Simulating the energy and heat transport in quantum systems

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We state the equations necessary to calculate the heat current in a tight-biding system with the help of tkwant. Short explanations of the implementation are given.

I. INTRODUCTION – PARTICLE CURRENT AND T-KWANT

KWANT (https://kwant-project.org/) [1] is a software package to easily build a tight-binding system and calculate all kinds of properties, mostly needed for transport calculations. E.g., the scattering matrix is obtained by calculating the scattering states in the leads and the system.

t-KWANT [2, 3] is an extension that allows for the calculation of transport properties in time-dependent tight-binding systems, e.g. by applying a voltage pulse in one of the leads. The Hamiltonian in general reads

$$H(t) = \sum_{ij}^{\text{sites}} H_{ij}(t) c_i^\dagger c_j. \tag{1}$$

The implementation of t-KWANT is based on the discovery that the lesser Greens function $G^<$ can be expressed in terms of the time-dependent scattering states $\Psi^{\alpha E}$ from lead α with energy E as (see e.g. Eq. (2.29) in B. Gaury's thesis):

$$G^<_{ij}(t,t') = \frac{i}{\hbar}\langle c_j^\dagger(t') c_i(t)\rangle = i\sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) \Psi_i^{\alpha E}(t) \Psi_i^{\alpha E}(t')^\dagger, \tag{2}$$

with f_α being the Dirac-Fermi function. The time-evolution of the scattering states is given by Schrödinger equation

$$i\hbar\partial_t \Psi^{\alpha E}(t) = H(t)\Psi^{\alpha E}(t) \tag{3}$$

where the Hamiltonian $H(t) = H_{\text{static}} + V(t)$ is composed of a static and a time-dependent term.

With the help of Eq. (2), we can write the particle current I^N_{ij} between sites i and j in terms of the scattering states (see e.g. Eq. (4.13) in B. Gaury's thesis):

$$I^N_{ij}(t) = -2\text{Im}\sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) \Psi_i^{\alpha E}(t)^\dagger H_{ij}(t) \Psi_j^{\alpha E}(t). \tag{4}$$

Technically, in t-Kwant, $\Psi^{\alpha E}(t)$ is calculated by solving Eq. (3), by default with a Dormand-Prince method which is a special Runge-Kutta method. Then, the integrand $\Psi_i^{\alpha E}(t)^\dagger H_{ij}(t)\Psi_j^{\alpha E}(t)$ is calculated with the help of the class `kwant.operator.Current`. The integration is done with the help of the class `tkwant.manybody.Solver`, where an adaptive Gauss-Kronrod(7/15) method is used. The reason for the adaptive method is to calculate the integrand at as few energies as possible for a given allowed error since obtaining $\Psi^{\alpha E}(t)$ is rather slow.

Instead of the particle current, we want to calculate the heat current in a time-dependent system. The major part of the t-KWANT calculations will be usable and we only have to define new operators, i.e. different integrands in Eq. (4) as shown in the subsequent sections.

The operators so far available in in kwant are:

- `kwant.operator.Density`: $\phi_i^\dagger M_{ii}\psi_i$,
- `kwant.operator.Current`: $\phi_i^\dagger H_{ij} M_{jj}\psi_j$,
- `kwant.operator.Source` : $\phi_i^\dagger H_{ii} M_{ii}\psi_i$,

where M is a user-defined onsite matrix.

II. LEAD HEAT CURRENT

A. Without I_c

The heat current I^h in lead l is defined as

$$I_l^h = I_l^E - \mu_l I_l^N (+I_c), \tag{5}$$

where μ_l is the chemical potential in the lead l and I_c is a coupling term, which we will omit in this section and discuss only in the next section.

The energy current I_l^E is defined as

$$I_l^E = \frac{d\langle H_l \rangle}{dt} = \left\langle \frac{\partial H_l}{\partial t} \right\rangle - \frac{i}{\hbar} \langle [H_l, H] \rangle \tag{6}$$

with the commutator $[\cdot, \cdot]$. Using the commutation relations of annihilation and creation operators and the definition of the lesser Green's function in Eq. (2), we obtain

$$I_l^E(t) = \sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) \sum_{ij \in l} \sum_{q \in \bar{0}} (-2) \mathrm{Im} \left\{ \Psi_q^{\alpha E}(t)^\dagger H_{qi} H_{ij} \Psi_j^{\alpha E}(t) \right\}, \tag{7}$$

where $\bar{0}$ denotes the sites in the scattering region, i.e. the system without the leads. Compared to I^N in Eq. (4), the overall structure is quite similar with the difference that now, we have two Hamiltonian terms, which does not match any `kwant.operator` so far (see end of Sec. I). For implementation reasons, we split the sum in Eq. (7) into the term with $i = j$, which we call 'onSite', and $i \neq j$, called 'offSite':

$$I_l^{E,\mathrm{on}}(t) = \sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) \sum_{i \in l} \sum_{q \in \bar{0}} (-2) \mathrm{Im} \left\{ \Psi_q^{\alpha E}(t)^\dagger H_{qi} H_{ii} \Psi_i^{\alpha E}(t) \right\}, \tag{8}$$

$$I_l^{E,\mathrm{off}}(t) = \sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) \sum_{i \neq j \in l} \sum_{q \in \bar{0}} (-2) \mathrm{Im} \left\{ \Psi_q^{\alpha E}(t)^\dagger H_{qi} H_{ij} \Psi_j^{\alpha E}(t) \right\}, \tag{9}$$

where now, the 'onSite' term has the same structure as needed for `kwant.operator.Current` with the onsite-matrix $M = H$. The 'offSite' term on the other hand still does not match directly any `kwant.operator` term. One could define a new wave function $\psi_i = \sum_j H_{ij} \Psi_j^{\alpha E}$ and use `kwant.operator.current` to calculate it, but we/I decided to create a new operator-class instead which is able to calculate the 'offSite'-term:

- `offEnergyCurrent`: $\sum_{i \neq j \in l} \sum_{q \in \bar{0}} (-2) \mathrm{Im} \left\{ \phi_q^\dagger H_{qi} H_{ij} \psi_j \right\}$,

Note that since we are computing the energy current for the whole lead, as compared to the local quantities in `kwant.operator`, we have the sums directly in the operator.

As a side not, we see that both the 'onSite'-term as well as μI^N depend on the choice of the zero point of the energy (e.g. band minimum or Fermi energy or anything else), whereas the 'offSite'-term does not, since only hoppings appear there. However, it turns out numerically that the difference of 'onSite'-term and μI^N is again independent of the energy offset, which has to be the case.

B. With I_c

According to Ref. [4], the additional coupling term I_c in the heat current of Eq. (5) is given by

$$I_c = 0.5 \times \frac{d\langle H_{l\bar{0}} + H_{\bar{0}l} \rangle}{dt} = 0.5 \times \left(\frac{\partial \langle H_{l\bar{0}} + H_{\bar{0}l} \rangle}{\partial t} - \frac{i}{\hbar} \langle [H_{l\bar{0}} + H_{\bar{0}l}, H] \rangle \right), \tag{10}$$

where $H_{l\bar{0}}$ is the part of the Hamiltonian that couples the scattering region $\bar{0}$ to the lead l.

The explicit time-dependence in Eq. (10) leads to

$$\frac{\partial \langle H_{l\bar{0}} + H_{\bar{0}l} \rangle}{\partial t} = \sum_{i \in \bar{0}} \sum_{j \in l} 2\mathrm{Re} \sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) \Psi_i^{\alpha E}(t)^\dagger \frac{\partial H_{ij}}{\partial t} \Psi_j^{\alpha E}(t), \tag{11}$$

which again cannot be directly described by the available `kwant.operator`. That is why we create another operator that calculates:

- `CurrentWithArbitHop`: $\phi_i^\dagger O_{ij} M_{jj} \psi_j$,

where M is again user-defined onsite-term and O_{ij} is a user-defined 'hopping'-term, which would be the time-derivative of the Hamiltonian for Eq. (11).

The term with the commutator in Eq. (10) leads to two additional terms:

$$-\frac{i}{\hbar}\langle[H_{l\bar{0}} + H_{\bar{0}l}, H]\rangle = \sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) 2\mathrm{Im}\Big\{ \sum_{ij\in l}\sum_{q\in\bar{0}} \Psi_q^{\alpha E}(t)^\dagger H_{qi} H_{ij} \Psi_j^{\alpha E}(t) \quad + \sum_{ij\in\bar{0}}\sum_{q\in l} \Psi_q^{\alpha E}(t)^\dagger H_{qi} H_{ij} \Psi_j^{\alpha E}(t) \quad \Big\} \tag{12}$$

$$= \sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) \quad \Big\{ \quad - I_l^{E,\mathrm{off}} \quad - \quad I_l^{E,\mathrm{off,shift}} \quad \Big\}, \tag{13}$$

which have both the same structure as the `offEnergyCurrent`, the first term being exactly the same but with a different sign, the second one being shifted towards the scattering region since the sums have changed. Thus, for the commutator part, no additional `kwant.operator` has to be created, but only the sites where to calculate the `offEnergyCurrent` has to be modified.

The total heat current then yields

$$I_l^h = 0.5 I_l^E - \mu_l I_l^N - 0.5 I_l^{E,\mathrm{off,shift}} + 0.5 \frac{\partial \langle H_{l\bar{0}} + H_{\bar{0}l}\rangle}{\partial t}, \tag{14}$$

which can be calculated with the help of tkwant using the above mentioned operator classes.

III. TECHNICAL DETAILS

A. Add two lead unit cells to the system

In case of a time-dependent voltage in the lead, a gauge transformation is used to move the time-dependence to the hopping between lead and voltage. Since this hopping is now different from the other lead hoppings, it has to be excluded from the lead and included into the scattering region in kwant. The function `tkwant.leads.add_voltage` takes care of both, changing the hopping phase and adding the additional sites to the system.

In the case of the lead heat current, we always have to access sites in the lead [compare Eq. (7)]. One way to enable to do so is to add two lead unit cells to the central system. This is done by the function `operatorsHeatCurrent.add_two_lead_unit_cells` which allows additionally to add directly the phase for a time-dependent voltage. Internally `tkwant.leads.add_voltage` is called twice.

The returned values of `operatorsHeatCurrent.add_two_lead_unit_cells` are two lists of the added sites – one for the first lead unit cell, the other one for the second lead unit cell. These lists can be given directly to the `operatorsHeatCurrent.heatCurrentWithIc` which creates the needed hopping lists to calculate the lead heat current.

B. The path finding – book-keeping

to be added

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[4] María Florencia Ludovico, Jong Soo Lim, Michael Moskalets, Liliana Arrachea, and David Sánchez, "Dynamical energy transfer in ac-driven quantum systems," Phys. Rev. B **89**, 161306 (2014).