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 as well as a comparison to the literature (Crépieux et al and Eich et al).

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] 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):

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

(Probably inconsistent use of $\hbar$, i.e. it might be missing somewhere.) The time-evolution of the scattering states is given by (see e.g. Eq. (2.44) in B. Gaury's thesis)

$$i\partial_t \Psi^{\alpha E}(t) = [H(t) + \Sigma^R(E)]\Psi^{\alpha E}(t) + V(t)\mathrm{e}^{-iEt}\Psi^{\alpha E}_{\text{st(atic?)}}, \tag{3}$$

where the Hamiltonian $H(t) = H_{\text{static}} + V(t)$ is composed of a static and a time-dependent term. **Attention: This differential equation is not completely true for the defined quantities, but I was too lazy to find out all the correct definitions, etc. All I wanted to show here is that the differential equation to obtain $\Psi^{\alpha E}(t)$ is in principle known and is solved numerically by t-KWANT. That's all we have to care about at the moment, since we won't touch that part of t-KWANT.**

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

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

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. HEAT CURRENT - WITHOUT I_c

A. Formulas

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. **Probably, the classes should be named in a way such that one can directly see that its only for a lead and not for local quantities at the moment.**

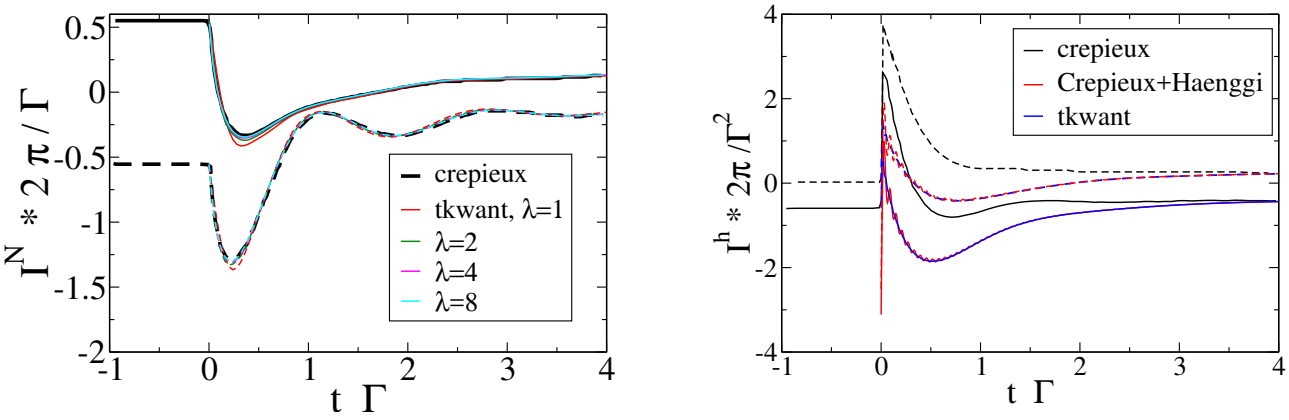
As a side not, we see that both the 'onSite'-term as well as μI^N depend on the choice of the zero point of the energy (e.g. band minimum or Fermi energy or anything else), whereas the 'offSite'-term does not, since only hoppings appear there. However, it turns out numerically that the difference of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

B. Comparison to Crepieux et al

One of the first papers about time-dependent thermo-electricity is by Crépieux, Simcovic, Cambon and Michelini [3], where they consider a quantum dot whose energy level is time-dependent and which is attached to leads. With the help of the Keldysh formalism, they are able to calculate analytically time-dependent particle and energy currents in the wide band limit.

The time-dependence of the onsite-term ε_0 of the dot in their case is a step function

$$\varepsilon_0(t) = \tilde{\varepsilon}_0 + \tilde{\gamma}_0 \Theta(t - t_0). \tag{10}$$



(a) (b)

FIG. 1: Comparison between Fig. 3 in Ref. [3] and our t-KWANT calculations for (a) I^N and (b) I^h, where solid lines belong to the left lead and dashed lines to the right lead. The coefficient λ states how close we are in to the wide band limit, which would be $\lambda \to \infty$. Although for I^N, everything matches well, we do not obtain the same results for I^h. Only with the additional term found in Ref. [4] (red line), the results coincide with t-KWANT. Note that the jump at $t = 0$ in the red line is unphysical and due to the wide band limit as discussed in Ref. [5]. Moreover, the oscillations of the red line for small times are most likely due to brute force numerical integration of the not very well behaved integrand.

As unit of energy, they use the coupling between leads and dot $\Gamma = \Gamma_L + \Gamma_R = 4t_c/t$, where t is the hopping in the leads and t_c is the hopping between lead and dot (in our tight-binding system).

In Fig. 1, we compare the particle and heat currents obtained by Crépieux et al. (see Fig. 3 in Ref. [3]) with our t-KWANT results. The parameters are $t_0 = 0$, $\tilde{\varepsilon} = 0.5\Gamma$, $\tilde{\gamma} = 2.5\Gamma$, $k_B T_L = 1 \times \Gamma$, $T_R = 0$, $\mu_L = 0.5\Gamma$ and $\mu_R = -0.5\Gamma$.

The main difference is from a physical point of view, that we are not in the wide band limit, which means that the coupling does not depend on the energy (or that the density of states in the leads is a constant of energy). The larger we choose λ which rescales our parameters to be closer to the wide band limit, the better the results match for I^N in Fig. 1a. On the other hand, for I^h in Fig. 1b, the results match only after adding an additional term found in Ref. [4]. **We are not sure where this term comes from and we have to check that!**

Note: There was an errata from Crepieux et al. confirming our results.

III. HEAT CURRENT - WITH I_c

A. Formulas

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

$$I_c = 0.5 \times \frac{d\langle H_{l\bar{0}} + H_{\bar{0}l}\rangle}{dt} = 0.5 \times \left(\frac{\partial \langle H_{l\bar{0}} + H_{\bar{0}l}\rangle}{\partial t} - \frac{i}{\hbar} \langle [H_{l\bar{0}} + H_{\bar{0}l}, H] \rangle \right), \tag{11}$$

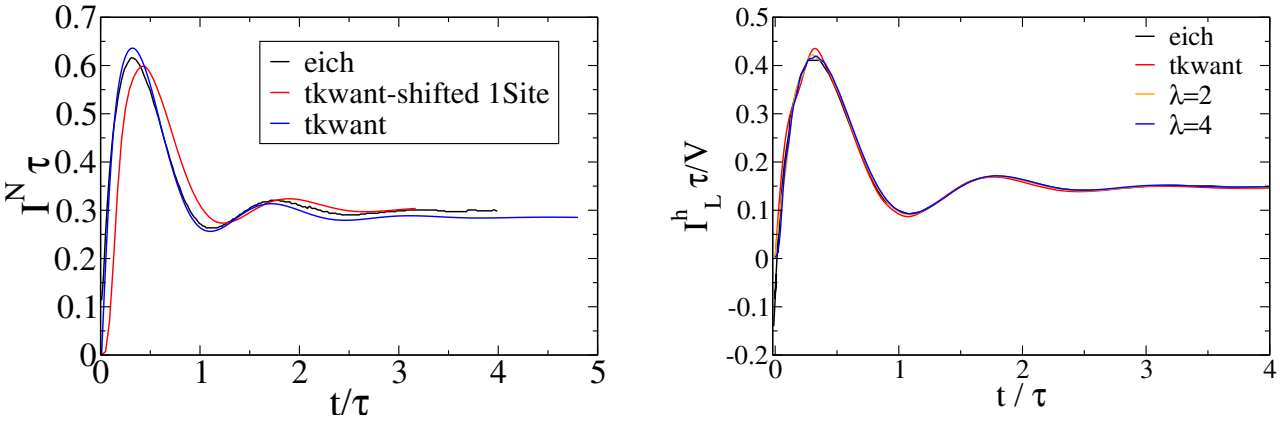
where $H_{l\bar{0}}$ is the part of the Hamiltonian that couples the scattering region $\bar{0}$ to the lead l. **(On the first look, it seems that all the other papers have the same I_c, e.g. Moskalets etc.)**

The explicit time-dependence in Eq. (11) leads to

$$\frac{\partial \langle H_{l\bar{0}} + H_{\bar{0}l}\rangle}{\partial t} = \sum_{i\in\bar{0}} \sum_{j\in l} 2\mathrm{Re} \sum_{\alpha} \int \frac{dE}{2\pi} f_\alpha(E) \Psi_i^{\alpha E}(t)^\dagger \frac{\partial H_{ij}}{\partial t} \Psi_j^{\alpha E}(t), \tag{12}$$

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

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



(a) (b)

FIG. 2: Comparison between t-KWANT and Ref. [3] for (a) I^N [their Fig. 8(a)] and (b) I^h [their Fig. 9(b)]. The results match in general very well, although we do not obtain exactly the same results in (a) mostly due to the fact that the Eich-data was obtained graphically which introduces some small errors due to finite line width, etc. The red line in (a) shows the t-KWANT result for the case when we define our lead-dot interface one site shifted into the lead, which is why it does not match perfectly. **This red line is only in (a) because it was the first result which I got for that system. Probably, I should have removed this line from the plot.**

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. (12).

The term with the commutator in Eq. (11) leads to two additional terms:

$$-\frac{i}{\hbar}\langle[H_{l\bar{0}}+H_{\bar{0}l},H]\rangle = \sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) 2\mathrm{Im}\Big\{ \sum_{ij\in l}\sum_{q\in\bar{0}} \Psi_q^{\alpha E}(t)^\dagger H_{qi}H_{ij}\Psi_j^{\alpha E}(t) \quad + \sum_{ij\in\bar{0}}\sum_{q\in l} \Psi_q^{\alpha E}(t)^\dagger H_{qi}H_{ij}\Psi_j^{\alpha E}(t) \quad \Big\} \tag{13}$$

$$= \sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) \quad \Big\{ \quad -I_l^{E,\mathrm{off}} \quad - \quad I_l^{E,\mathrm{off,shift}} \quad \Big\}, \tag{14}$$

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

$$I_l^h = 0.5 I_l^E - \mu_l I_l^N - 0.5 I_l^{E,\mathrm{off,shift}} + 0.5\frac{\partial\langle H_{l\bar{0}}+H_{\bar{0}l}\rangle}{\partial t}, \tag{15}$$

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

In the code, I need a different sign for the explicitly time-dependent term and I am not sure where it comes from! Answer: Eich's result is not gauge invariant, whereas with the choice above, the heat current is gauge invariant.

B. Comparison to Covito, Eich et al

We want to compare our results to the latest related publication, which is Ref. [5], mostly Fig. 8(a) for I^N and Fig. 9(b) for I^h. There, they consider a quantum dot attached to leads, where a voltage in the left lead is suddenly swichted on:

$$U_L(t) = U\Theta(t-t_0). \tag{16}$$

The hopping from lead to dot $V = V_L = V_R$ is chosen as unit of energy (= t_c in our tight-binding calculations). The parameters are $U = 2V$, the dot level $\varepsilon_c = 0.2V$, the hoppings in the lead are $t = 5V$, $\mu_{L/R} = 0$ and $k_B T_{L/R} = 0.01V$. The results match very well. The only problem is the graphical read out of the data of their Fig. 8(a) which naturally comes with some error tolerance due to finite line width etc. and that we are not yet in the wide band limit ($\lambda = 1$ in Fig. 2a).

IV. SUMMARY OF UNCLEAR THINGS

- where does missing term in Crépieux come from? DONE (more or less)
- check signs in Eq. (15), which means check all the signs for every new defined quantity. DONE
- why do I have problems in t-KWANT for large λ
- calculating currents for some hopping and for an adjacent hopping is often not only a shift (in time) but sometimes has a rather different structure. **(That's a little exagerated. However, relative peak hights might change, not only due to spreading but in a more complicated way.)**
- check if I_c is defined everywhere in the literature in the same way
- in general, be aware in which direction the energy flows. Crepieux and Eich have a different (minus) definition as compared to Eq. (6)

V. TECHNICAL DETAILS

`kwant.add_voltage` 2 mal: `add_two_lead_unit_cells` .

fuer init muss nur der output uebergeben werden. Daraus werden dann alle noetigen hoppings berechnet, indem alle hoppings zu den `i`-sites gefunden werden (ueber `fsyst.graph.out_edge_ids(i)`) und die verbundenen sites dann je nach scat oder lead sortiert werden ($\mathcal{O}((\text{width of lead})^2)$). Hoppings, die zum gleichen `i` gehoeren findet man mitHilfe der `where_idx` Liste.

Concerning `where_idx`:

$$\texttt{where\_idx[0/1][i]} = [\text{list of positions of connected sites to } \texttt{i} \text{ in } \texttt{where}] \tag{17}$$

'0' as index in `where_idx` means a hopping between lead and scattering region, whereas '1' indicates a lead-lead hopping.

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