Quantum effects in devices

• The MC method described so far solves the BTE by sampling
• The solution converges to the solution of the BTE in the large ensemble/long time limit
• However, some effects are missing—tunneling and quantization
• Including quantum effects is necessary in order to capture:
  1. Electrons tunneling through the oxide in a MOSFET, causing gate leakage
  2. High gate voltage causes separation of subbands in the inversion layer
  3. Ultra thin body (UTB) or NW devices have volume inversion
• Capturing these effects within the MC/BTE formalism can be done:
  1. Quantum corrections
  2. Extended treatments based on the Wigner Transport Equation
  3. Coupled treatments solving the Poisson and Schroedinger equations together
Quantum correction approaches

• Add in a potential which captures the difference between the classical and quantum solution

\[ Q = -\frac{\hbar^2}{2mR} \nabla^2 R \rightarrow -\frac{\hbar^2}{2m\sqrt{n}} \frac{\partial^2 \sqrt{n}}{\partial x^2} \]

• Bohm potential:

• Wigner potential (sometimes called the density gradient correction):

\[ V_Q = -\frac{\hbar^2}{8m} \frac{\partial^2 (\ln n)}{\partial x^2} \]

• Effective potential:

\[ V_{\text{eff}}(x) = \frac{1}{\sqrt{2\pi a_0}} \int_{-\infty}^{\infty} V(x') \exp\left(-\frac{(x - x')^2}{2a_0^2}\right) dx' \]

Where \( a_0 \) is the spread (size) of the wavepacket.
Overview of quantum effects in devices

• As device dimensions are reduced, the particle-wave duality emerges
• So far we covered the semi-classical theory
  • treated electrons as particles having position and momentum
  • Both position and momentum (hence energy, velocity) were continuous variables
  • Included QM scattering from Fermi’s Golden Rule as perturbations
• Next we want to delve deeper into the quantum regime
• Two types of quantum effects:
  • Single electron effects, such as confinement and quantization
  • Many-body effects due to the electron-electron interaction
• In general, we need to incorporate the wave nature of electrons
Devices relying on quantum effects

• Ultra-thin body and nanowire FETs (confinement and quantization)
• Point contact and Coulomb blockade devices
• Resonant Tunneling Diodes
• Tunnel FETs (TFETs)
Particle-wave comparison

• For the description of quantum effects in devices, we will need to treat electrons as waves

• The simplest wave is a plane wave

• However, a plane wave is the opposite of a particle—it is everywhere!

• Nonetheless, it has a precisely defined momentum $k$ like a particle

• A collection of plane waves can be assembled into a wave packet with a finite spread in space:

  $$\psi(r,t) = \int \int \int \Psi_0(k) \exp \left[ i(k \cdot r - \omega(k)t) \right] d^3k$$

  --uncertainty principle requires $\Delta k \Delta x > 1/2$
The time-dependent Schroedinger equation is usually presented as:

\[ i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = -\frac{\hbar^2}{2m_0} \nabla^2 \psi(\mathbf{r}, t) + V(\mathbf{r})\psi(\mathbf{r}, t) \]

However, the wavefunction can be complex-valued. The TDSE can be written as a set of two coupled equations for the real and imaginary parts of the wavefunction:

\[ \hbar \frac{\partial \Re(\psi)}{\partial t} = -\frac{\hbar^2}{2m_0} \nabla^2 \Im(\psi) + V(\mathbf{r})\Im(\psi) \]

\[ \hbar \frac{\partial \Im(\psi)}{\partial t} = \frac{\hbar^2}{2m_0} \nabla^2 \Re(\psi) - V(\mathbf{r})\Re(\psi) \]
Schroedinger wave equation, cont.

• Formally, time-dependent Schroedinger equation is readily solved

\[ \psi(r, t) = \exp \left(-\frac{i}{\hbar} H t \right) \psi(r, 0) \]

• Where $H$ is the Hamiltonian operator composed of kinetic+potential energy terms:

\[ H = -\frac{\hbar^2}{2m} \nabla^2 + V(r) \]

• In discretized form, this becomes an explicit time-stepping scheme:

\[ \tilde{\psi}(t + \Delta t) = \exp(-\frac{i}{\hbar} H^* \Delta t) \tilde{\psi}(0) \]

• This equation describes the (unitary) time evolution from an initial condition
Matrix exponentials and eigenvalues

• How do we take an exponential of a matrix/operator?

\[ e^A = I + A + \frac{1}{2!} A^2 + \frac{1}{3!} A^3 + \cdots = \sum_{k=0}^{\infty} \frac{1}{k!} A^k \]

• However, a better way is via the eigenvalues:
• If lambda is an eigenvalue with eigenvector v, then

\[ e^{tA}v = e^{\lambda t}v \]

• So if the initial condition \( \psi(0) \) is an eigenvalue, it will simply stay in that eigenvalue
• To take an exponential of an operator (matrix in discretized form), we need to know its eigenvalues

\[ e^{tA}v = e^{\lambda t} \left( v + t(A - \lambda I)v + \frac{t^2}{2!}(A - \lambda I)^2v + \cdots + \frac{t^{k-1}}{(k-1)!}(A - \lambda I)^{k-1}v \right) \]
Time-independent Schroedinger equation

• The eigenvalues and eigenvectors of the Hamiltonian are given by

$$H\Psi = E\Psi$$

where $\Psi$ is the wavefunction and $E$ is the corresponding energy.

• In matrix language, the solution $E$ to this problem is an eigenvalue of the Hamiltonian operator while the $\Psi$ is the corresponding eigenvalue.

• Once this problem is solved, the eigenvalue/eigenvector pairs can be used to construct a time-dependent solution

• However, there are other approaches to the TDSE
Envelope function approximation

• We already talked about the steady state problem $H_0 \Psi = E \Psi$
• Solved this for the atomic potential (or pseudopotential) in Ch1
• Near the band minima we can replace the atomic potential with effective mass $m^*$
• Now we have to add an external potential $V(x)$ to the problem
• Solving the problem $(H_0 + V) \Psi = (E_0 + E') \Psi$ is equivalent to solving

$$\left[ -\frac{\hbar^2}{2m^*} \nabla^2 + V(x) \right] \Psi(x) = E \Psi(x)$$

with effective mass capturing the bandstructure.
• Then the solution $\Psi$ is called an envelope function because it is multiplying the much faster varying Bloch function
Discretizing the effective mass Hamiltonian

- We can use finite differences to discretize the Hamiltonian
- Problem: effective mass can vary across material interfaces
- Solution: bring the mass inside the operator

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

- Then we can use quantities at midpoints

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

- Finally we can discretize the Hamiltonian operator $H$ as

\[ -\frac{\hbar^2}{2} \left[ \frac{\psi(i + 1) - \psi(i)}{m^*(i + 1/2)} - \frac{\psi(i) - \psi(i - 1)}{m^*(i - 1/2)} \right] / \Delta x^2 \]
Boundary conditions for the Hamiltonian

- Hamiltonian is a 2\textsuperscript{nd} order operator (has a second derivative)
- Need to apply 2 boundary conditions (one at each end of the domain)
- If our domain is \( i=1:N \), then need \( \Psi(0) \) and \( \Psi(N+1) \)
- Dirichlet BCs: if the potential goes to infinity at \( V(0) \) and \( V(N+1) \), then set \( \Psi(0)=\Psi(N+1)=0 \)
- Otherwise, we need to enforce continuity of the function and its derivatives at the boundaries
- Then the first derivative \( d\Psi/dx \) is equal at the two sides of the boundary—the BC implies the second derivative is zero
Coupled Schroedinger Poisson

• We can solve the TISE given a potential using the effective mass and finite difference discretization

• Where does the potential come from? Solve the Poisson eqn.

• The Poisson equation requires densities—how do we fold the solution \( \Psi \) of the TISE into the RHS for the Poisson equation?

• Each solution of the TISE gives an eigenvalue (energy \( E \)) and eigenvector (wavefunction \( \Psi \))

• The charge density is \( \Psi^*\Psi = |\Psi|^2 \). But is the state occupied?

• Use equilibrium statistics from the Fermi Dirac distribution

\[
 n(x) = \int_{E_i} \sum_i |\Psi_i(x)|^2 f_{FD}(E - E_F) g(E) \, dE
\]

• Multiply the density at each position by the probability \( \Psi^*\Psi \)
Time-dependent Schroedinger solvers

• Discretizing the TDSE

\[ j\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + V(x)\psi(x, t) \]

using finite differences with an explicit forward method in time

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

• This method can be viewed in operator notation as

\[ \tilde{\psi}(n+1) = \left( I - \frac{j}{\hbar} H^*\Delta t \right) \tilde{\psi}(n) \]

which is not unitary and hence not stable

• Using, instead, a three level explicit scheme with \( n+1, n, \) and \( n-1 \) gives

\[ \psi(i; n+1) = \psi(i; n - 1) + j2\Delta t \left( \frac{\hbar}{2m} \left( \frac{\psi(i - 1; n) - 2\psi(i; n) + \psi(i + 1; n)}{\Delta x^2} \right) - \frac{V(i)}{\hbar} \psi(i; n) \right) \]

Which has a stable unitary propagator

\[ \tilde{\psi}(n+1) = \frac{I - j\Delta t H^*/\hbar}{I + j\Delta t H^*/\hbar} \tilde{\psi}(n - 1) \]
Crank-Nicholson method for the TDSE

• We can also use a semi-implicit approach like the one we used to stabilize the continuity equations

• Evaluate the RHS as the average of current and next time step

\[ \overline{\Delta t} \psi(i; n + 1) - \psi(i; n) = \frac{1}{2}[RHS(n + 1) + RHS(n)] \]

• The method is said to be “implicit” because it requires the knowledge of the solution at n+1 in order to solve for the next n+1 step

• Often, implicit methods require us to solve for the next time step rather than updating explicitly from the solution at step n
Crank-Nicholson method for the TDSE, cont.

• The resulting discretization is (with $C_o = \frac{4m\Delta x^2}{\hbar \Delta t}$)

$$
\psi(i - 1; n + 1) + \left(jC_o - \frac{2m\hbar^2}{\hbar^2} V(i) - 2\right) \psi(i; n + 1) + \psi(i + 1; n + 1) = \\
-\psi(i - 1; n) + \left(jC_o + \frac{2m\hbar^2}{\hbar^2} V(i) + 2\right) \psi(i; n) - \psi(i + 1; n)
$$

• The propagator can be written as

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

which is again stable and unitary.

• Where is the “solve”—how are we required to solve a linear problem?
Crank-Nicholson method for the TDSE, cont.

• The solve can be seen by rearranging

\[ \psi(n + 1) = \frac{I - \frac{1}{2}jH^*\Delta t}{I + \frac{1}{2}jH^*\Delta t} \psi(n) \]

to move the operator in from the denominator to the LHS:

\[ \left( I + \frac{1}{2}jH^*\Delta t \right) \psi(n + 1) = \left( I - \frac{1}{2}jH^*\Delta t \right) \psi(n) \]

• Now we can form the RHS directly from

\[ b(n) = \left( I - \frac{1}{2}jH^*\Delta t \right) \psi(n) \]

but then we have to solve the linear problem

\[ A\psi(n + 1) = b(n) = A^T\psi(n) \]

• The T here signifies a Hermitian (complex transpose) operation

• The matrix A is tridiagonal with has diagonal elements

\[ d(j) = \frac{\hbar^2}{m^*\Delta x^2} + V(i) \]

• Off diagonal elements (above and below) are

\[ a(j) = -\frac{\hbar^2}{2m^*\Delta x^2} \]
2-d TDSE solvers

- We can easily extend our discretization to 2d assuming a uniform mesh $\Delta x=\Delta y=\Delta$. For the 3-level explicit scheme we get:

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

$$
-4\psi(i, j; n) + \psi(i + 1, j; n) + \psi(i, j + 1; n) - \frac{j^2\Delta tV(i)}{\hbar} \psi(i, j; n)
$$

- The Crank-Nicholson implicit method produces the discretization

$$
\psi(i, j; n + 1) - \psi(i, j; n) = -\frac{\Delta t}{2\hbar} [C_0(\psi(i - 1, j; n + 1) + \psi(i, j - 1; n + 1)) - 4\psi(i, j; n) + \psi(i + 1, j; n) + \psi(i, j + 1; n)) + V(i, j)\psi(i, j; n + 1) + C_0(\psi(i - 1, j; n) - \psi(i, j - 1; n) - 4\psi(i, j; n) + \psi(i + 1, j; n)) + V(i, j)\psi(i, j; n)]
$$

where the constant is given by $C_0 = -\hbar^2/(2m\Delta^2)$
Split-step ADI scheme

• Alternating Direction Implicit is a popular numerical approach

• Divide the implicit step into two sub-steps of size $\Delta t/2$

• Then update at time $n+1/2$ with a horizontal sweep

$$\psi(i, j; n + \frac{1}{2}) + \frac{\Delta t}{2h} \left[ C_0(\psi(i-1, j; n + \frac{1}{2}) - 2\psi(i, j; n + \frac{1}{2}) + \psi(i+1, j; n + \frac{1}{2}) + \frac{V(i, j)}{2} \psi(i, j; n + \frac{1}{2}) \right] =$$

$$\psi(i, j - 1; n) - \frac{\Delta t}{2h} \left[ C_0(\psi(i, j; n) - 2\psi(i, j; n) + \psi(i, j + 1; n) + \frac{V(i, j)}{2} \psi(i, j; n) \right]$$

• Followed by a vertical weep to get to $n+1$

$$\psi(i, j; n + 1) + \frac{\Delta t}{2h} \left[ C_0(\psi(i, j - 1; n + 1) - 2\psi(i, j; n + 1) + \psi(i, j + 1; n + 1) + \frac{V(i, j)}{2} \psi(i, j; n + 1) \right] =$$

$$\psi(i, j; n + \frac{1}{2}) - \frac{\Delta t}{2h} \left[ C_0(\psi(i-1, j; n + \frac{1}{2}) - 2\psi(i, j; n + \frac{1}{2}) + \psi(i+1, j; n + \frac{1}{2}) + \frac{V(i, j)}{2} \psi(i, j; n + \frac{1}{2}) \right]$$

• The ADI scheme only requires a tri-diagonal solve at each iteration
Calculating the current from TDSE solution

- Continuity equation says
  \[
  \frac{\partial \rho}{\partial t} = -q \frac{\partial |\psi|^2}{\partial t} = \nabla \cdot \mathbf{J}
  \]

- Using the property
  \[
  \frac{\partial |\psi|^2}{\partial t} = \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}
  \]

- We can introduce the Schroedinger equation to write the above as
  \[
  \frac{\partial |\psi|^2}{\partial t} = \psi^* \left( \frac{j\hbar}{2m^*} \nabla^2 \psi + \frac{1}{j\hbar} V(r) \psi \right) - \psi \left( \frac{j\hbar}{2m^*} \nabla^2 \psi^* + \frac{1}{j\hbar} V(r) \psi^* \right) = \frac{j\hbar}{2m^*} (\psi^* \nabla^2 \psi - \psi \nabla^2 \psi^*)
  \]

- We can simplify the above using
  \[
  \nabla \cdot (\psi^* \nabla \psi) = \psi^* \nabla^2 \psi + \nabla \psi^* \cdot \nabla \psi
  \]
to get
  \[
  \frac{\partial |\psi|^2}{\partial t} = \frac{j\hbar}{2m^*} \nabla \cdot (\psi^* \nabla \psi - \psi \nabla \psi^*)
  \]
  which means the current is
  \[
  \mathbf{J} = \int \frac{q\hbar}{2m^*} (\psi^* \nabla \psi - \psi \nabla \psi^*)
  \]
Open boundary conditions for the SE

- Open quantum systems is a broad and challenging topic
- We will consider the case of open boundaries for the SE
- Usually this is done using a plane wave basis

\[ \psi(x) = A(x) \exp[\pm j k_x(x) x] \]

- Then we can test the transmission through a nanostructure for different wavevectors \( k_x \)
- Set the amplitude at one end and observe the resulting amplitude at the other as the wave is partially reflected due to potential variation
- For a perfect reservoir at the contact, we assume \( k_x(0)=k_x(1) \) and also at the other end \( k_x(N+1)=k_x(N) \) — no potential variation in the contact
- Setting the amplitude \( A(N)=1 \), \( \psi(N) = \exp[j k_x(N) L] \) means

\[ \psi(N + 1) = \exp[j k_x(N)(L + \Delta x)] \]
Open boundary conditions for the SE, cont.

- Potential variation inside the device $V(i)$ means there will be some internal reflection, referenced from $V(1)=0$ so that $E = \hbar^2 k_x^2(1)/2m^*$

- We can write the solution as a superposition of a transmitted and reflected wave

$$\psi(i) = I(i) \exp[jk_x(i)i\Delta x] + R(i) \exp[-jk_x(i)i\Delta x]$$

- If the contacts are perfect, they will cause no reflection so at the end we have $R(N)=0$ so $I(N)=A(N)$

- At the left contact we have a combination of incident and reflected

$$\psi(0) = I(0) + R(0) = I(1)\exp[-jk_x(1)\Delta x] + R(1)\exp[jk_x(1)\Delta x]$$

- The above can be rearranged to obtain the incident amplitude

$$I(1) = \frac{\psi(1) \exp(jk_x(1)\Delta x) - \psi(0)}{2j \sin[k_x(1)\Delta x]}$$
Calculating the current from TDSE solution, cont.

- The current in discretized form is then given by

\[ i = \frac{q\hbar}{2m^*} \sum_n n(k_i) \Delta k \left( \psi_i^*(x) \frac{\partial \psi_i(x)}{\partial x} - \psi_i(x) \frac{\partial \psi_i^*(x)}{\partial x} \right) \]

- In general the density is given by an integral over k-space

\[ n = \frac{1}{4\pi^3} \int \int \int_{-\infty}^{\infty} dk_x dk_y dk_z \frac{1}{1 + \exp[(E - E_F)/k_BT]} \]

- Breaking up the energy integral into

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

- Which produces

\[ n = \frac{m^*}{2\pi^2 \hbar^2} \int_{-\infty}^{\infty} dk_x \int_{0}^{\infty} dE_\perp \frac{dE_\perp}{1 + \exp[(E_\perp + E_x - E_F)/k_BT]} \]

- The integral can be done explicitly

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

\[ n(k_x) = \frac{m^* k_BT}{2\pi^2 \hbar^2} \log \left[ 1 + \exp \left( \frac{E_F - \hbar^2 k_x^2 / 2m^*}{k_BT} \right) \right] \]
Recursive methods for the TISE

- We will discuss two recursive methods for the solution of the TISE
  1. Transfer matrix approach
  2. Usuki method

- Both of the aforementioned are aimed at solving the time independent SE using a recursion from the boundary condition

- Both allow us to study the propagating states of an open system

- There is no time dependence; instead we “move” the wavefunction from one region to another by transmission and reflection

- Allow us to capture the effect of the potential on the wavefunction
Transfer matrix approach

• Consider the simplest QM problem of tunneling through a barrier
• \( V(x)=0 \) for \( x<0 \) and \( x>L \) while \( V(x)=V_0 \) inside \( 0<x<L \)
• Then the solutions to the TISE outside the barrier are plane waves
  \[ \psi_1(x) = A e^{i k x} + B e^{-i k x} \] and
  \[ \psi_3(x) = E e^{i k x} + F e^{-i k x} \]
  where \( k = \sqrt{2 m^* E / \hbar^2} \)
• In the barrier, the solution is exponentially decaying
  \[ \psi_2(x) = C e^{\gamma x} + D e^{-\gamma x} \] with \( \gamma = \sqrt{2 m^* (E - V_0) / \hbar^2} \)
• To find a solution, we match wavefunction and its derivatives at the boundaries \( x=0 \) and \( x=L \)
Transfer matrix method, cont.

• We have two coefficients in each region and 2 sets of BCs
• Set up a matrix problem

\[
\begin{bmatrix}
A \\
B
\end{bmatrix} = M_1 \begin{bmatrix}
C \\
D
\end{bmatrix} \quad \text{and} \quad \begin{bmatrix}
C \\
D
\end{bmatrix} = M_2 \begin{bmatrix}
E \\
F
\end{bmatrix}
\]

so that

\[
\begin{bmatrix}
A \\
B
\end{bmatrix} = M_1 M_2 \begin{bmatrix}
E \\
F
\end{bmatrix}
\]

where the matrix coefficients $m_{ij}$ are determined from the BCs

• We can generalize the procedure for any problem
• Break up the potential into small piece-wise constant regions
• The we have $\Psi_R = M \Psi_L = P_m B_{m-1} P_{m-1} \ldots P_1 B_1$
• P is the propagation matrix to propagate across each region
• B the boundary matrix to connect two consecutive regions
Dissipative quantum transport

• We have studied quantum systems based on the Schroedinger eqn.
  • A closed system meant we set the boundaries to zero
  • Electrons cannot enter or leave via the contacts, no net current flow

• An open system meant we have a non-zero boundary condition
  • Electrons can enter/leave via contacts, there can be a net current flow
  • However the electrons remain “coherent”—there is no scattering
  • Coherent processes are captured by the phase of the wave function

• There is another way a quantum system can be open
  • Electrons can also couple to the environment via the “heat bath” or phonons
  • Net flux of energy between the electrons and the environment occurs

• Methods we have covered so far based on TDSE cannot account for dissipation and coupling to the environment other than contacts

• Need to include scattering!
Density matrix

• Coherent processes are captured by evolving the wavefunction
• Also need to capture incoherent processes which exchange energy and mix different wavefunctions
• Define a “density matrix” operator \( \rho(x, x') = \sum_i P_i \Psi_i(x)\Psi_i^*(x') \)
• The \( P_i \) are the probabilities of occupying each of the states “i”
• Psi’s are not necessarily the solutions of the TISE (eigenvectors of H)
• We need a method to capture the time-dependence of the \( P_i \)
• Particle density is then given by the trace of the density matrix \( n(x) = \rho(x, x) \)
• Current density is given by \( J(x) = \lim_{x' \to 0} \frac{\epsilon \hbar}{jm^*} \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right) \rho(x, x') \)
Liouville-von Neummann equation

• The density matrix evolves in time the same way the wavefunctions evolve

• The evolution is governed by the Liouville-von Neumann eqn:
  \[ \frac{d}{dt} \rho = -\frac{j}{\hbar} [H, \rho] = -\frac{j}{\hbar} [H\rho - \rho H] = L_\rho \rho \]
  where the bracket indicates a “commutator”
  L is the Liouville operator

• In a purely classical system, the density matrix is replaced by the distribution function f(x,k)

• The classical Liouville equation is similar to the BTE
  \[ \frac{d}{dt} f = L_c f = \frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} - \frac{\partial V}{\partial x} \frac{\partial f}{\partial p} \]
Master equation method

• The evolution of the probabilities $P_i$ is based on perturbation theory

• Fermi’s Golden Rule establishes the transition rates

$$S_{ij} = \frac{2\pi}{\hbar} |\langle j|H'|i \rangle|^2 \delta(E_i - E_j)$$

where $H'$ is the perturbation Hamiltonian describing the coupling to the environment

• The rate of loss of one state is equal to the gain of another

$$dP_i = -dP_j = S_{ji}P_j dt$$

• We also have the gain from transitions in the opposite direction

$$\frac{dP_i}{dt} = \sum_j [S_{ji}P_j - S_{ij}P_i]$$

• Written in matrix form $\frac{dP}{dt} = MP$ where the master matrix is $M_{ij} = \begin{cases} S_{ij} & i \neq j \\ -\sum_{i \neq j} S_{ij} & i = j \end{cases}$
Master equation, cont.

- The ME is said to be “Markovian” because it is memoryless—
  - Future states of the system (given by probabilities $P_i$) depend only on their current state, not the past
  - Transitions are instantaneous and “memoryless”
  - Monte Carlo is an example of a Markov Process—the final state after scattering depends only on the state before scattering, not any previous state
  - We cannot reconstruct the past states from the present

- The ME has a stationary solution given by $P_i^{eq} = \frac{\sum_j S_{ji}P_j}{\sum_i S_{ij}}$

- The ME always converges to this solution, regardless of the starting point

- Such a solution is said to be the “equilibrium distribution” of the ME
Wigner function and Wigner-Weyl transform

• We can obtain a Wigner distribution which resembles a classical distribution by performing a Wigner transform on the density matrix.

• We first create a new set of coordinates \( r \) and \( r' \):
  • center of mass: \( r = (x + x')/2 \)
  • “spread” around the center of mass: \( r' = x - x' \)

• Then we take a Fourier transform of \( r' \) to get momentum \( k \):

\[
f_W(r, k) = \int_{-\infty}^{\infty} dr' \rho \left( \frac{r + r'}{2}, r - \frac{r'}{2} \right) e^{-ikr'}
\]

• The Wigner function \( f_W \) is NOT a probability distribution because it can take on negative values.

• However, it has several nice properties.
The Wigner equation

- We can obtain a transport equation for the Wigner function
- Perform a Wigner-Weyl transform on the Liouville-von Neumann eqn:

\[
\frac{\partial f_W}{\partial t} + \frac{\hbar k}{m^*} \frac{\partial f_W}{\partial r} + \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dk' V_W(r, k - k') f_W(r, k') = C f_W
\]

where the Wigner potential \( V_W \) is a Wigner transform of the potential \( V(x) \)

\[
V_W(r, k) = \int_{-\infty}^{\infty} dr' \left[ V \left( r + \frac{r'}{2} \right) - V \left( r - \frac{r'}{2} \right) \right] e^{-ikr'}
\]

- The RHS term is the collision integral—exactly like the BTE:

\[
C f_W = \int dk' [S(k', k)f_W(k') - S(k, k')f_W(k)]
\]
Wigner transport equation vs. BTE

• The Wigner transport equation and the BTE have many similarities
  • Same coordinates (position and momentum)
  • Same collision term which derives from the Master equation/FGR
  • Same “drift” term $\frac{\hbar k}{m^*} \frac{\partial f}{\partial r}$
  • Same “interpretation” where $n(r) = \int dk \, f(r, k)$ and $P(k) = \int dr \, f(r, k)$

• Where they differ is critical for capturing quantum effects:
  • the BTE only considers the “force” term based on classical acceleration $\frac{\partial V}{\partial r} \frac{\partial f}{\partial k}$
  • The WTE replaces this with the Wigner transformed potential $V_W$
  • The WTE captures quantum effects such as tunneling through barriers
  • The WTE also captures decoherence and scattering
The Wigner-Boltzmann equation

- Wigner-Boltzmann equation splits the potential into a “classical” or slowly varying and a “quantum” or rapidly varying part.
- The slowly varying part contributes only the force term through the electric field.
- The quantum part still requires a transform but may only need to be done once.
- Hence the Wigner potential acts as a position-dependent scattering-out term.

\[
\frac{\partial f_w(r,k,t)}{\partial t} + \mathbf{v} \cdot \nabla_r f_w + \frac{\mathbf{F}}{\hbar} \cdot \nabla_k f_w - \int dk' V_w(r, k - k') f_w(r, k', t) + \left( \frac{\partial f_w}{\partial t} \right)_{\text{coll}} = 0 ,
\]

- Hence the Wigner potential acts as a position-dependent scattering-out term.
Implementing the WTE

1. Direct discretization using an implicit or explicit time stepping
   • May only be possible in 1D, numerical integrals for the potential are expensive
   • Stability requires upwind or high order schemes

2. Monte Carlo-like methods
   • Full 3D WTE simulation is possible with MC techniques
   • Motion and scattering are treated exactly like MC
   • Additional treatment needed for the Wigner potential
   • Typically using “affinities” where each “electron” gets an additional “affinity” which evolves according to the Wigner potential
   • Another technique is using signed particles: since the Wigner function can be negative, allow “electrons” to change sign between positive and negative