent DFT (TDDFT). 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 have modified [3] our initial cluster embedding equations [1].

3 Quantum transport theory and cluster model

One of the approaches for calculation of electrical properties of nanodevices is quantum transport theory methods developed by Gross with co-workers [4]. We study possibility to combine our cluster approach with approach of Gross et al. Method of Gross implies that wave functions of nanodevice central part are orthogonal to the wave functions of the electrodes. We show [2] that approach for electric current calculation developed for orthogonal wave functions may be applied for non-orthogonal wave functions if we transform initial equations assuming that overlaps between wave functions are small ($S^2 \ll S$). Using this assumption we may combine our cluster embedding method with approach of Gross et al. and calculate electric parameters of nanodevices.

We can conclude that our cluster embedding method is compatible with electric current calculation method based on TDDFT [4] and we can propose calculation scheme for electric parameters of nanodevices using both methods.

4 Conclusions

We demonstrate that our cluster embedding method is compatible with DFT Kohn-Sham method. We conclude that our embedding scheme may be combined with TDDFT and electric current calculation method based on TDDFT. We use TDDFT based quantum transport theory method of Gross et al [4] and propose approach for calculation of electric parameters of nanodevices.

Quantum transport theory methods for electric current calculation may be applied if we deal with 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 consider temperature-dependent electron transitions. In this case one-electron density may be constructed and continuity equation for electric current may be obtained in the frameworks of one-electron approach if we use temperature-dependent occupation numbers for vacant and occupied one-electron states.

Situation is more complicated if we want to overcome limitations of one-electron approximation using approaches like 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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