I. FORMULATION OF THE QUANTUM TRANSPORT PROBLEM AS A SET OF LINEAR EQUATIONS

A. Scattering problem

Consider a system with a single lead (without loss of generality, several leads can be considered as one virtual lead) with a Hamiltonian

$$H = \begin{pmatrix} \ddots & V_L & & \\ V_L^\dagger & H_L & V_L & \\ & V_L^\dagger & H_L & V_L \\ & & V_L^\dagger & H_S \end{pmatrix} \tag{1}$$

where H_L is the onsite Hamiltonian of the lead, V_L the hopping between the lead unit cells, and H_S the (big) Hamiltonian of the scattering region.

We write a wave function as $(\ldots, \psi_{\mathrm{L}}(2), \psi_{\mathrm{L}}(1), \psi_S)$, where ψ_S is the wave function in the scattering region, and ψ_{L} the wave function in the i-th unit cell away from the scattering region in the lead. Using translational invariance of the lead we rewrite the wave function in the lead in terms of the eigenvectors of translation operator. Since the lead is assumed only half-infinite, evanescent modes are allowed. The decomposition gives

$$\psi_L(j) = U\Lambda^j \psi_L, \tag{2}$$

with ψ_L the wave function in mode basis, Λ a diagonal matrix of translation eigenvalues, and U a matrix of translation eigenvectors. We order the modes in the following manner: $\psi_L = (\psi_{\mathrm{in}}, \psi_{\mathrm{out}})$, with ψ_{in} modes incoming to the system, and ψ_{out} contains outgoing and evanescent modes. Since we do not consider modes diverging at infinite, Λ is bounded by one from above. Scattering problem is formulated as a matrix equation:

$$H \begin{pmatrix} \mathbb{1} \\ S \\ \psi_S \end{pmatrix} = 0, \tag{3}$$

where we have set the excitation energy to 0 for brevity. Here S is the scattering matrix of propagating and evanescent modes, and ψ_S the wave function inside the system. Writing down the tight binding equations for the scattering system and the 0th unit cell of the lead yields

$$H_S\psi_S + V_L^\dagger U_{\mathrm{out}}\Lambda_{\mathrm{out}} S = -V_L^\dagger U_{\mathrm{in}}\Lambda_{\mathrm{in}} \tag{4}$$

$$V_L\psi_S + (H_L U_{\mathrm{out}}\Lambda_{\mathrm{out}} + V_L^\dagger U_{\mathrm{out}}\Lambda_{\mathrm{out}}^2)S = -(H_L U_{\mathrm{in}}\Lambda_{\mathrm{in}} + V_L^\dagger U_{\mathrm{in}}\Lambda_{\mathrm{in}}^2). \tag{5}$$

This is the system of equations which has to be solved. One straighforward simplification of Eq. (5) is possible using the lead tight-binding equation:

$$V_L U + H_L U\Lambda + V_L^\dagger U\Lambda^2 = 0. \tag{6}$$

substituting it into the Eq. (5) we get

$$V_L\psi_S - V_L U_{\mathrm{out}} S = V_L U_{\mathrm{in}}. \tag{7}$$

We proceed to discuss various optimizations and strategies of solving this sytem of equations. For now we not that it is already very efficient to provide this system to existent blackbox sparse solvers.

B. Translation eigenvalues in the lead

C. Lead Hamiltonian and wave functions

We consider leads that are described by a unit cell Hamiltonian H_{lead} and a hopping from cell j to cell $j+1$ V_{lead}. The cells are numbered such that the index i increases as one moves away from the scattering region.

Because of Bloch's theorem, the lead eigenfunctions can be written as $\phi(j) = \boldsymbol{u}e^{ikj} = \boldsymbol{u}\lambda$, where $\lambda = e^{ik}$ (Note that k can be complex, describing evanescent modes). The Schrödinger equation for the lead then reads

$$\begin{aligned}(H_{\text{lead}} - E)\phi(j) + V_{\text{lead}}\phi(j-1) + V_{\text{lead}}^\dagger\phi(j+1) = \\ (H_{\text{lead}} - E)\boldsymbol{u} + V_{\text{lead}}\boldsymbol{u}\lambda^{-1} + V_{\text{lead}}^\dagger\boldsymbol{u}\lambda = 0\end{aligned} \tag{8}$$

A general wave function in the lead can then be written in a compact form as

$$\psi(j) = U_{\text{o}}\Lambda_{\text{o}}^j\boldsymbol{a} + U_{\text{i}}\Lambda_{\text{i}}^j\boldsymbol{b} \tag{9}$$

where $U_{\text{o/i}}$ is a matrix with all outgoing (going out of the scattering region into the lead)/incoming (going into the scattering region) modes $\boldsymbol{u}$ in the columns. $\Lambda_{\text{o,i}}$ is a diagonal matrix with the corresponding λ's, and $\boldsymbol{a}$ and $\boldsymbol{b}$ are vectors of amplitudes. Note that the choice of phase of $\boldsymbol{a}$ and $\boldsymbol{b}$ is arbitrary, here I chose them such that the phase described by Λ vanishes at $j = 0$ which is the "unit cell" that is already in the scattering region.

D. Formulating the scattering problem as a linear system

Consider a system with a single lead (without loss of generality, several leads can be considered as one virtual lead) with a Hamiltionian

$$H = \begin{pmatrix} \ddots & V_L & & \\ V_L^\dagger & H_L - E & V_L & \\ & V_L^\dagger & H_L - E & V_L \\ & & V_L^\dagger & H_S - E \end{pmatrix} \tag{10}$$

where H_L is the onsite Hamiltionian of the lead, V_L the hopping between the lead unit cells, and H_S the (big) Hamiltionian of the scattering region.

We write a wave function as $(\ldots, \psi_{\text{L}}(2), \psi_{\text{L}}(1), \psi_S)$, where ψ_S is the wave function in the scattering region, and ψ_{L} the wave function in the i-th unit cell away from the scattering region in the lead.

In the lead, the wave function can be written as

$$\psi_{\text{L}}(j) = U_{L,\text{o}}\Lambda_{L,\text{o}}^j\boldsymbol{S} + \Lambda_i^j\boldsymbol{U}_{i,\text{i}} \tag{11}$$

with S the scattering matrix of the problem (including evanescent modes).

Using Eq. (11) we can rewrite the infinite Schroedinger equation in terms of S and ψ_{S} only. We have

$$\begin{aligned}V_{\text{L}}^\dagger\psi_{\text{L}}(2) + (H_{\text{L}} - E)\psi_{\text{L}}(1) + V_{\text{L,S}}\psi_{\text{S}} = \\ (V_{\text{L}}^\dagger U_{\text{L,o}}\Lambda_{\text{L,o}}^2 + (H_{\text{L}} - E)U_{\text{L,o}}\Lambda_{\text{L,o}})\,\boldsymbol{r} + V_{\text{L,S}}\psi_{\text{S}} + \\ (V_{\text{L}}^\dagger\lambda_i^2 + (H_{\text{L}} - E)\lambda_i)\,\boldsymbol{u}_{i,\text{i}}\,.\end{aligned} \tag{12}$$

Using Eq. (8) this equation can be simplified to

$$-V_{\text{L}}U_{\text{L,o}}\,\boldsymbol{r} + V_{\text{L,S}}\psi_{\text{S}} = V_{\text{L}}\boldsymbol{u}_{i,\text{i}}\,. \tag{13}$$

In the same fashion we can rewrite the remaining equations and arrive at a finite linear system:

$$\begin{pmatrix} -V_{\text{L}}U_{\text{L,o}} & V_{\text{L}} \\ V_L^\dagger U_{\text{L,o}}\Lambda_{\text{L,o}} & H_{\text{S}} - E \end{pmatrix}\begin{pmatrix} \boldsymbol{S} \\ \psi_S \end{pmatrix} = \begin{pmatrix} V_L U_i \\ -V_{\text{L,S}}^\dagger\lambda_i U_i \end{pmatrix} \tag{14}$$

This formulation avoids the error-prone inversion of U. Note that since $V_{\text{R/L}}$ and $V_{\text{R/L,S}}$ are assumed to have the same structure, the first and the last row have the same completely zero rows if the hopping does not connect to all points of the unit cell.

E. Lead modes via current eigenstates

Since lead wave functions only enter the system

F. Open questions

- Can one get rid of the evanescent part of the $\boldsymbol{t}$ and $\boldsymbol{r}$? Propbably with Schur complement method (eliminate these variables). Not sure if it's worth it.
- Connection to Green's function formalism - most likely, if I eliminate the $\boldsymbol{r}$ and $\boldsymbol{t}$'s completely, I end up again with the self-energies (In fact, if V_{lead} is invertible, one sees it immediately. For singular hopping one probably needs to work with an SVD decomposition, as the components of $\boldsymbol{r}$ corresponding to the zero singular values of V_{lead} do not enter the equation). The other way round, to get this type of equation from the self-energies only seems not possible.
- Assume for the sake of argument (in fact in practice this will most likely be not necessary) that I include a part of the lead in the scattering region. In this case, the amplitudes of the fastest decaying modes will be exponentially small, and it is a good approximation to neglect them all together. In terms of the linear system this means taking out the columns corresponding to these modes. The resulting linear system is then overdetermined, and will not have an exact solution any more (we did an approdximation!). Still the problem is well posed, as one can look for the best approximation under the given contraints (least squares problem). There are in principle dense (QR), sparse (sparse QR) and iterative (LSQR) methods for this problem. Instead of acting on the full matrix, the special form makes it probably possible to act on the lead degrees of freedom only, and turn the problem into a regular linear system.

  One rationale for this approach would be to use iterative solvers for the lead modes (which is another problem, that we didn't solve very satisfactorily yet), where one would only calculate the modes with the longest decay length.

  Overall, this needs a bit more reading (never thought about least squares problems).

---

[1] D. Z.-Y. Ting, E. T. Yu, and T. C. McGill. Phys. Rev. B **45**, 3583 (1992).