Pseudopotential-based calculation of electronic structure and transport in nanostructures

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ABSTRACT/SYNOPSIS

This short course describes the use of empirical pseudopotentials (EPs) to study the electronic properties and transport in nanometer-scale structures, discussing the calculation of the band structure and wavefunctions, of the matrix elements determining scattering rates, and on open-boundary-condition quantum transport. The EP approach is compared to other approaches presented in these short courses (Density Functional Theory, DFT, tight-binding, and $\boldsymbol{k\cdot p}$ perturbation theory).

CRYSTAL HAMILTONIAN AND PSEUDOPOTENTIALS

The course begins with a brief overview of the main physical approximations required to simplify the 'exact' crystal Hamiltonian with emphasis on plane-wave methods: The adiabatic (Born-Oppenheimer) approximation to separate the ionic and electronic degrees of freedom; The single-electron and mean-field approximations (Hartree and Hartree-Fock); The concept of 'density functional' to handle exchange and correlation [1]; And, finally, 'model potentials' and 'pseudopotentials' [2,3], both self-consistent (DFT) and empirical. EPs, when suitably calibrated and using 'relaxed' atomic coordinates, are then argued to represent a satisfactory compromise between physical accuracy and computational efficiency.

EMPIRICAL PSEUDOPOTENTIALS AND NANOSTRUCTURES

As an illustration of the practical use of EPs, the case of bulk Si is discussed also in its numerical details [4]. The idea of 'supercell' is then introduced with examples relative to transport in two dimensions (thin Si bodies, III-V hetero-layers, graphene) and in one dimension (Si nanowires, carbon nanotubes, graphene nanoribbons) [5,6].

SCATTERING PROCESSES

Next, the discussion moves to the use of EPs to calculate matrix elements (and so, scattering or transition rates, or self-energies) for some important collision processes. In particular, the rigid-(pseudo)ion approximation [7] is used to compute the electron-phonon matrix elements in Si inversion layers and in graphene. Results from semiclassical full-band transport studies (mobility and Monte Carlo) are then presented. Next, we describe the use of EPs to model atomic roughness (and its effect on electronic transport) at surfaces/interfaces/line-edges in thin bodies, nanowires (NWs) and armchair-edge graphene nanoribbons (AGNRs).

BALLISTIC QUANTUM TRANSPORT WITH OPEN BOUNDARY CONDITIONS

The last section of this short course deals with the study of ballistic quantum transport in nanostructures. The treatment of open boundary conditions at the 'contacts' is discussed presenting a full-band extension of the 'Quantum Transmitting Boundary Method' [8] using EPs and the example of ballistic transport in a small Si NW.

REFERENCES

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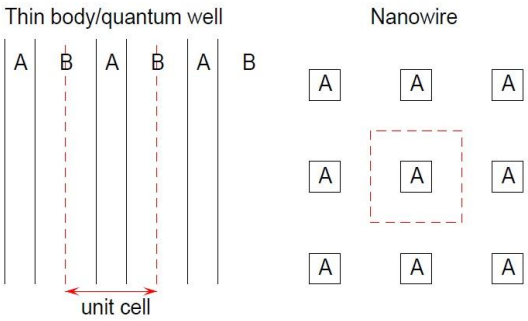

Fig. 1. Schematic diagram illustrating the concept of 'supercell': The nanostructure is replicated along one direction (*left*, thin body, 2DEG) or on the plane (*right*, nanowire/nanotube, 1DEG) to recover periodicity and make a plane-wave analysis possible.

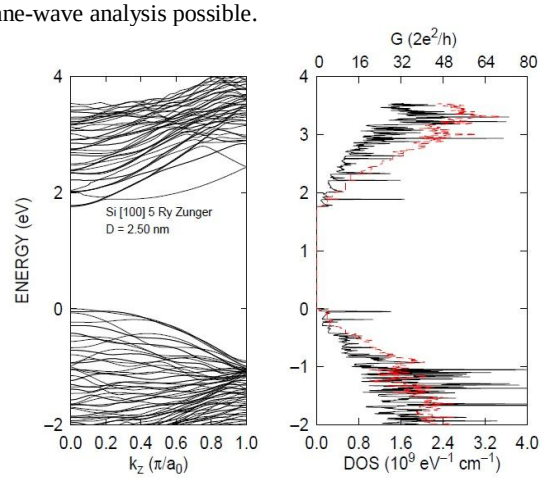

Fig. 2. Band structure (*left*) and density-of-states (*right*, solid black line, bottom scale) and ballistic conductance (*right*, dashed red line, top scale) for a 2.5 nm-diameter cylindrical [100] Si nanowire obtained using empirical pseudopotentials (M. V. Fischetti, unpublished).

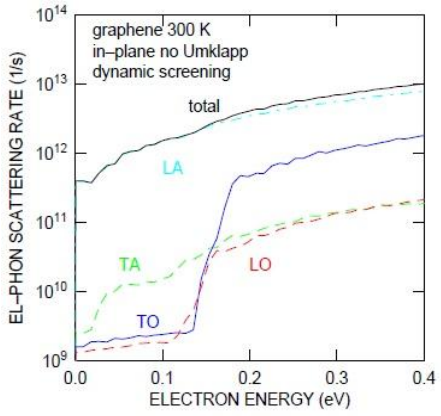

Fig. 3. Dynamically screened electron phonon scattering rate in graphene at zero density calculated using EPs and the rigid-ion approximation (M. V. Fischetti and S. Aboud, unpublished).

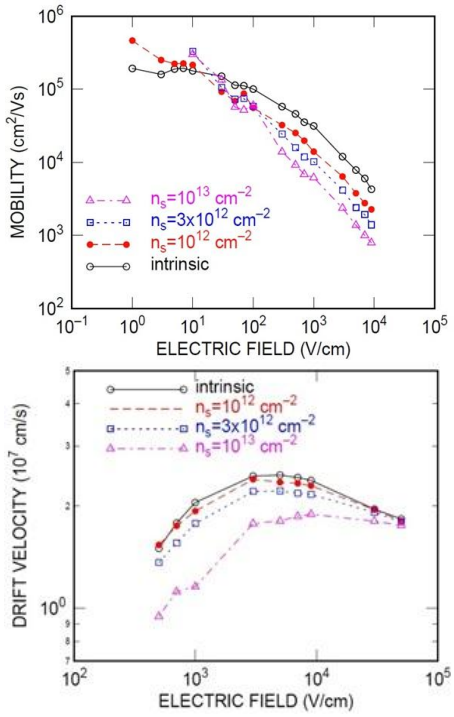

Fig. 4. Field-dependent mobility (*top*, calculated from the longitudinal diffusion coefficient) and drift-velocity (*bottom*) in graphene obtained using the rigid-ion scattering rates (courtesy S. Narayanan, UT-Dallas PhD Thesis).

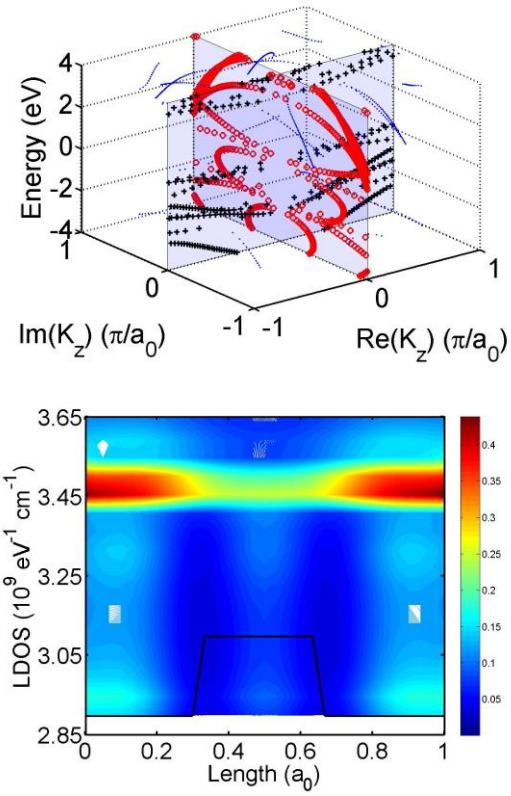

Fig. 4. *Top*: Complex band structure for a Si NW with 1 cell x1 cell square cross-section. This information is needed by the full-band QTBM. *Bottom*: Local density-of-states for the same Si NW in the presence of a rectangular potential barrier simulating the effect of a gate potential (courtesy Bo Fu, UT-Dallas Ph.D. Thesis).