Project for advancement of software usability in materials science

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1 Overview

From the 2015 fiscal year, the supercomputer center (SCC) has started "Project for advancement of software usability in materials science" [1]. In this project, for enhancing the usability of the supercomputer system in ISSP, we perform some software-advancement activity such as implementing a new function to an existing code, releasing a private code on Web, writing manuals. Target programs are publicly offered in December and selected in the review by the Steering Committee of SCC. The projects are carried out by the software development team composed of three members in ISSP.

In the 2015 fiscal year, since it is the first time to start the project, the public offering was announced in March 2015 and the following two projects were selected in April 2015: One is adding new functions to compute eigenchannels and the real space current density into the first-principles program package OpenMX [2]. The other is releasing a numerical solver package for a wide range of quantum lattice models $\mathcal{H}\Phi$ [3]. In this package, the Lanczos algorithm for finding ground states and newly developed Lanczos-based algorithm for finite-temperature properties [4] are implemented for parallel computing. In the following sections, we report the details of the contents of these projects, respectively.

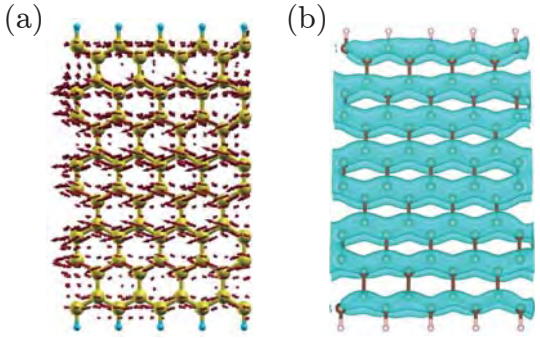

Figure 1: (a) Current density in 8-zigzag graphene nanoribbon with an antiferromagnetic junction under a finite bias voltage of 0.3 V. (b) Isosurfaces of the **a**-compontent of that.

2 Eigenchannel and real space current density in OpenMX

In a nanoscale electronic transmission phenomena, it is important to realize the path of transmitting electrons. Transmission eigenchannel analysis is suitable to obtain real space microscopic picture of that phenomena; this channel is represented as a special transmission wavefunction which maximizes the transmission probability. On the other hand, when we scope the spatial variation of the direction of transmission, the real space current density analysis is preferred. A program package which can perform easily these calculation have been required.

OpenMX (Open source package for Material eXplorer) [2] is a software package for nano-scale material simulations based on density functional theories (DFT); it uses

norm-conserving pseudopotentials and pseudo-atomic localized basis functions [5]. This program package supports the simulation of the electronic conduction phenomena in a nanoscale device; this simulation is performed by using the *ab initio* nonequilibrium Green's function (NEGF) theorem. We implemented functions to compute the transmission eigenchannels [6] and the real space current density [7] in the framework of the NEGF theory; this calculation is performed as a post process of the calculation of NEGF.

As an example, we apply these functions to 8-zigzag graphene nanoribbon with an antiferromagnetic junction; the spin polarization at the edge of this system and the dual spin filter effect are predicted by previous first-principles study [8]. We show the currentdensity in 8-zigzag graphene nanoribbon with an antiferromagnetic junction under a finite bias voltage of 0.3 V in Fig. 1. Figure 2 shows eigenchannels of this system under a finite bias voltage of ± 0.3 V besides the spin dependent transmission probability at each energy.

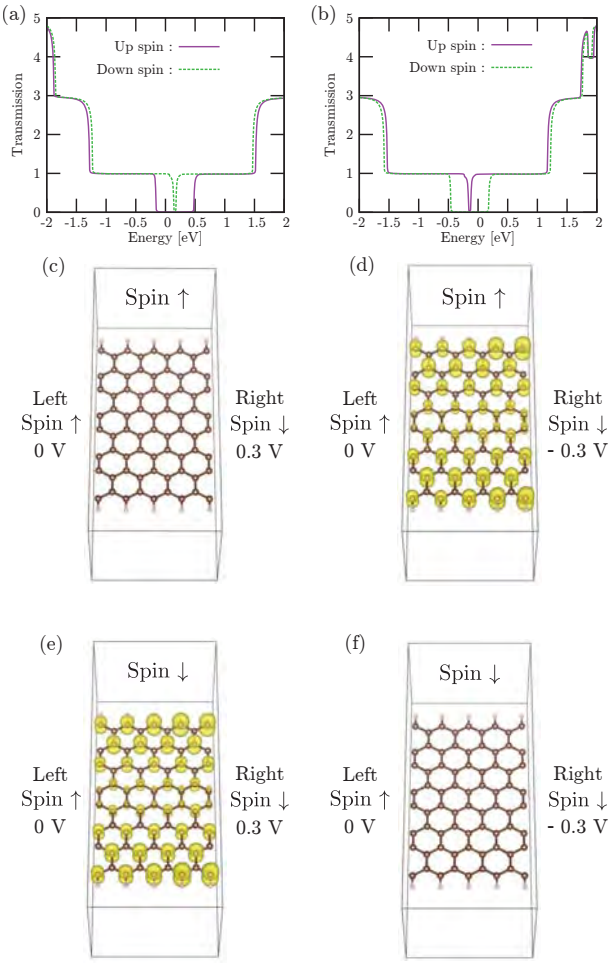

Figure 2: (a) Spin dependent transmission under a bias voltage of 0.3 V, (b) Spin dependent transmission under a bias voltage of -0.3 V, (c) An eigenchannel at a energy of 0 eV, spin ↑, and 0.3 V as a bias voltage, (d) An eigenchannel at a energy of 0 eV, spin ↑, and - 0.3 V as a bias voltage, (e) An eigenchannel at a energy of 0 eV, spin ↓, and 0.3 V as a bias voltage, and (f) An eigenchannel at a energy of 0 eV, spin ↓, and - 0.3 V as a bias voltage in 8-zigzag graphene nanoribbon with an antiferromagnetic junction (The spin is ↑ in the left region and it is ↓ in the right region.) are depicted. The level of isosurfaces are identical in these figures; when the transmission is small, the eigenchannel itself is also small.

3 $\mathcal{H}\Phi$: Solver for general quantum lattice models

For the quantitative comparison with experimental data, the numerical exact diagonalization of a quantum lattice system [9] is one of the most reliable tools without any approximation for small systems. This method can be used also for benchmarks of other numerical methods (such as DMRG, DMFT, VMC, QMC, tensor network, etc.). In addition, recent advances in quantum statistical mechanics [4, 10, 11, 12] enable us to calculate finite-temperature properties of quantum many-body systems without an ensemble average. This method enables us to compare theoretical results for temperature dependence of, for example, specific heat and magnetic susceptibility with experimental results quantitatively [13]. To utilize the parallel computing infrastructure with narrow bandwidth and distributed-memory architectures, an efficient, user-friendly, and highly parallelized diagonalization packages are highly desirable.

In this project, we released a flexible diagonalization package $\mathcal{H}\Phi$[3] for solving quantum

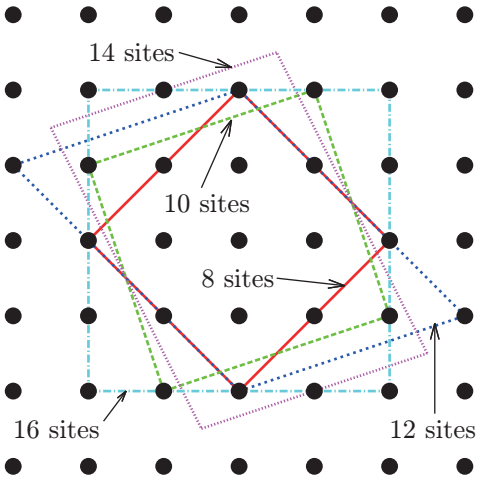

Figure 3: Shapes of numerical cells having 8, 10, 12, 14, 16 sites.

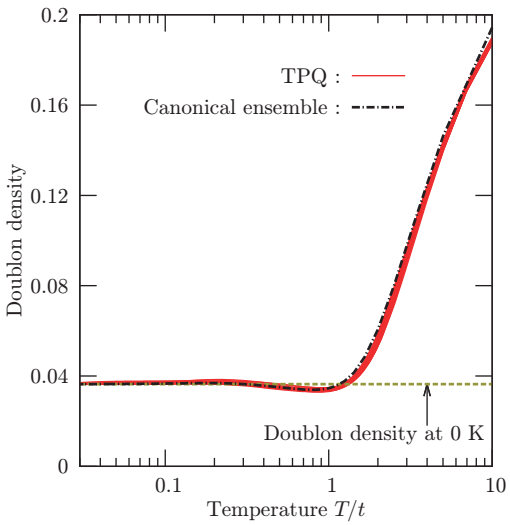

Figure 4: Temperature dependence of the doublon density calculated from the TPQ state and the canonical ensemble obtained by the full diagonalization method on 8 sites Hubbard model. We perform the TPQ calculation 20 times and depict each results. The yellow horizontal line indicates the doublon density at 0 K, which is calculated with the Lanczos method.

lattice hamiltonians; the Lanczos method for calculations of the ground state and a few excited states properties, and finite temperature calculations based on thermal pure quantum (TPQ) states [4] are implemented in this program package. We designed its user-interface to use easily by theoretical/experimental researchers and students. By using $\mathcal{H}\Phi$, a wide range of quantum lattice hamiltonians including simple Hubbard and Heisenberg models, multi-band extensions of the Hubbard model, exchange couplings that break SU(2) symmetry of quantum spins such as Dzyaloshinskii-Moriya and Kitaev interactions, and Kondo lattice models describing itinerant electrons coupled with quantum spins can be analized. $\mathcal{H}\Phi$ calculates a variety of physical quantities such as internal energy at zero temperature or finite temperatures, temperature dependence of specific heat, charge/spin structure factors, and so on. A broad spectrum of users including experimental scientists is cordially welcome.

As an example of using $\mathcal{H}\Phi$, we compute the temperature dependence of the doublon density in a Hubbard model ($U/t = 8$) for 8, 10, 12, 14, 16 sites; the shape of the numerical cell is depicted in Fig. 3. We can easily construct these Hamiltonian by using $\mathcal{H}\Phi$.

Figure 4 shows the temperature dependence of the doublon density calculated from the TPQ state and the canonical ensemble obtained by the full diagonalization method on Hubbard model with 8 sites; we perform the TPQ calculation 20 times and depict each results. These two results show a good agreement. In Fig. 5, we show the doublon density calculated from TPQ states on Hubbard model with 8, 10, 12, 14, 16 sites; we performed the TPQ calculation 20 times in each size and found that the result almost converges about the number of sites.

In the project for advancement of software usability in materials science for 2016 fiscal year, we are planning to implement a function to compute an optical spectrum of the quantum lattice system in $\mathcal{H}\Phi$. With this function, we will be able to compare the theoretical results and data of some spectroscopic experiments such as ARPES, the neutron scattering, and so on.

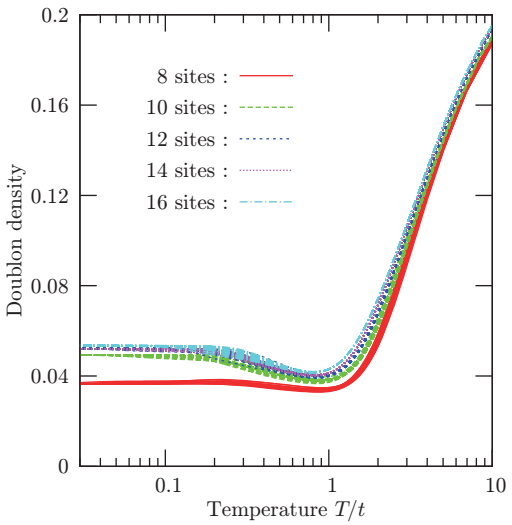

Figure 5: The doublon density calculated from TPQ states on Hubbard model with 8, 10, 12, 14, 16 sites; we perform the TPQ calculation 20 times in each size and plot all of them.

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