Numerical methods for the solution of Schrödinger equation for ballistic transport

Umberto Ravaioli

Beckman Institute and
Department of Electrical and Computer Engineering
University of Illinois at Urbana-Champaign
Urbana, IL 61801, USA

Time-dependent Schrödinger Equation

- **Goal of quantum mechanics is to give a quantitative description on a microscopic scale of individual elementary objects (electrons, photons, atoms,…) which behave both like particles and waves, exhibiting diffraction and interference phenomena.**

- **Propagation cannot be described by a trajectory $r(t)$ as for a classical particle, but by a field-like quantity $\psi(r,t)$ called wave function. The simplest wave function is a plane wave**

$$\psi(\vec{r},t) = \Psi_0 \exp\left[\hat{j}\left(\vec{k}\cdot\vec{r} - \omega t\right)\right]$$

with mechanical and wave parameters related as

$$\vec{p} = \hbar\vec{k}\,; \quad E = \hbar\omega\,; \qquad \underbrace{\omega = \omega(k)\,; \quad E = E(\vec{p})}_{\textit{dispersion relations}}$$

- For an electron in vacuum, the energy dispersion relation assumes the parabolic form which gives the kinetic energy

$$E = \frac{p^2}{2m_0} = \frac{\hbar^2 k^2}{2m_0} \qquad m_0 = 9.1 \times 10^{-31} \quad [kg]$$

A plane wave represents a mathematical limit, since it extends infinitely in space and time. A realistic particle could be constructed as a superposition of plane waves

$$\psi(\vec{r},t) = \iiint \Psi_0(\vec{k}) \exp\left[\hat{j}\left(\vec{k}\cdot\vec{r} - \omega(\vec{k})\,t\right)\right] \quad d^3k$$

The wave function plays the role of a probability amplitude, from which we assume the normalization for the probability density

$$\iiint |\psi(\vec{r},\,t)|^2 \, d^3\vec{r} = 1$$

- **The evolution of the wave function is described by the Schrödinger equation**

$$\hat{j}\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}=-\frac{\hbar^2}{2m_0}\nabla^2\psi(\vec{r},t)+V(\vec{r})\,\psi(\vec{r},t)$$

which is actually a system of two equations for the real and imaginary part of the wave function

$$\psi=\Re(\psi)+\hat{j}\,\Im(\psi)$$

$$\hbar\frac{\partial\Re(\psi)}{\partial t}=-\frac{\hbar^2}{2m_0}\nabla^2\Im(\psi)+V(\vec{r})\,\Im(\psi)$$

$$\hbar\frac{\partial\Im(\psi)}{\partial t}=-\frac{\hbar^2}{2m_0}\nabla^2\Re(\psi)+V(\vec{r})\,\Re(\psi)$$

- In operator notation the solution to Schrödinger equation is

$$\psi(\vec{r},t) = \exp\left(-\frac{\hat{j}}{\hbar}\bar{H}\,t\right)\psi(\vec{r},0)$$

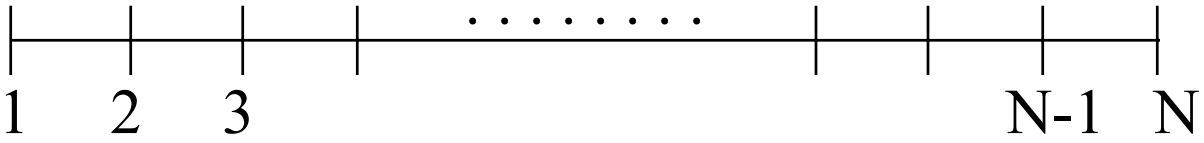
with the system Hamiltonian

$$\bar{H} = -\frac{\hbar^2}{2m_0}\nabla^2 + V(\vec{r})$$

This represents a formal solution of the Schrödinger equation as a first order differential equation in time. Except for trivial cases, we cannot find an analytical form for the exponential term containing the Hamiltonian.

All numerical solutions must find a suitable approximation of the exponential on a set of discrete points.

- **Consider a discretization of the domain involving N mesh points**



The discretized form of the solution is

$$\bar{\psi}(t+\Delta t) = \exp\left(-\frac{\hat{j}}{\hbar}\underline{H}\,\Delta t\right)\,\bar{\psi}(0)$$

$\underline{H}^{*}$ = **matrix representing the discretized Hamiltonian**

$\bar{\psi}(t)$ = **solution array defined on the mesh points**

- We need to find a numerical approximation for the exponential of the discretized operator

$$\exp\left(-\frac{\hat{j}}{\hbar}\underline{H}\,\Delta t\right)$$

satisfying:

a) stability of the iteration

b) conservation of the wave function probability

c) consistency (we really solve the intended equation)

1-D time-dependent Schrödinger equation

$$\hat{j}\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m_0}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(\vec{r})\psi(x,t)$$

Let's illustrate the properties of numerical solutions by using finite-differences on a uniform mesh.

A discretization may require

Explicit numerical methods – if it only requires a direct substitution of values in the formulation

Implicit methods – if it involves solution of a linear system of equations

A. Simple (naïve) explicit method

A simple direct finite difference discretization gives

$$\hat{j}\hbar\,\frac{\psi(i;n+1)-\psi(i;n)}{\Delta t}=-\frac{\hbar^2}{2m_0}\,\frac{\psi(i-1;n)-2\psi(i;n)+\psi(i+1;n)}{\Delta x^2}+V(i)\,\psi(i;n)$$

$$\psi(i;n+1)=\psi(i;n)+\hat{j}\Delta t\left(\frac{\hbar}{2m_0}\,\frac{\psi(i-1;n)-2\psi(i;n)+\psi(i+1;n)}{\Delta x^2}+\frac{V(i)}{\hbar}\,\psi(i;n)\right)$$

In operator notation

$$\bar{\psi}(n+1)=\left(I-\frac{\hat{j}}{\hbar}\bar{H}\Delta t\right)\quad\bar{\psi}(n)$$

UNSTABLE and NON-CONSERVING

B. Three-time-levels explicit method

A centered time difference is applied

$$\psi(i;n+1)=\psi(i;n-1)+2\hat{j}\Delta t\left(\frac{\hbar}{2m_0}\frac{\psi(i-1;n)-2\psi(i;n)+\psi(i+1;n)}{\Delta x^2}+\frac{V(i)}{\hbar}\psi(i;n)\right)$$

To obtain the operator algorithm, we need to eliminate the intermediate solution at iteration n

$$\frac{\bar{\psi}(n+1)-\bar{\psi}(n-1)}{2}=\bar{\psi}(n)$$

$$\Rightarrow \qquad \bar{\psi}(n+1)\approx\frac{\left(I-\hat{j}\bar{H}\,\Delta t/\hbar\right)}{\left(I+\hat{j}\bar{H}\,\Delta t/\hbar\right)}\;\bar{\psi}(n-1)$$

STABLE and UNITARY (CONSERVING)

C. Fully implicit method

Discretize space operator at timestep *(j+1)* leading to a system that requires a matrix inversion

$$\psi(i;n+1)+\hat{j}\Delta t\left(\frac{\hbar}{2m_0}\frac{\psi(i-1;n+1)-2\psi(i;n+1)+\psi(i+1;n+1)}{\Delta x^2}+\frac{V(i)}{\hbar}\psi(i;n+1)\right)$$
$$=\psi(i;n-1)$$

In operator notation

$$\bar{\psi}(n+1)=\left(I+\frac{\hat{j}}{\hbar}\bar{H}\Delta t\right)^{-1}\quad\bar{\psi}(n)$$

STABLE but NON-UNITARY (NON-CONSERVING)

D. Semi-implicit method (Crank-Nicholson, also Cayley)

The right hand side is discretized as an average of operators at the two timesteps

$$\hat{j}\hbar\frac{\psi(i;n+1)-\psi(i;n)}{\Delta t}=\frac{1}{2}\left[RHS(n+1)+RHS(n)\right]$$

$$\Rightarrow\quad \psi(i-1;n+1)+\left(\hat{j}\frac{4m_0\Delta x^2}{\hbar\Delta t}-\frac{2m_0\Delta x^2}{\hbar^2}V(i)-2\right)\psi(i;n+1)+\psi(i+1;n+1)$$

$$=\psi(i-1;n)+\left(\hat{j}\frac{4m_0\Delta x^2}{\hbar\Delta t}+\frac{2m_0\Delta x^2}{\hbar^2}V(i)+2\right)\psi(i;n)+\psi(i+1;n)$$

In operator notation

$$\bar{\psi}(n+1)=\frac{I-\hat{j}\bar{H}\Delta t/(2\hbar)}{I+\hat{j}\bar{H}\Delta t/(2\hbar)}\quad\bar{\psi}(n)$$

STABLE and UNITARY (CONSERVING)

Of the schemes analyzed, only the three time steps explicit

$$\bar{\psi}(n+1) \approx \frac{\left(I - \hat{j}\bar{H}\Delta t/\hbar\right)}{\left(I + \hat{j}\bar{H}\Delta t/\hbar\right)} \quad \bar{\psi}(n-1)$$

and the Crank Nicholson semi-implicit method

$$\bar{\psi}(n+1) = \frac{I - \hat{j}\bar{H}\Delta t/(2\hbar)}{I + \hat{j}\bar{H}\Delta t/(2\hbar)} \quad \bar{\psi}(n)$$

are suitable.

One can see that the numerical operators are essentially equivalent.

The unitary finite difference schemes can be readily extended to 2D. Let's assume for simplicity a uniform mesh

$$\Delta = \Delta x = \Delta y$$

The three times level scheme becomes

$$\psi(i,j;n+1) = \psi(i,j;n-1) + \hat{j}\frac{\Delta t}{\Delta^2}\frac{\hbar}{m_0}(\psi(i-1,j;n) + \psi(i,j-1;n)$$
$$-4\psi(i,j;n) + \psi(i+1,j;n) + \psi(i,j+1;n)) - \hat{j}\frac{2\Delta t}{\hbar}V(i)\psi(i,j;n)$$

The numerical solution is still obtained by a simple recursion, without having to solve a matrix problem.

The Crank-Nicholson algorithm is

$$\psi(i,j;n+1)-\psi(i,j;n)=-\hat{j}\frac{\Delta t}{2\hbar}\Big[V(i,j)\psi(i,j;n+1)+V(i,j)\psi(i,j;n)$$
$$-\frac{\hbar^2}{2m_0\Delta^2}\big(\psi(i-1,j;n+1)-2\psi(i,j;n+1)+\psi(i+1,j;n+1)+$$
$$\psi(i-1,j;n)-2\psi(i,j;n)+\psi(i+1,j;n)+$$
$$\psi(i,j-1;n+1)-2\psi(i,j;n+1)+\psi(i,j+1;n+1)$$
$$\psi(i,j-1;n)-2\psi(i,j;n)+\psi(i,j+1;n+1)\big)\Big]$$

The algorithm can be rewritten for matrix implementation, by moving all terms at timestep (n+1) to the left and all terms at timestep n to the right. Numerical solution of a 5-diagonal matrix problem is required at each iteration.

To alleviate the requirements of the matrix solution, it is possible to use an Alternate Direction Implicit (ADI) scheme. The time step is split into two sub-steps of half duration, and two consecutive sets of solutions are performed:

Horizontal sweep

$$\psi(i,j;n+1/2)+\hat{j}\frac{\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m_0\Delta^2}\left(\psi(i-1,j;n+1/2)-2\psi(i,j;n+1/2)\right.\right.$$
$$\left.\left.+\left(\psi(i+1,j;n+1/2)\right)+\frac{V(i,j)}{2}\psi(i,j;n+1/2)\right]=\right.$$
$$\psi(i,j;n)-\hat{j}\frac{\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m_0\Delta^2}\left(\psi(i,j-1;n)-2\psi(i,j;n)\right.\right.$$
$$\left.\left.+\left(\psi(i,j+1;n)\right)+\frac{V(i,j)}{2}\psi(i,j;n)\right]\right.$$

Vertical sweep

$$\psi(i,j;n+1)+\hat{j}\frac{\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m_0\Delta^2}\left(\psi(i,j-1;n+1)-2\psi(i,j;n+1)\right.\right.$$
$$\left.\left.+\left(\psi(i,j+1;n+1)\right)+\frac{V(i,j)}{2}\psi(i,j;n+1)\right]=\right.$$
$$\psi(i,j;n+1/2)-\hat{j}\frac{\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m_0\Delta^2}\left(\psi(i-1,j;n+1/2)-2\psi(i,j;n+1/2)\right.\right.$$
$$\left.\left.+\left(\psi(i+1,j;n+1/2)\right)+\frac{V(i,j)}{2}\psi(i,j;n+1/2)\right]\right.$$

The ADI procedure decouples adjacent rows and columns of mesh points. For every sweep, a set of tridiagonal systems is solved.

Because of the decoupling, the tridiagonal solutions in each sweep can be carried out independently, therefore the approach is suitable for supercomputing applications (vectorization, parallelization).

In the numerical scheme shown here, the contribution by the potential is equally divided between the implicit part (left hand side) and the explicit part (right hand side) of the algorithm.

Note: the intermediate solution after a horizontal sweep is still very biased. Only solutions obtained after two consecutive sweeps should be considered.

Possible discussion items:

How can one implement a self-consistent solution (Poisson equation solved at each iteration to update the potential) in a three-time-step explicit method or in a semi-implicit method, where the potential should be known for the "next" timestep already?

What trade-offs and approximations are possible/reasonable?

Systems with variable effective mass

In the effective mass approximation, the potential V in the Schrödinger equation is assumed to be only the electrostatic potential, since the effect of the periodic crystal is accounted for by the effective mass itself.

However, some of the most interesting applications of quantum systems involve spatially varying materials and heterojunctions. The effective mass approximation can still be used with some caution.

When the effective mass is space-dependent, the major issue is to find the Hamiltonian operator, so that it remains Hermitian.

If we just insert a space dependent mass in the Schrödinger as is we know that the Hamiltonian is not Hermitian. Also, this method would be mathematically applicable only to slowly varying mass.

A widely used Hermitian form brings the effective inside the Laplacian differential operator

$$-\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m^*}\nabla\psi\right)$$

This operator can be used also for transport across abrupt heterojunctions, as long as the materials on the two sides have similar properties and band structure (e.g. AlGaAs/GaAs).

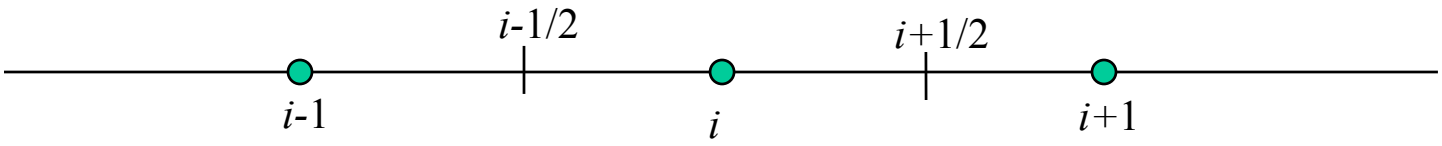
But one has to keep in mind that very close to the heterojunction the physical properties, described by the effective mass Schrödinger equation, are not necessarily well defined.

Let's consider a 1-D situation with uniform mesh. We can discretize first the outer differential operator considering the mid-points of the intervals around the mesh point i, using center differences

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial x}\left[\frac{1}{m^*}\frac{\partial \psi}{\partial x}\right] \approx -\frac{\hbar^2}{2\Delta x}\left[\left(\frac{1}{m^*}\frac{\partial \psi}{\partial x}\right)_{i+1/2} - \left(\frac{1}{m^*}\frac{\partial \psi}{\partial x}\right)_{i-1/2}\right]$$

Then the derivatives on the mid-points are also evaluated with center differences

$$-\frac{\hbar^2}{2(\Delta x)^2}\left[\frac{\psi(i+1)-\psi(i)}{m^*(i+1/2)} - \frac{\psi(i)-\psi(i-1)}{m^*(i-1/2)}\right]$$



The effective mass only needs to be known at the mid-points. If an abrupt heterojunction is located at point l, the abrupt change of effective mass is treated correctly in mathematical terms and without ambiguity. We avoid having to assume an effective mass value exactly at the heterojunction.

There are other possible Hamiltonians for the space-dependent mass case, which are Hermitian. The following operator is Hermitian, and is obtained as linear combination of two non-Hermitian operators

$$-\frac{\hbar^2}{4}\left[\frac{1}{m^*}\nabla^2\psi+\nabla^2\left(\frac{1}{m^*}\ \psi\right)\right]$$

Let's compare the two Hamiltonians, in a 1-D formulation

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial x}\left[\frac{1}{m^*}\frac{\partial \psi}{\partial x}\right] = -\frac{\hbar^2}{2}\left[\frac{1}{m^*}\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial \psi}{\partial x}\frac{\partial}{\partial x}\left(\frac{1}{m^*}\right)\right]$$

$$-\frac{\hbar^2}{4}\left[\frac{1}{m^*}\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2}{\partial x^2}\left(\frac{1}{m^*}\,\psi\right)\right] =$$

$$-\frac{\hbar^2}{2}\left[\frac{1}{m^*}\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial \psi}{\partial x}\frac{\partial}{\partial x}\left(\frac{1}{m^*}\right)\right.$$

$$\left. + \underbrace{\frac{1}{2}\psi\frac{\partial^2}{\partial x^2}\left(\frac{1}{m^*}\right)}_{\text{extra term}}\right]$$

For smoothly varying mass, the two approaches are approximately equivalent. One can see that it is awkward to directly discretize with finite differences the numerical operators on the right hand side. The proper procedure is to use box integration, over the interval [*i-1/2; i+1/2*]. Integration by parts can be applied

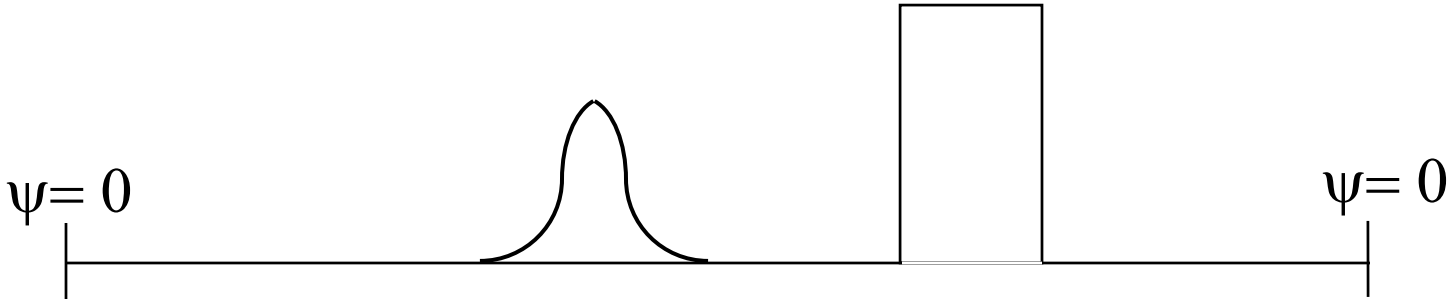
$$-\frac{\hbar^2}{2\Delta x}\int_{i-1/2}^{1+1/2} dx\left[\frac{1}{m^*}\frac{\partial^2\psi}{\partial x^2}+\frac{\partial\psi}{\partial x}\frac{\partial}{\partial x}\left(\frac{1}{m^*}\right)\right]=$$

$$\underbrace{-\frac{\hbar^2}{2\Delta x}\left[\left[\frac{1}{m^*}\frac{\partial\psi}{\partial x}\right]_{1-1/2}^{1+1/2}\right.}_{\text{same as previous result}}-\cancel{\int_{i-1/2}^{1+1/2} dx\frac{\partial\psi}{\partial x}\frac{\partial}{\partial x}\left(\frac{1}{m^*}\right)}$$

$$\left.+\cancel{\int_{i-1/2}^{1+1/2} dx\frac{\partial\psi}{\partial x}\frac{\partial}{\partial x}\left(\frac{1}{m^*}\right)}\right]$$

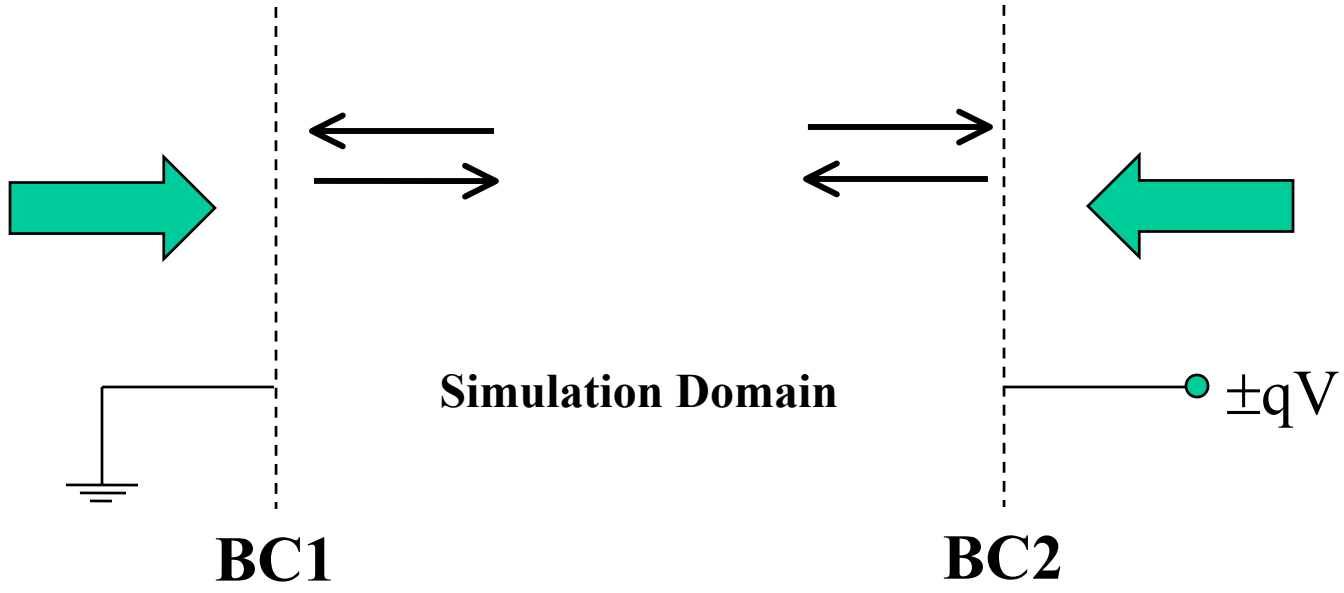
Absorbing boundary conditions

Numerical solution of the time-dependent Schrödinger equation is often accomplished by assuming a gaussian wave packet distribution describing the particle. The boundaries of the systems are taken to be far away from the simulated region, and the wave function there is fixed to zero.



As the simulation progresses, the wave packet spreads and intercats with potential variations, originating reflected wavepackets. Over a sufficient number of simulation steps, the wave may reach the boundaries, where the condition of zero wave function corresponds to perfect reflection!

In order to let the wave function exist the domain, we need to implement absorbing boundary conditions.



$$\psi_1 = \underbrace{A\exp(\hat{j}\,k_x x)}_{input} + B(x)\exp(-\hat{j}\,k_x x)$$

Assume $B(x)$ approximately linear near the boundary BC1

$$\hat{j}\hbar\frac{\partial\psi(0,t)}{\partial t} = -\frac{\hbar^2}{2m_0}\frac{\partial^2\psi(0,t)}{\partial x^2} + \cancel{V(0)\psi(0,t)}$$

$$= -\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial x^2}\left(A e^{\hat{j}k_x x} + B(x) e^{-\hat{j}k_x x} \right)$$

$$= \frac{\hbar^2 k_x^2}{2m_0}\psi(x,t) + \hat{j}\frac{\hbar^2 k_x}{m_0} e^{-\hat{j}k_x x}\frac{\partial B(x)}{\partial x} + \ldots$$

The formal solution of the differential equation in time gives

$$\psi\left(t=\Delta t\right)\approx\psi\left(t=0\right)e^{-\hat{j}\left(E/\hbar\right)\Delta t}$$
$$+\frac{\hbar k_x}{m^*}\frac{\partial B\left(x\right)}{\partial t}e^{-\hat{j}k_x x}\Delta t$$

At BC2 similar treatment with

$$k_{BC2}=\frac{\sqrt{2m^*\left[E-qV\right]}}{\hbar}$$

Create a new discretized equation near the boundaries

$$\frac{\partial B(x)}{\partial t} = \frac{B(\Delta x) - B(0)}{\Delta x} \qquad BC1$$

$$= \frac{B(x_{\max}) - B(x_{\max} - \Delta x)}{\Delta x} \qquad BC2$$

In a Crank-Nicholson scheme

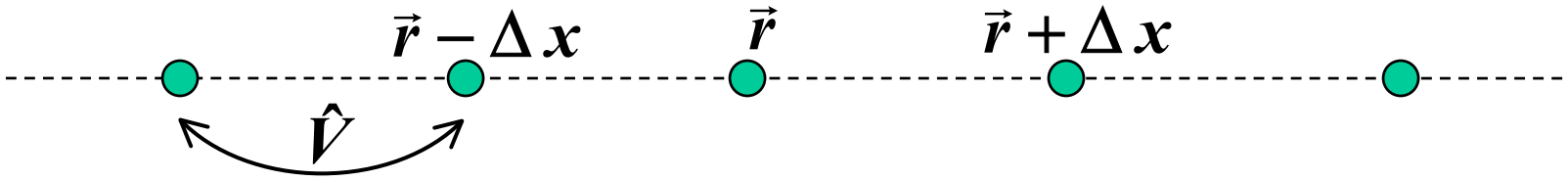
$$\frac{\partial B(x)}{\partial t} = \frac{1}{2}\left[\left(\frac{\partial B(x)}{\partial x}\right)^{t} + \left(\frac{\partial B(x)}{\partial x}\right)^{t+\Delta t}\right]$$

In general

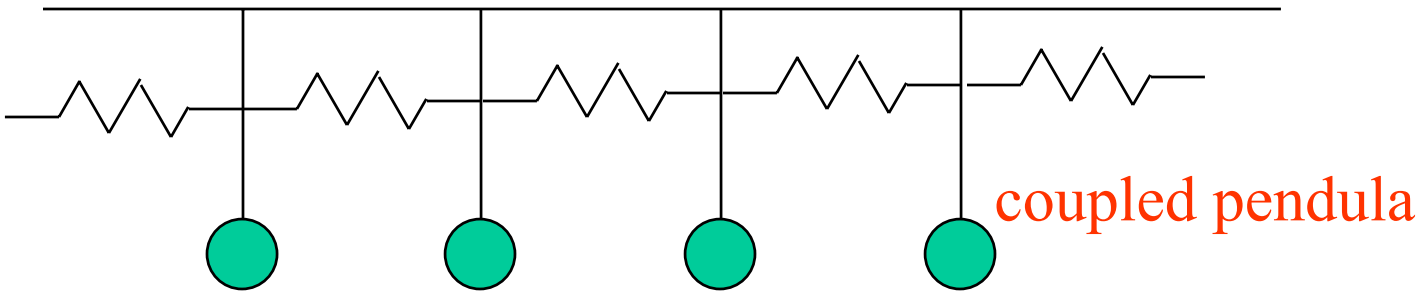
$$\psi_{BC} = A\, e^{\hat{j} k_i x} + B(x)\, e^{-\hat{j} k_R x}$$

The numerical value of the reflected momentum may differ slightly from the incident momentum, during a transient, particularly in 2D and 3D situations.

Issue: discretization changes the relationship between (simulated) energy and momentum! Discetization creates a virtual lattice where transport is described by the Tight-Binding Hamiltonian



$$\hat{H}=\sum_{\vec{r}}\left(|l><E_{\vec{r}}<l|+|l>\hat{V}<l+1|+|l>\hat{V}<l-1|\right)$$



Potential for transferring an electron from one site to a neighbor

$$\hat{V} = -\frac{\hbar^2}{2m^*}\frac{1}{(\Delta x)^2} = \text{hopping potential}$$

Energy of an electron located at a lattice site

$$E_{\vec{r}} = \underbrace{V(\vec{r})}_{\substack{\textit{potential} \\ \textit{energy}}} - 2\hat{V}$$

Atomic-like orbital centers at the sites $\vec{r}$ (forming a regular lattice)

$$|l>$$

In the continuum limit

$$\hat{H} \rightarrow H = -\frac{\hbar^2}{2m^*}\frac{d^2}{dr^2} + V(\vec{r})$$

$$\hat{H} = \text{finite difference approximation}$$

For a periodic lattice

$$V(\vec{r}) = 0$$

$$|\vec{k}> = \frac{1}{\sqrt{N}}\sum_l \exp\left(\hat{j}\,k\,l\Delta x\right)|l>$$

$$E(k) = E_0 + \sum_l V_{0l}\exp\left(\hat{j}\,k\,l\Delta x\right)$$

l ← neighbors

Consider a periodic chain with constant energy parameters and mass, and uniform potential energy distribution. The discretized Hamiltonian is described by a tridiagonal matrix

$$\begin{vmatrix} E_0 & \hat{V} & 0 & 0 & 0 \\ \hat{V} & E_0 & \hat{V} & 0 & 0 \\ 0 & \hat{V} & E_0 & \hat{V} & 0 \\ 0 & 0 & \hat{V} & E_0 & \hat{V} \\ 0 & 0 & 0 & \hat{V} & E_0 \end{vmatrix}$$

Eigenvalues of the tridiagonal matrix

$$E_n = E_0 + 2\hat{V}\cos\left(\frac{n\pi}{N+1}\right)$$

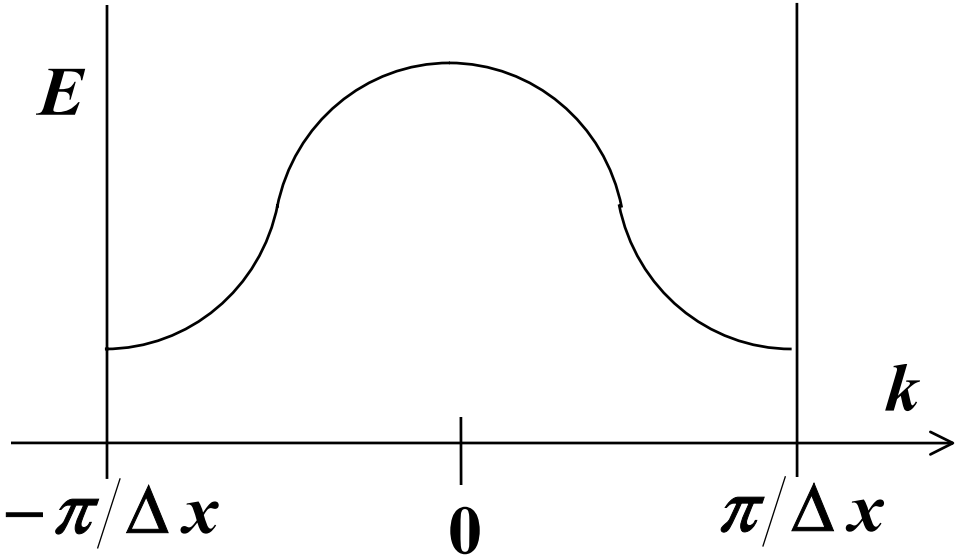
Dispersion relationship for the discretized Hamiltonian is not parabolic!

Absorbing boundary conditions for a discretized Hamiltonian should be derived in the tight-binding formalism.

$$E(k) = E_0 + \hat{V}\sum_l \exp(\hat{j}\,k\,l)$$

$$= E_0 + \hat{V}\left(\exp(\hat{j}\,k\,\Delta x) + \exp(-\hat{j}\,k\,\Delta x)\right)$$

$$= E_0 + 2\hat{V}\cos(k\Delta x)$$



$BC1 \rightarrow l = 0 \qquad E_0 = \text{constant} \qquad \Delta x = a$

$$\langle 0|\hat{H}|\psi\rangle = E_0\langle 0|\psi\rangle + \hat{V}\left[\langle 1|\psi\rangle + \langle -1|\psi\rangle\right] =$$

$$= E_0\langle 0|\psi\rangle + \hat{V}\left[Ae^{\hat{j}ka} + B(1)e^{-\hat{j}ka} + Ae^{-\hat{j}ka} + B(-1)e^{\hat{j}ka} \right]$$

$$\left.\begin{aligned} B(1) &= B(0) + \Delta B \\ B(-1) &= B(0) - \Delta B \end{aligned}\right\} B(x) \text{ linear at boundary}$$

$$\langle 0|\hat{H}|\psi\rangle = E_0\langle 0|\psi\rangle + \hat{V}\left[e^{\hat{j}ka} \underbrace{\left(A + B(0)\right)}_{\langle 0|\psi\rangle} + \right.$$

$$\left. + e^{-\hat{j}ka}\left(A + B(0)\right) + \hat{V}\Delta B\left(e^{-\hat{j}ka} - e^{\hat{j}ka}\right)\right]$$

$$\langle 0|\hat{H}|\psi\rangle = \underbrace{\left[E_0 + 2V\cos(ka)\right]}_{E(k)\text{ for TBH}}\langle 0|\psi\rangle - \hat{j}\,2\hat{V}\,\Delta B\sin(ka)$$

$$\Delta B = B(1) - B(0) = B(0) - B(-1)$$

$$\Delta B = \langle 1|\psi_R\rangle e^{\hat{j}\,ka} - \langle 0|\psi_R\rangle =$$

$$= \underbrace{\left(\langle 1|\psi\rangle - \langle 1|\psi_{in}\rangle\right)}_{reflected} e^{\hat{j}\,ka} - \left(\langle 0|\psi\rangle - \langle 0|\psi_{in}\rangle\right)$$

$$= \left(\langle 1|\psi\rangle e^{\hat{j}\,ka} - \langle 0|\psi\rangle\right) - \langle 0|\psi_{in}\rangle\left(e^{2\hat{j}\,ka} - 1\right)$$

$$= \langle 1|\psi\rangle e^{\hat{j}\,ka} - \langle 0|\psi\rangle - 2\,\hat{j}\,e^{\hat{j}\,ka}\sin(ka)\langle 0|\psi_{in}\rangle$$

Final results for absorbing boundary conditions at input

$$\langle 0|\hat{H}|\psi\rangle = \left[E_0 + 2V\cos(ka)\right]\langle 0|\psi\rangle$$
$$+ \hat{j}\,2\hat{V}\sin(ka)\langle 0|\psi\rangle - \hat{j}\,2\hat{V}\sin(ka)\langle 1|\psi\rangle e^{\hat{j}\,ka}$$
$$- 4\hat{V}e^{\hat{j}\,ka}\sin^2(ka)\langle 0|\psi_{in}\rangle$$

ψ_R **has been eliminated**

An even more refined methodology for absorbing boundary conditions can be found at:

L.F. Register, U. Ravaioli and K. Hess, *J. Applied Physics*, vol. 69, pp. 7153-7158, 1991 (+ small corrections at the Erratum section of: *J. Applied Physics*, vol 71, p. 1555, 1992),

Time-independent transport with Schrödinger equation

We consider her an open system in steady-state conditions. The open system consists of a finite region connected to reservoirs of particles (contacts).

Waves (particles) flow between the system and the reservoirs, with reflection and transmission properties depending on the potential profile. Waves entering from any separate reservoir contact are studied with an independent solution.

Assuming stationary states

$$\Psi(\vec{r},t) = \psi(\vec{r})\exp(-\hat{j}\omega t) = \psi(\vec{r})\exp(-\hat{j}\frac{E}{\hbar}t)$$

the steady-state Schrödinger equation has the form

$$-\frac{\hbar^2}{2m_0}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

Let's consider a 1-D domain with uniform grid and mesh size Δx. The time independent Schrödinger equation is discretized with finite differences

$$-\frac{\hbar^2}{2m_0}\frac{\psi(i-1)-2\psi(i)+\psi(i+1)}{(\Delta x)^2}+\left[V(i)-E\right]\psi(i)=0$$

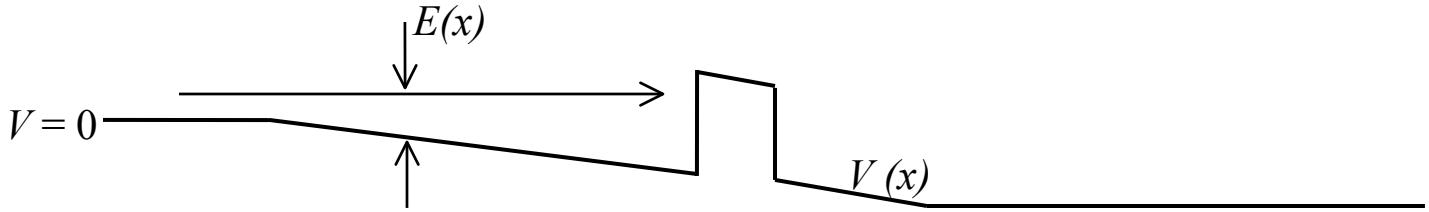
E represents the total energy, so that $V(i)$ - E is the kinetic energy. It is often convenient to set the reference zero of the potential $V(x)$ at the inflow boundary, so that E corresponds to the incident kinetic energy.

The kinetic energy varies spatially according to the potential changes, and the wavenumber $k_x(x)$ varies accordingly. The knowledge of k_x at the reservoir ends, allows the specification of boundary conditions.

The travelling wave at the specified energy can be assumed to be a plane wave of the form

$$\psi(x) = A(x)\exp\left[\pm\hat{j}\,k_x(x)\,x\right]$$

where the sign indicates the direction of propagation. Boundary conditions are derived from this expression for both forward and backward wave.



The exponentials are completely specified in the boundary conditions by the knowledge of E and $V(x)$. The prefactor A is set to a conventional reference (e.g., A=1) at the one boundary, and the value at the other end is the outcome of the solution. The solution for the pre-factor A may be complex, and it contains the information on reflection and transmission coefficients.

In 1-D, all is needed for the solution is a recursion algorithm. For a forward travelling wave which enters the open system at $x = 0$, we can set $A(L) = 1$ (L is the length of the domain) and obtain the boundary condition

$$\psi(N) = \exp\left[\hat{j}\, k_x(N) L\right]$$

N is the index corresponding to the output boundary. Assuming that the domain is subdivided into N mesh intervals, the index for the left boundary is i = 0. To solve the open system problem, we need to assume a perfect reservoir with a constant potential (ohmic contact) and no change in the wavevector k_x

$$k_x(N) = k_x(N+1) \quad \Rightarrow \quad \psi(N+1) = \exp\left[\hat{j}\, k_x(N)\left(L + \Delta x\right)\right]$$

The knowledge of the wave function N and $N+1$ is sufficient to calculate the value of ψ $(N-1)$ using the discretized Schrödinger equation.

The general recursion algorithm can be easily obtained by rewriting the discretized Schrödinger equation

$$\psi_{i-1} = \left[2 + \frac{2m_0 (\Delta x)^2}{\hbar^2} \left(V(i) - E \right) \right] \psi_i - \psi_{i+1}$$

The potential reference is $V(0) = 0$, so that E represents the kinetic energy

$$E = \frac{\hbar^2 k_x^2(0)}{2 m_0}$$

as well as the total energy at the inflow point $i = 0$.

Because of reflection due to the potential variations, throughout the device one can express the wave function as the superposition of an incident and a reflected wave

$$\psi(i) = I(i)\exp\left[\hat{j}\,k_x(i)\,i\,\Delta x\right] + R(i)\exp\left[-\hat{j}\,k_x(i)\,i\,\Delta x\right]$$

At the output, because of the constant potential in the reservoir, we assume that there is no reflection

$$R(N) = 0 \qquad \text{and} \qquad I(N) = A(N)$$

At the input we can express the total wave function as

$$\psi(0) = A(0) = I(0) + R(0)$$

To find the amplitude of incident and reflected waves, we need an additional solution at a mesh point inside the input reservoir. With the same assumptions as for the output reservoir

$$x = -\Delta x\,; \quad i = -1 \qquad \Rightarrow \qquad \psi(-1) = I(-1) + R(-1)$$

$$\psi(-1) = I(0)\exp\left[-\hat{j}\,k_x(0)\,\Delta x\right] + R(0)\exp\left[\hat{j}\,k_x(i)\,\Delta x\right]$$

By combining the above with

$$\psi(0) = A(0) = I(0) + R(0)$$

we obtain

$$I(0) = \frac{\psi(0)\exp\left[\hat{j}\,k_x(0)\Delta x\right] - \psi(-1)}{2\hat{j}\sin\left(k_x(0)\Delta x\right)}$$

Once $I(0)$ is determined, the wave function throughout the device can be re-normalized to make the total probability unitary.

The procedure for inflow from the right boundary is essentially the same, with appropriate sign changes for the waves. The recursion relation becomes

$$\psi_{i+1} = \left[2 + \frac{2m_0 (\Delta x)^2}{\hbar^2} \left(V(i) - E \right) \right] \psi_i - \psi_{i-1}$$

with the starting point

$$\psi(0) = 1 \quad \text{and} \quad \psi(-1) = \exp\left[-\hat{j} k_x(0) \, \Delta x \right]$$

The recursions are solved for a set of energies and for inflow from both boundaries. In order to find the total result, one still needs to specify injection condition, that provide the weights for adding all the separate recursion results.

We consider now a simple case for an n-type semiconductor, where the two reservoirs are assumed in quasi-equilibrium, with a specific Fermi level E_F.

The equilibrium particle density, including the effect of spin, is

$$n = \frac{1}{4\pi^3} \iiint_{-\infty}^{\infty} dk_x dk_y dk_z \frac{1}{1 + \exp\left[\left(E - E_F\right)/k_B T\right]}$$

Assuming for simplicity an isotropic mass, the particle energy is

$$E = E_x + E_\perp = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2\left(k_y^2 + k_z^2\right)}{2m^*}$$

To determine the density for the injection direction, we need to integrate over the transverse direction

The integration is performed over the transverse momentum components, in polar coordinates

$$n = \frac{1}{4\pi^3}\int_{-\infty}^{\infty} dk_x \int_0^{2\pi} d\theta \int_0^{\infty} d\left|\mathbf{k}_\perp\right| \frac{\left|\mathbf{k}_\perp\right|}{1+\exp\left[\left(E_\perp + E_x - E_F\right)/k_B T\right]}$$

The integration over the angle provides simply a factor 2π and a change of variable is performed

$$\left|\mathbf{k}_\perp\right| \rightarrow E_\perp \qquad \left|\mathbf{k}_\perp\right| = \frac{\sqrt{2m^* E_\perp}}{\hbar}$$

$$d\left|\mathbf{k}_\perp\right| = \frac{\sqrt{2m^*}}{2\hbar\sqrt{E_\perp}} dE_\perp$$

We obtain

$$n = \frac{m^*}{2\pi^2\hbar^2}\int_{-\infty}^{\infty} dk_x \int_0^{\infty} \frac{dE_\perp}{1+\exp\left[\left(E_\perp + E_x - E_F\right)/k_B T\right]}$$

The integration can be carried out exactly according to

$$\int \frac{dx}{1+\exp(x)} = -\log\left[1+\exp(x)\right]$$

from which

$$n = \frac{m^* k_B T}{2\pi^2\hbar^2}\int_{-\infty}^{\infty} dk_x \;\; \log\left[1+\exp\left(\frac{E_F - E_x}{k_B T}\right)\right]$$

From this result, deduce that the electron density corresponding to an incident momentum k_x is

$$n = \frac{m^* k_B T}{2\pi^2 \hbar^2} \log\left[1 + \exp\left(\frac{E_F - \hbar^2 k_x^2 / 2m^*}{k_B T}\right)\right]$$

The expression above can be used as a weight to combine the incident waves which are injected from the reservoir momentum distribution.

The Fermi-Dirac distribution in the contacts is valid close to equilibrium. Far from equilibrium, one can still use the approach to get a qualitative solution. However, in a general situation, the boundary conditions for the injection distribution should be adapted self-consistently to the bias.

Let's trace the same steps for a classical distribution of particles from a Maxwellian distribution

$$n = \left(\frac{m}{2\pi k_B T}\right)^{3/2} \iint \int_{-\infty}^{\infty} dv_x dv_y dv_z \; e^{-\frac{mv_x^2}{2k_B T}} e^{-\frac{mv_\perp^2}{2k_B T}}$$

$$n = \left(\frac{m}{2\pi k_B T}\right)^{3/2} \int_{-\infty}^{\infty} dv_x \int_0^{2\pi} d\theta \int_0^{\infty} d|v_\perp| \quad |v_\perp| e^{-\frac{mv_x^2}{2k_B T}} e^{-\frac{mv_\perp^2}{2k_B T}}$$

$$|v_\perp| = \sqrt{\frac{2E_\perp}{m}} \qquad d|v_\perp| = \sqrt{\frac{2}{m}} \frac{1}{2\sqrt{E_\perp}} dE_\perp$$

After changing variables

$$n = \left(\frac{m}{2\pi k_B T}\right)^{3/2} 2\pi \int_{-\infty}^{\infty} dv_x \int_{0}^{\infty} dE_\perp \sqrt{\frac{2E_\perp}{m}} \sqrt{\frac{2}{m}} \frac{1}{2\sqrt{E_\perp}} e^{-\frac{E_\perp - E_x}{k_B T}}$$

$$n = \left(\frac{m}{2\pi k_B T}\right)^{3/2} \frac{2\pi}{m} \int_{-\infty}^{\infty} dv_x \int_{0}^{\infty} dE_\perp \quad e^{-\frac{E_\perp - E_x}{k_B T}}$$

$$n = \left(\frac{m}{2\pi k_B T}\right)^{3/2} \frac{2\pi}{m} \int_{-\infty}^{\infty} dv_x \underbrace{\left[-k_B T \quad e^{-\frac{E_\perp - E_x}{k_B T}} \right]_0^{\infty}}_{0 - \left(-k_B T \exp\left(0 + E \ / k_B T\right)\right)}$$

Finally

$$n = \left(\frac{m}{2\pi k_B T}\right)^{3/2} \frac{2\pi k_B T}{m} \int_{-\infty}^{\infty} dv_x \; e^{-\frac{mv_x^2}{2k_B T}}$$

$$n = \left(\frac{m}{2\pi k_B T}\right)^{1/2} \int_{-\infty}^{\infty} dv_x \; e^{-\frac{mv_x^2}{2k_B T}}$$

$$n = \int_{-\infty}^{0} dv_x \underbrace{\left(\frac{m}{2\pi k_B T}\right)^{1/2} e^{-\frac{mv_x^2}{2k_B T}}}_{\text{negative } v_x} + \int_{0}^{\infty} dv_x \underbrace{\left(\frac{m}{2\pi k_B T}\right)^{1/2} e^{-\frac{mv_x^2}{2k_B T}}}_{\text{positive } v_x}$$

Here are the injecting distributions for the two cases

$$n = \frac{m^* k_B T}{2\pi^2 \hbar^2} \int_0^\infty dk_x \;\; \log\left[1 + \exp\left(\frac{E_F - E_x}{k_B T}\right)\right]$$

$$n = \left(\frac{m}{2\pi k_B T}\right)^{1/2} \int_0^\infty dv_x \;\; e^{-\frac{m v_x^2}{2 k_B T}}$$

Once the wave function is determined, it is possible to evaluate the current flowing in the structure. Again using a parabolic dispersion relation, the electron current associated with a specific momentum component is defined as

$$\vec{J} = \rho \vec{v}\left(\vec{\mathbf{k}}\right) = -q\,\psi\,\psi^{*}\,\frac{\hbar\,\vec{\mathbf{k}}}{m^{*}}$$

For a plane wave

$$\nabla\psi = \hat{j}\,\vec{\mathbf{k}}\,\psi$$

from which we obtain the alternative expression

$$\vec{J} = -q\,\frac{\hbar}{m^{*}}\,\Im\left(\psi^{*}\,\nabla\psi\right)$$

The continuity equation for electrons has the form

$$\frac{\partial \rho}{\partial t} = -q\frac{\partial |\psi|^2}{\partial t} = -\nabla \cdot \vec{J}$$

where

$$\frac{\partial |\psi|^2}{\partial t} = \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}$$

From Schrödinger equation

$$\frac{\partial |\psi|^2}{\partial t} = \psi^* \left(\frac{\hat{j}\,\hbar}{2m^*}\nabla^2\psi + \frac{1}{\hat{j}\,\hbar}V(\vec{r})\,\psi \right)$$

$$-\psi \left(\frac{\hat{j}\,\hbar}{2m^*}\nabla^2\psi^* + \frac{1}{\hat{j}\,\hbar}V(\vec{r})\,\psi^* \right) = \frac{\hat{j}\,\hbar}{2m^*}\left(\psi^*\nabla^2\psi - \psi\,\nabla^2\psi^* \right)$$

Then, since

$$\nabla \cdot \left(\psi^* \nabla \psi \right) = \psi^* \nabla^2 \psi + \nabla \psi^* \cdot \nabla \psi$$

we have

$$\frac{\partial |\psi|^2}{\partial t} = \frac{\hat{j}\,\hbar}{2m^*} \nabla \cdot \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right)$$

and from the continuity equation itself

$$\frac{\partial \rho}{\partial t} = -q \frac{\partial |\psi|^2}{\partial t} = -\nabla \cdot \vec{J}$$

we get yet another expression for the current density

$$\vec{J} = \frac{\hat{j}\,q\,\hbar}{2m^*} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right)$$

Here are together all the expressions for current that we found

$$\vec{J} = \rho \vec{v}\left(\vec{\mathbf{k}}\right) = -q\,\psi\,\psi^{*}\,\frac{\hbar\,\vec{\mathbf{k}}}{m^{*}}$$

$$\vec{J} = -q\,\frac{\hbar}{m^{*}}\,\Im\left(\psi^{*}\,\nabla\,\psi\right)$$

$$\vec{J} = \frac{\hat{j}\,q\,\hbar}{2m^{*}}\left(\psi^{*}\nabla\,\psi - \psi\,\nabla\,\psi^{*}\right)$$

In practice, one cannot select all possible values of the incident momentum and the momentum axis is discretized. Assuming a uniform discretization step Δk_x we can take the mid-value of the interval as the average momentum for that mesh. We can expressed the following quantities for a 1-D system

$$n(x) = \sum_i n(k_i)\ \Delta k\ \ \psi_i^*(x)\,\psi_i(x)$$

$$J(x) = -\frac{q\hbar}{m^*}\sum_i n(k_i)\,\Delta k\,\Im\left(\psi_i^*(x)\frac{\partial \psi_i(x)}{\partial x}\right)$$

$$= \hat{j}\,\frac{q\hbar}{2m^*}\sum_i n(k_i)\,\Delta k\left(\psi_i^*(x)\frac{\partial \psi_i(x)}{\partial x} - \psi_i(x)\frac{\partial \psi_i^*(x)}{\partial x}\right)$$

Note that these formulas are general and can be applied to both time-independent and time-dependent formulations

Possible discussion items:

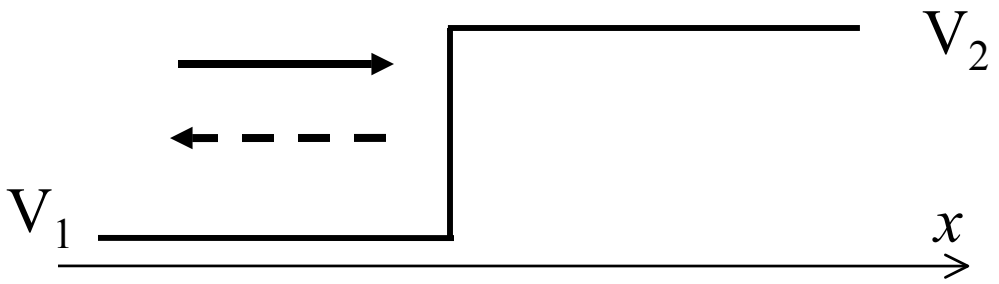
What can we do to formulate boundary conditions when quasi-equilibrium is not a good assumption?

How can we formulate a self-consistent simulation?

Video animation: Switching in a quantum nanostructure

1D quantum simulation using transmission line theory

Consider a single barrier system



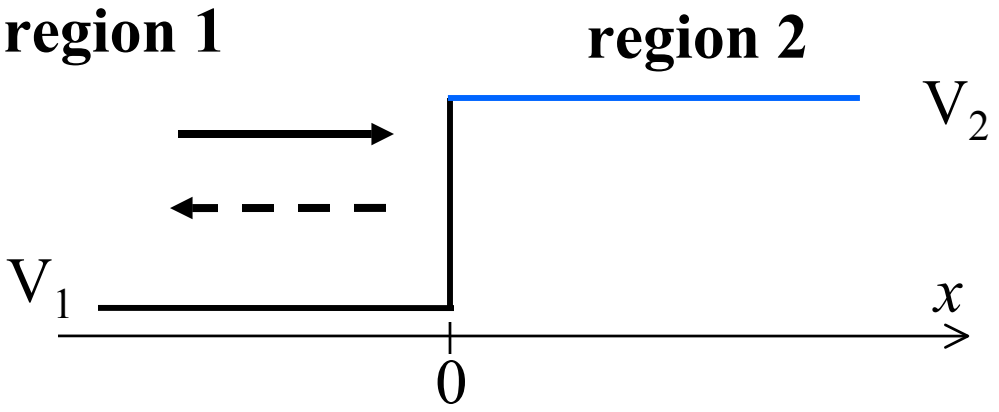
The wave function can be written as

$$\psi(x) = A\left[\exp(\gamma x) - \Gamma \exp(-\gamma x)\right]$$

$$\gamma = \alpha + \hat{j}\beta = \hat{j}\sqrt{\left(2m^*/\hbar^2\right)(E - V)}$$

Γ = amplitude reflection coefficient

The system behaves like a standard transmission line



$$\psi_1(x) = A_1\left[\exp(\gamma_1 x) - \Gamma\exp(-\gamma_1 x)\right]$$

$$\gamma_1 = \hat{j}\sqrt{\left(2m_1^*/\hbar^2\right)(E - V_1)}$$

$$\psi_2(x) = A_2\exp(\gamma_2 x)$$

$$\gamma_2 = \hat{j}\sqrt{\left(2m_2^*/\hbar^2\right)(E - V_2)}$$

By applying continuity conditions, we obtain Γ

$$\psi_1(0) = \psi_2(0)$$

$$\frac{1}{m_1^*}\frac{d}{dx}\psi_1(0) = \frac{1}{m_2^*}\frac{d}{dx}\psi_2(0)$$

$$\Rightarrow \Gamma = \frac{\left(\gamma_2 / m_2^*\right) - \left(\gamma_1 / m_1^*\right)}{\left(\gamma_2 / m_2^*\right) + \left(\gamma_1 / m_1^*\right)}$$

Then, we define the following auxiliary function

$$\phi(x) = \frac{\hbar}{j m^*}\frac{d\psi_1(x)}{dx} = \frac{\hbar}{j m^*}\gamma_1 \; A_1\left[\exp(\gamma_1 x) + \Gamma \exp(-\gamma_1 x)\right]$$

This function is anologous to electric voltage in a transmission line

$$\phi(x) = \frac{\hbar}{j m^*} \gamma_1 \, A_1 \left[\exp(\gamma_1 x) + \Gamma \exp(-\gamma_1 x) \right]$$

The wave function is analogous to electric current in a transmission line

$$\psi_1(x) = A_1 \left[\exp(\gamma_1 x) - \Gamma \exp(-\gamma_1 x) \right]$$

and the scaling factor behaves like characteristic impedance

$$Z_0 = \frac{\hbar}{j m^*} \gamma_1$$

The probability current flow density is analogous to time average power in a transmission line

$$\frac{\vec{J}}{q} = \frac{\hbar}{2\hat{j}m^*}\left(\psi^*\nabla\psi - \psi\,\nabla\psi^*\right) = \frac{1}{2}\Re\left\{\phi\,\psi^*\right\}$$

At any location one can define the line impedance as

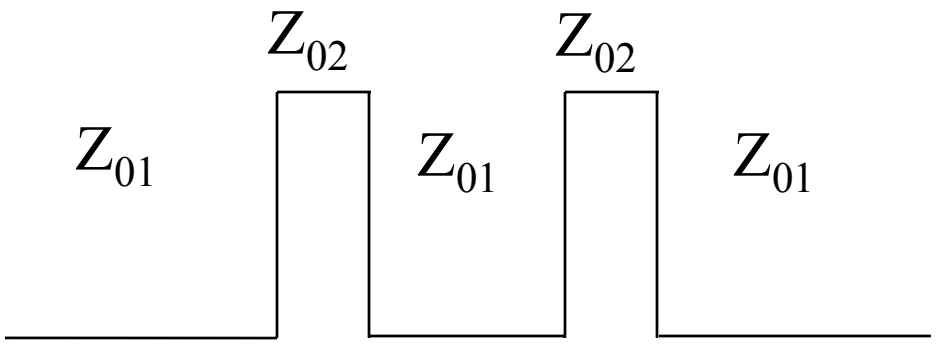
$$Z(x) = \frac{\phi(x)}{\psi(x)}$$

Indicate the load impedance as $Z_L = Z_2$ the input impedance of the system is

$$Z_{in} = Z_0\frac{Z_2\cosh(\gamma L) - Z_0\sinh(\gamma L)}{Z_0\cosh(\gamma L) - Z_2\sinh(\gamma L)}$$

$$\text{where} \quad x_{in} = -L$$

If a system consists of a sequence of different material layers, each layer can be treated as a transmission line with different characteristic impedance, which depends on the effective mass. The reflection coefficient of the structure can be obtained with the same algebra of transmission lines.



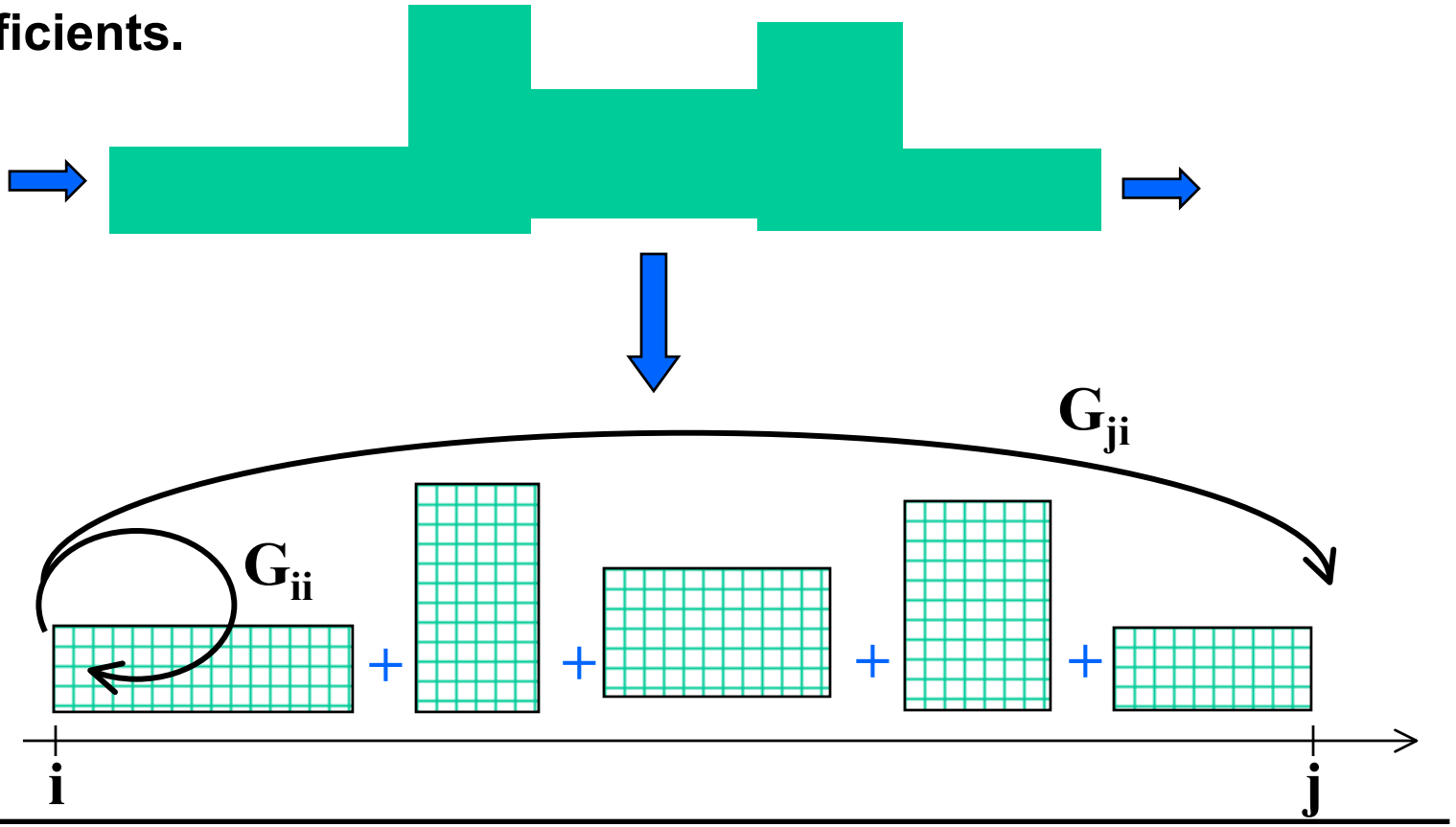
Possible discussion items:

What are the limitations of this approach?

How can we include bias and self-consistency?

2D Solution with iterative tight-binding Green's functions.

Let's assume a 2-D electron gas system define by a wave guide like pattern, and perform a uniform discretization (tight-binding lattice). Assume a flat potential floor for simplicity. We are looking for the structure's reflection and transmission coefficients.



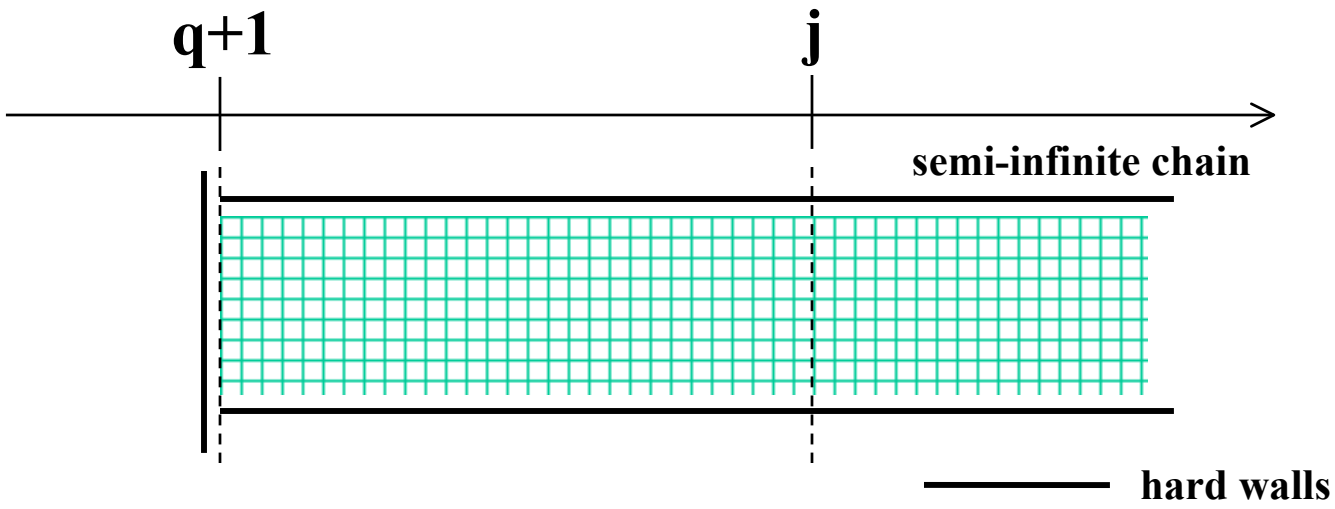
Scattering eigenstate in the input lead

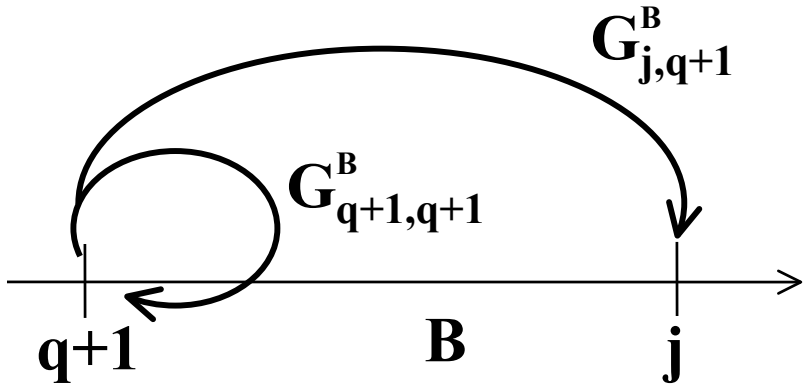
$$\Psi_{E,m}(x,y) = \underbrace{\frac{1}{\sqrt{k_m}} e^{\hat{j}k_m x}\,\psi_m(y)}_{\text{incident wave}} + \underbrace{\sum_n \Gamma_{nm} \frac{1}{\sqrt{k_n}} e^{\hat{j}k_n x}\,\psi_n(y)}_{\text{reflected waves}} \qquad x \to -\infty$$

Scattering eigenstate in the output lead

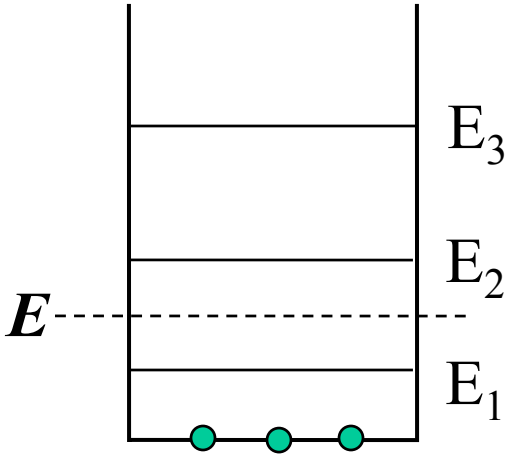
$$\Psi_{E,m}(x,y) = \underbrace{\sum_n \tau_{nm} \frac{1}{\sqrt{k_n}} e^{\hat{j}k_n x}\,\psi_n(y)}_{\text{transmitted waves}} \qquad x \to \infty$$

Start with output lead as an isolated section





The Green's function is a matrix [n × n] where "n" is the number of modes in the trasverse chain (same as the number of discretization nodes, 3 in the example)



$$\begin{bmatrix} G_1 & 0 & 0 \\ 0 & G_2 & 0 \\ 0 & 0 & G_3 \end{bmatrix}_{\substack{q+1,\, q+1 \\ j,\, q+1}}$$

$$\theta = \cos^{-1}\left(\frac{E}{2\hat{V}}\right) \qquad \text{Energy above cut-off}$$

$$\alpha = \cosh^{-1}\left(\frac{E}{2\hat{V}}\right) \qquad \text{Energy below cut-off}$$

Green's functions for the semi-infinite chain

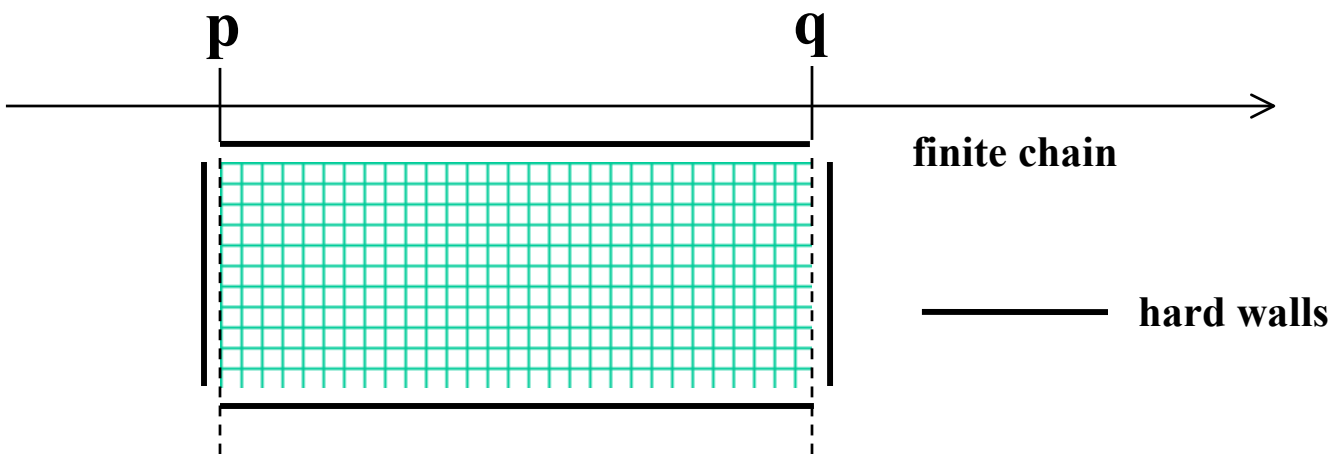
$$\left(G_i\right)^{\mathrm{B}}_{\mathrm{q+1,q+1}} = \frac{e^{\hat{j}\theta}}{\hat{V}} \quad \text{above cut-off}$$

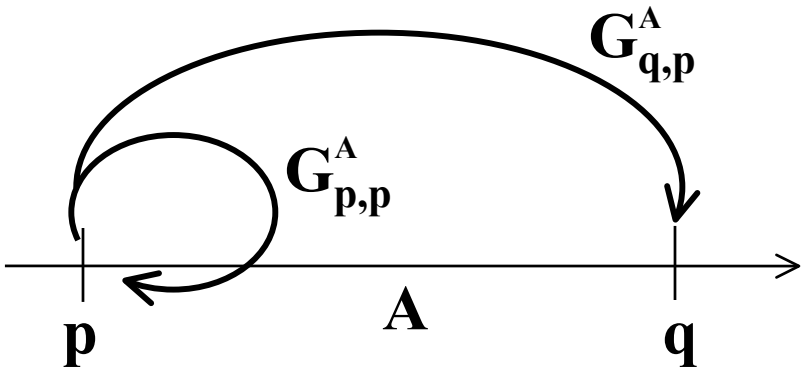
$$\left(G_i\right)^{\mathrm{B}}_{\mathrm{q+1,q+1}} = \frac{e^{-\alpha}}{\hat{V}} \quad \text{below cut-off}$$

$$\left(G_i\right)^{\mathrm{B}}_{\mathrm{j,q+1}} = \frac{e^{\hat{j}\left|\mathrm{j-q}\right|\theta}}{\hat{V}} \quad \text{above cut-off}$$

$$\left(G_i\right)^{\mathrm{B}}_{\mathrm{j,q+1}} = \frac{e^{-\alpha\left|\mathrm{j-q}\right|}}{\hat{V}} \quad \text{below cut-off}$$

Then, treat the next section as an isolated finite chain





Green's function for the finite chain

$$\left(G_i\right)^{\mathrm{A}}_{\mathrm{pp}} = \frac{\sin\left(N\theta\right)}{\hat{V}\sin\left[\left(N+1\right)\theta\right]} \quad \text{above cut-off}$$

$$\left(G_i\right)^{\mathrm{A}}_{\mathrm{pp}} = \frac{\sinh\left(N\alpha\right)}{\hat{V}\sinh\left[\left(N+1\right)\alpha\right]} \quad \text{below cut-off}$$

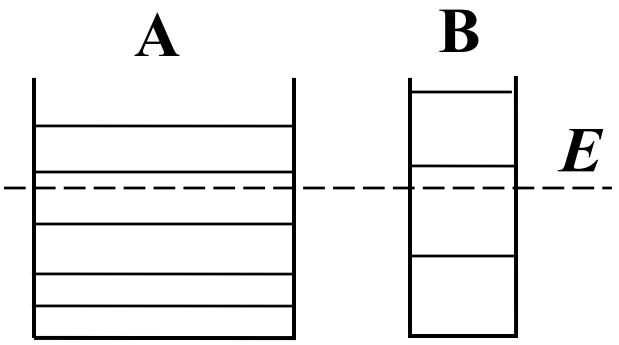
$$\left(G_i\right)^{\mathrm{A}}_{\mathrm{qp}} = \frac{\sin\left(\theta\right)}{\hat{V}\sin\left[\left(N+1\right)\theta\right]} \quad \text{above cut-off}$$

$$\left(G_i\right)^{\mathrm{A}}_{\mathrm{qp}} = \frac{\sinh\left(\alpha\right)}{\hat{V}\sinh\left[\left(N+1\right)\alpha\right]} \quad \text{below cut-off}$$

$$\left(G_i\right)^{\mathrm{A}}_{\mathrm{pp}} = \left(G_i\right)^{\mathrm{A}}_{\mathrm{qq}} \quad \text{(symmetry)} ; \quad N = \text{ nodes along the chain}$$

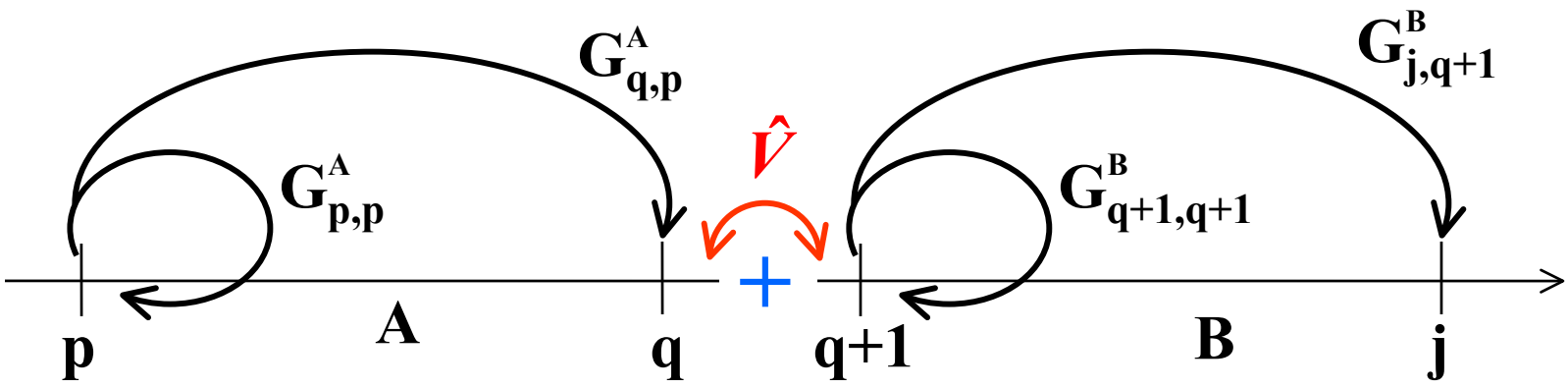
G^A is a matrix [m × m] where m is the number of transverse modes (number of transverse discretization nodes)

$$\begin{bmatrix} G_1^A & 0 & 0 & 0 & 0 & 0 \\ 0 & G_2^A & 0 & 0 & 0 & 0 \\ 0 & 0 & \bullet & 0 & 0 & 0 \\ 0 & 0 & 0 & \bullet & 0 & 0 \\ 0 & 0 & 0 & 0 & G_{m-1}^A & 0 \\ 0 & 0 & 0 & 0 & 0 & G_m^A \end{bmatrix}$$



In wider section, more modes are above cut-off

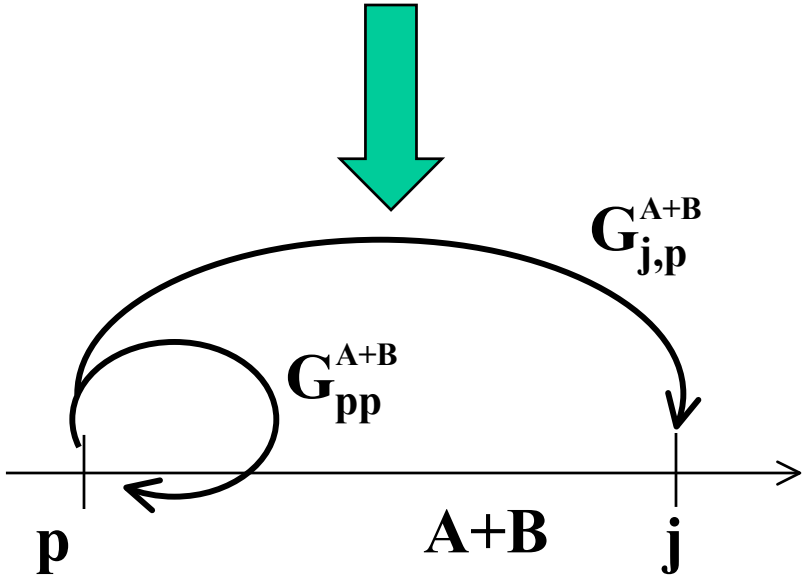
Now, add sections A and B - Application of Dyson's equation



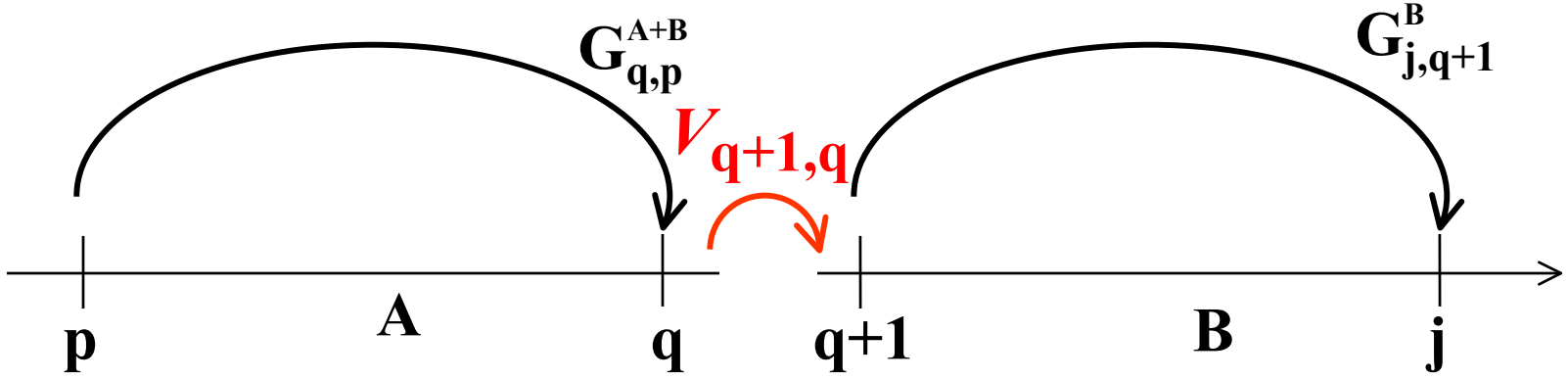
$$\underbrace{H}_{\text{total Hamiltonian}} = \underbrace{H_0}_{\text{isolated regions}} + \underbrace{\hat{V}}_{\text{connections}}$$

Dyson's equation for the Green's function

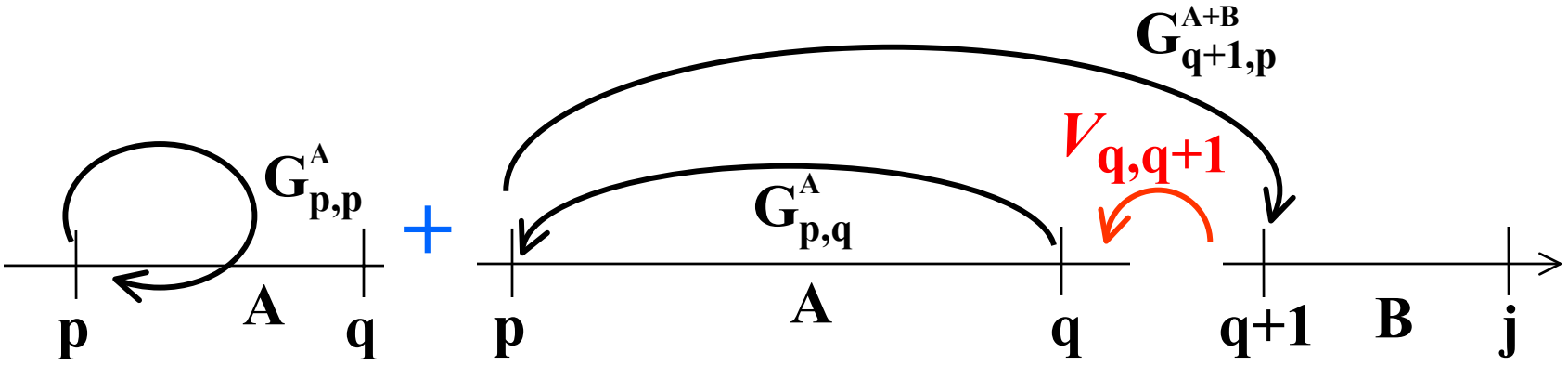
$$G = G^0 + G^0 \hat{V} G$$



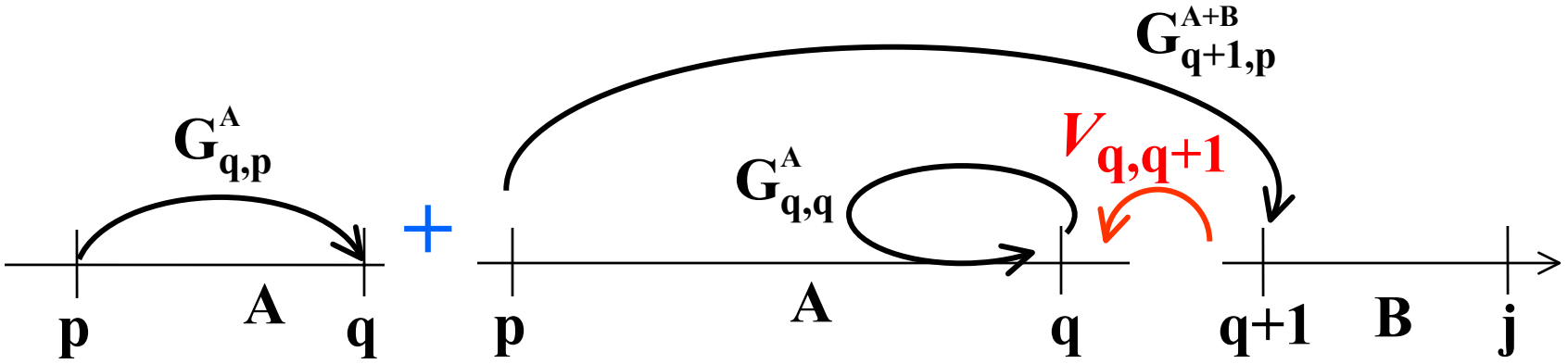
$$G^{A+B}_{jp} = G^{B}_{j,q+1}\,\hat{V}_{q+1,q}\,G^{A+B}_{qp}$$



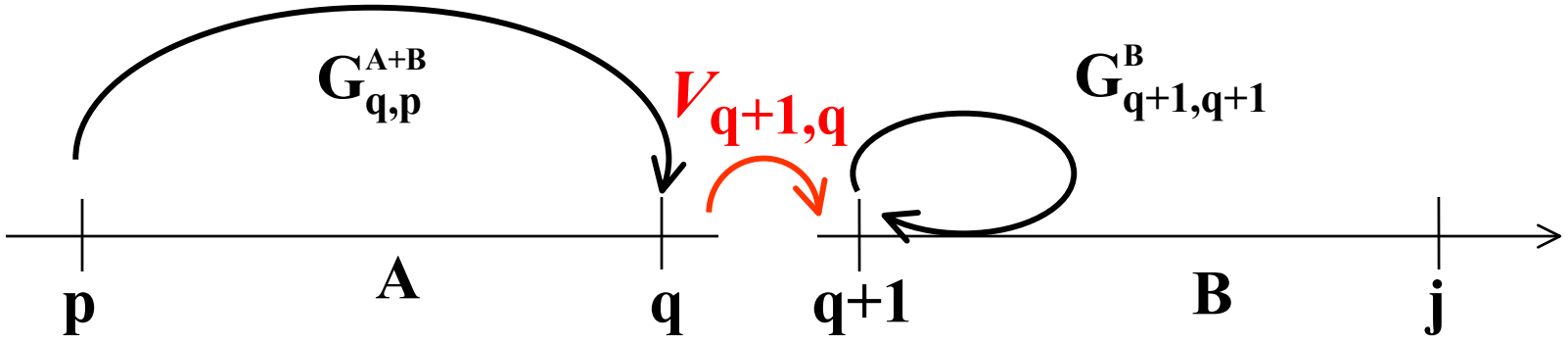
$$G^{A+B}_{pp} = G^{A}_{pp} + G^{A}_{pq}\,\hat{V}_{q,q+1}\,G^{A+B}_{q+1,p}$$



$$G^{A+B}_{qp} = G^{A}_{qp} + G^{A}_{qq}\,\hat{V}_{q,q+1}\,G^{A+B}_{q+1,p}$$



$$G^{A+B}_{q+1,p} = G^{B}_{q+1,q+1}\,\hat{V}_{q+1,q}\,G^{A+B}_{qp}$$



Add sections A and B

$$G^{A+B}_{jp} = G^{B}_{j,q+1}\,\hat{V}_{q+1,q}\,G^{A+B}_{qp}$$

$$G^{A+B}_{pp} = G^{A}_{pp} + G^{A}_{pq}\,\hat{V}_{q,q+1}\,G^{A+B}_{q+1,p}$$

$$\Rightarrow G^{A+B}_{qp} = G^{A}_{qp} + G^{A}_{qq}\,\hat{V}_{q,q+1}\,G^{A+B}_{q+1,p}$$

$$\Rightarrow G^{A+B}_{q+1,p} = G^{B}_{q+1,q+1}\,\hat{V}_{q+1,q}\,G^{A+B}_{qp}$$

$$G^{A+B}_{qp} = G^{A}_{qp} + G^{A}_{qq}\,\hat{V}_{q,q+1}\,G^{B}_{q+1,q+1}\,\hat{V}_{q+1,q}\,G^{A+B}_{qp}$$

$$\left(1 - G^{A}_{qq}\,\hat{V}_{q,q+1}\,G^{B}_{q+1,q+1}\,\hat{V}_{q+1,q}\right)G^{A+B}_{qp} = G^{A}_{qp}$$

$$\Rightarrow G^{A+B}_{qp} = \left(1 - G^{A}_{qq}\,\hat{V}_{q,q+1}\,G^{B}_{q+1,q+1}\,\hat{V}_{q+1,q}\right)^{-1} G^{A}_{qp}$$

Get the first Green's function for the coupled system

$$G_{jp}^{A+B} = G_{j,q+1}^{B}\,\hat{V}_{q+1,q}\,G_{qp}^{A+B}$$

$$G_{qp}^{A+B} = \left(1 - G_{qq}^{A}\,\hat{V}_{q,q+1}\,G_{q+1,q+1}^{B}\,\hat{V}_{q+1,q}\right)^{-1} G_{qp}^{A}$$

$$\Downarrow$$

$$G_{jp}^{A+B} = G_{j,q+1}^{B}\,\hat{V}_{q+1,q}\left(1 - G_{qq}^{A}\,\underbrace{\hat{V}_{q,q+1}\,G_{q+1,q+1}^{B}\,\hat{V}_{q+1,q}}_{S_q^B}\right)^{-1} G_{qp}^{A}$$

S_q^B = Self-energy for the transverse chain at location q, due to presence of B

Get the second Green's function for the coupled system

$$G^{A+B}_{qp} = \left(1 - G^{A}_{qq}\, S^{B}_{q}\right)^{-1} G^{A}_{qp}$$

$$G^{A+B}_{q+1,p} = G^{B}_{q+1,q+1}\, \hat{V}_{q+1,q}\, G^{A+B}_{qp}$$

$$\Downarrow$$

$$G^{A+B}_{q+1,p} = G^{B}_{q+1,q+1}\, \hat{V}_{q+1,q} \left(1 - G^{A}_{qq}\, S^{B}_{q}\right)^{-1} G^{A}_{qp}$$

$$G^{A+B}_{pp} = G^{A}_{pp} + G^{A}_{pq}\, \hat{V}_{q,q+1}\, G^{A+B}_{q+1,p}$$

$$= G^{A}_{pp} + G^{A}_{pq} \underbrace{\hat{V}_{q,q+1}\, G^{B}_{q+1,q+1}\, \hat{V}_{q+1,q}}_{S^{B}_{q}} \left(1 - G^{A}_{qq}\, S^{B}_{q}\right)^{-1} G^{A}_{qp}$$

Here are the Green's function results we were looking for

$$G^{A+B}_{jp} = G^{B}_{j,q+1}\,\hat{V}_{q+1,q}\left(1 - G^{A}_{qq}\,S^{B}_{q}\right)^{-1} G^{A}_{qp}$$

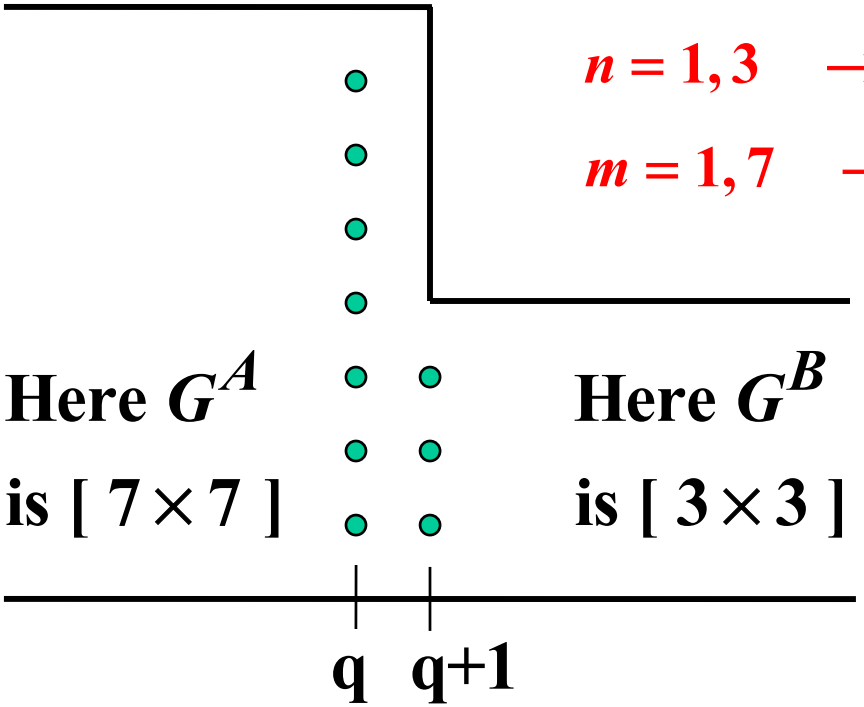
$$G^{A+B}_{pp} = G^{A}_{pp} + G^{A}_{pq}\,S^{B}_{q}\left(1 - G^{A}_{qq}\,S^{B}_{q}\right)^{-1} G^{A}_{qp}$$

NOTE

$G^{A}_{..}$ and $G^{B}_{..}$ are diagonal matrices

G^{A+B}_{pp} and $G^{A+B}_{q+1,p}$ are non-diagonal matrices

Example of coupling matrices



$n = 1, 3 \rightarrow$ 3 modes on section q+1

$m = 1, 7 \rightarrow$ 7 modes on section q

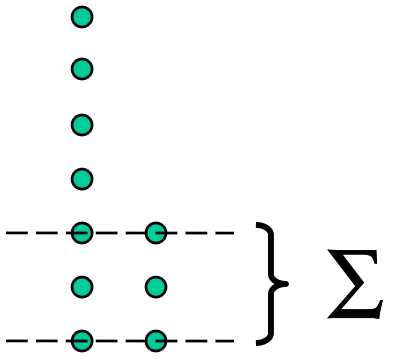
$V_{q,q+1}$ is [7×3]

$V_{q+1,q}$ is [3×7]

$$V_{q,q+1} = \left[V_{q+1,q} \right]^T$$

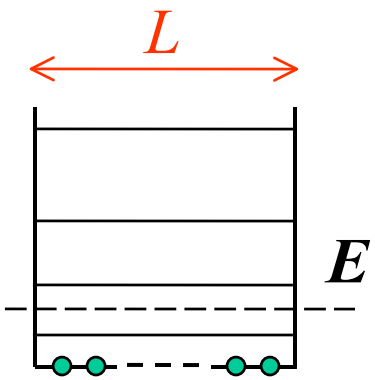
Overlap integral

$$\left(V_{q,q+1} \right)_{nm} = \hat{V} \sum_l \psi_n^*(l) \; \psi_m(l)$$



Transverse Eigenvalues and Eigenfunctions

The simplest approach is to use an infinite square well model for the transverse direction. But one could also solve a 2-D self-consistent Schrödinger/Poisson solution on the cross section and feed the eigenenergies and eigenfunctions (wave functions) to the Green's function code. The tight-binding model gives as many eigevalues as nodes. Typically, 20 nodes are sufficient to resolve realistic structures.



Discretized Hamiltonian with V(x) = 0 (flat potential)

$$\frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2}\begin{bmatrix} 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & \bullet & \bullet & 0 & 0 \\ 0 & 0 & \bullet & \bullet & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

Transverse Eigenvalues

$$\gamma\begin{bmatrix} a & b & 0 & 0 \\ c & a & b & 0 \\ 0 & c & a & b \\ 0 & 0 & c & a \end{bmatrix} \Rightarrow \qquad E_n = \gamma\left[a + 2\sqrt{bc}\cos\left(\frac{n\pi}{N+1}\right)\right]$$

$$n \in [1, N]$$

$$a = 2; \quad b = c = -1; \quad \gamma = \frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2}$$

$$E_n = \frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2}\left[2 - 2\cos\left(\frac{n\pi}{N+1}\right)\right]$$

Continuum model

$$E_n = \frac{\hbar^2\pi^2}{2m}\frac{n^2}{L^2} = \frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2}\left[\frac{\pi^2(\Delta x)^2}{L^2/n^2}\right] = \frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2}\left[\frac{\pi^2}{(N+1)^2/n^2}\right]$$

Transverse Eigenfunctions

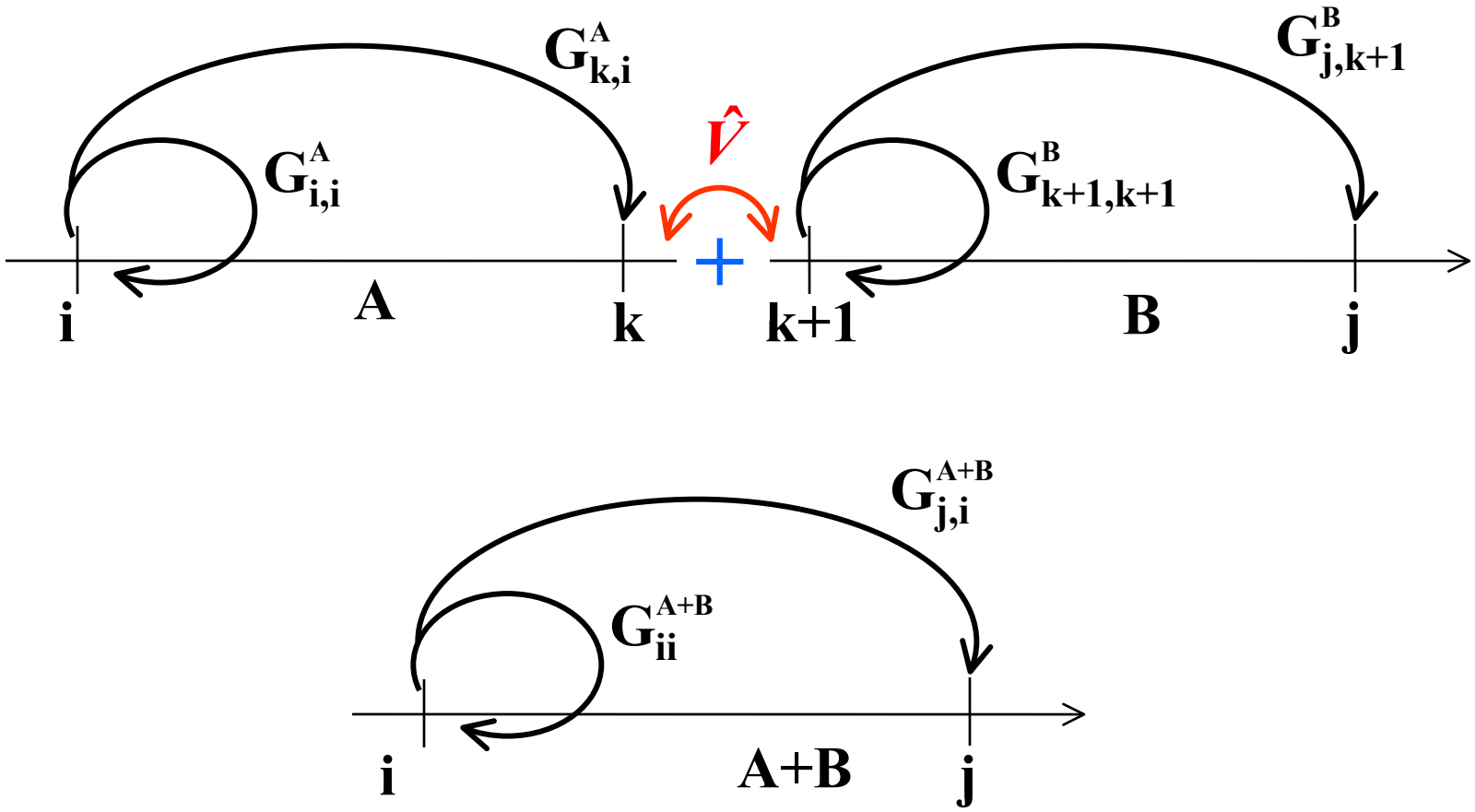
Hard walls, zero wave function at the wall.

$$\psi_n(l) = A_n \sin\left[\frac{n\pi l}{N+1}\right]$$

$$A_n = \frac{1}{\sqrt{\left[\frac{N}{2} + \frac{1}{2}\Re\left(\frac{1-\exp\left(\hat{j}\,2\pi n\,N/(N+1)\right)}{1-\exp\left(\hat{j}\,2\pi\,n/(N+1)\right)}\right)\right]}}$$

$$\langle \psi_n | \psi_m \rangle = \delta_{nm}$$

Last iteration - Add input lead (semi-infinite)



Last iteration - Add input lead (semi-infinite)

$$\left(G_i\right)^{\mathrm{A}}_{\mathrm{i,i}} = \frac{e^{\hat{j}(\mathrm{i\text{-}k\text{-}1})\theta}}{\hat{V}} \frac{\sin\left[(\mathrm{i\text{-}k\text{-}1})\theta\right]}{\sin\theta} \quad \text{above cut-off}$$

$$\left(G_i\right)^{\mathrm{A}}_{\mathrm{i,i}} = \frac{e^{-(\mathrm{i\text{-}k\text{-}1})\alpha}}{\hat{V}} \frac{\sinh\left[(\mathrm{i\text{-}k\text{-}1})\alpha\right]}{\sinh\alpha} \quad \text{below cut-off}$$

$$\left(G_i\right)^{\mathrm{A}}_{\mathrm{k,i}} = \frac{e^{\hat{j}(\mathrm{i\text{-}k\text{-}1})\theta}}{\hat{V}} \quad \text{above cut-off}$$

$$\left(G_i\right)^{\mathrm{B}}_{\mathrm{k,i}} = \frac{e^{-(\mathrm{i\text{-}k\text{-}1})\alpha}}{\hat{V}} \quad \text{below cut-off}$$

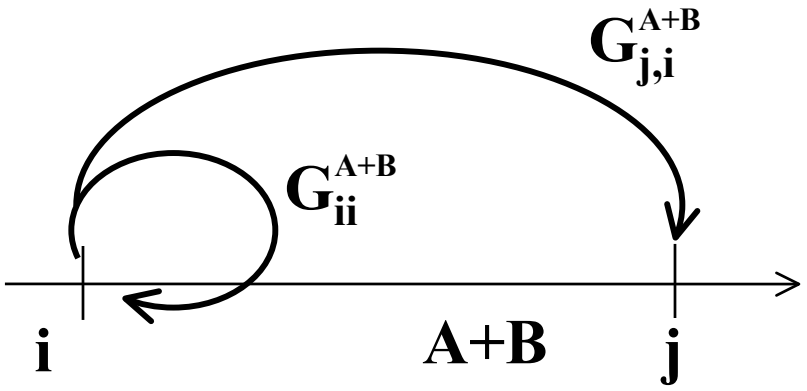
With the application of the same algorithm obtain

$G^{AB}_{i,i}$ = [m × m] matrix (m = nodes in input lead)

gives the reflection coefficients

$G^{AB}_{j,i}$ = [n × n] matrix (n = nodes in output lead)

gives the transmission coefficients



Reflection and transmission coefficients are evaluated for all modes in the input and output leads

transmission coefficients

$$\tau_{m,n} = -\hat{j}\,2\hat{V}\sqrt{\sin\theta_n \sin\theta_m}\; e^{\hat{j}(\theta_m \mathrm{i} - \theta_n \mathrm{j})} \underbrace{\langle n | G_{\mathrm{ji}} | m \rangle}_{\text{element of } G_{\mathrm{ji}}}$$

reflection coefficients

$$\Gamma_{m,n} = -\sqrt{\sin\theta_n / \sin\theta_m}\; e^{\hat{j}\,2(\theta_m + \theta_n)\mathrm{i}}$$

$$\times\left(\hat{j}\,2\hat{V}\sin\theta_m \underbrace{\langle n | G_{\mathrm{ii}} | m \rangle}_{\text{element of } G_{\mathrm{ii}}} + \delta_{nm}\right)$$

$$\delta_{nm} = \begin{cases} 1 & \text{for } m = n \\ 0 & \text{for } m \neq n \end{cases}$$

Possible discussion items:

- How to include realistic structures?
- Quasi-3D simulation
- Full self-consistent 3-D simulation

Available Software: TBGreen code

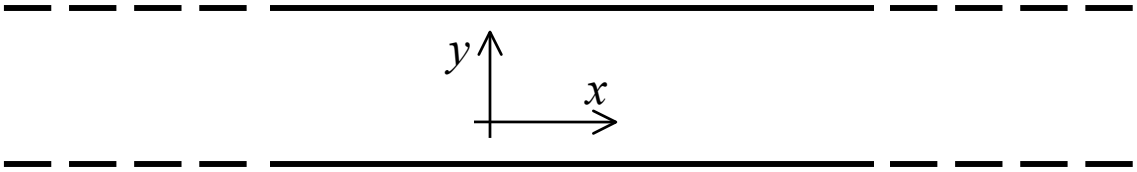
Mode-matching method

The structure is partitioned into slices in which the potential profile is constant along the longitudinal direction.

A 1-D Schrödinger equation is solved in each section to obtain transverse eigenmodes and eigenvalues.

The continuity of the wavefunction and of its normal derivative is enforced at each interface between different sections.

The equations are then projected onto appropriate sets of transverse modes and solved using numerical procedures.



$$\psi(x,y) = \sum_n a_n \, \varphi_n(x) \chi(n)$$

$$\varphi_n(x) = \frac{1}{\sqrt{k_n}} e^{\pm \hat{j} k_x x}$$

$$\chi(n) = \sqrt{\frac{2}{L}} \sin\left(\frac{n k_y y}{L}\right)$$

$$\frac{\hbar^2}{2m^*}\left(k_x^2 + k_y^2\right) = \frac{k_n^2}{2m^*} = E_n$$

Current normalization

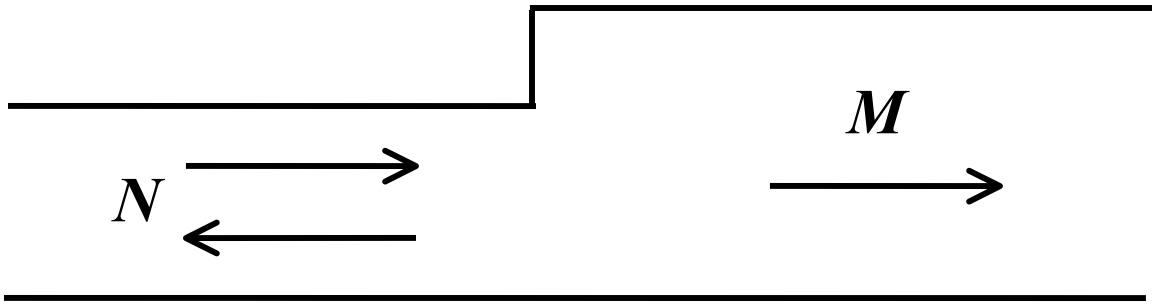
$$J = \frac{\hbar}{2\hat{j}\,m^*}\left(\psi^*\nabla\psi - \psi\,\nabla\psi^*\right)$$

$$= \frac{\hbar}{2\hat{j}\,m^*}\left(C^* e^{-\hat{j}k_x x}\;\hat{j}k_x C\, e^{\hat{j}k_x x} + C\, e^{\hat{j}k_x x}\;\hat{j}k_x C^*\, e^{-\hat{j}k_x x}\right)$$

$$\frac{\hbar}{2\hat{j}\,m^*}\left(|C|^2\, 2\hat{j}k_x\right) = \frac{\hbar}{m^*}|C|^2 k_x$$

In units of $\hbar/m^*$

$$C = \frac{1}{\sqrt{k_x}}$$ **to have unitary flux for each impinging mode**



N Reflection coefficients

M Transmission coefficients

N+M unknowns

M equations from the continuity of wave functions

N equations from the continuity of the normal derivative

M+N equations

Leftmost interface ($x = x_A$)

$$\frac{1}{\sqrt{k_i}} e^{\hat{j} k_i x_A} \psi_i(y) = -\sum_n R_n \frac{1}{\sqrt{k_n}} e^{\hat{j} k_n x_A} \psi_n(y)$$

$$+\sum_m c_m \frac{1}{\sqrt{\nu_m}} e^{\hat{j} \nu_m x_A} \chi_m(y) + \sum_m d_m \frac{1}{\sqrt{\nu_m}} e^{-\hat{j} \nu_m x_A} \chi_m(y)$$

$$\sqrt{k_i}\, e^{\hat{j} k_i x_A} \psi_i(y) = \hat{j} \sum_n R_n \sqrt{k_n}\, e^{\hat{j} k_n x_A} \psi_n(y)$$

$$+\hat{j} \sum_m c_m \sqrt{\nu_m}\, e^{\hat{j} \nu_m x_A} \chi_m(y) - \hat{j} \sum_m d_m \sqrt{\nu_m}\, e^{-\hat{j} \nu_m x_A} \chi_m(y)$$

Leftmost interface (assume $x = x_A = 0$)

wave function continuity condition

$$\frac{1}{\sqrt{k_i}}\int_0^L \psi_p(y)\psi_i(y)\,dy = -\sum_n R_n \frac{1}{\sqrt{k_n}}\int_0^L \psi_p(y)\psi_n(y)\,dy + \sum_m T_m \frac{1}{\sqrt{\nu_m}}\int_0^L \psi_p(y)\,\chi_m(y)\,dy$$

$$\Rightarrow \quad \frac{1}{\sqrt{k_i}}\delta_{p,i} = -R_p \frac{1}{\sqrt{k_p}} + \sum_m T_m \frac{1}{\sqrt{\nu_m}}\int_0^L \psi_p(y)\,\chi_m(y)\,dy$$

Leftmost interface (assume $x = x_A = 0$)

derivative continuity condition

$$\hat{j}\sqrt{k_i}\int_0^{L'}\chi_p(y)\psi_n(y)\,dy = \hat{j}\sum_n R_n\sqrt{k_n}\int_0^{L'}\chi_p(y)\psi_n(y)\,dy + \hat{j}\sum_m T_m\sqrt{\nu_m}\int_0^{L'}\chi_p(y)\chi_m(y)\,dy$$

$$\Rightarrow \quad \hat{j}\sqrt{k_i}\int_0^{L'}\chi_p(y)\psi_n(y)\,dy = \hat{j}\sum_n R_n\sqrt{k_n}\int_0^{L'}\chi_p(y)\psi_n(y)\,dy + \hat{j}\,T_p\sqrt{\nu_p}$$