Objective:
To illustrate the limitations of the model described in Lectures 2,3 and introduce a completely different approach based on the concept of Fock space.

I believe this will be a key concept in the next stage of development of transport physics.

Approach based on

Reference: QTAT, Chapter 3.4.
Current through a very small conductor

\[ F = \left[ \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \right] \]

\[ I = \frac{q}{h} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \left[ f_1 - f_2 \right] \]

\[ \text{max } I = \frac{q}{h} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \left[ f_1 - f_2 \right] \]

\[ \Rightarrow \frac{q \gamma_1}{2h} \text{ if } \gamma_2 = \gamma_1 \]

Normalized Current

\[ -qV_D \Rightarrow \]

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Conductance of a very small conductor

Assume $\gamma_2 = \gamma_1$

$$2\gamma_1 + 4k_BT \Rightarrow \frac{q\gamma_1}{2\hbar}$$

Conductance

$$\frac{\partial I}{\partial V_D}$$

$$\sim \frac{q\gamma_1/2\hbar}{2\gamma_1 + 4k_BT}$$

$$\sim \frac{q^2}{4\hbar} \text{ if } \gamma_1 \gg k_BT$$

Conductance quantum

$$\sim \frac{q^2}{2\pi\hbar}$$
Assume $\gamma_2 = \gamma_1$

$U_0 = 0.5 \text{ eV}$

$\gamma_1 / \hbar$  $\gamma_2 / \hbar$

Assume $U_0 \gg k_B T, \gamma_1, \gamma_2$

$U_0 / 2$  $\Rightarrow$  $q \gamma_1 / 2 \hbar$

$-qV_D \Rightarrow$

$\Rightarrow$  $\frac{q \gamma_1}{2 \hbar}$

Level floats up by $U_0 \frac{\gamma_2}{\gamma_1 + \gamma_2}$

$U_0 :$ Increase in potential due to SINGLE electron

$U_0 >> k_B T, \gamma_1, \gamma_2$
SCF with self-interaction correction

Assume $\gamma_2 = \gamma_1$

$U_0 = 0.5 \text{ eV}$

$$U_i = U_0 (N - N_i)$$

Self-interaction Correction

Level does NOT float up
2 levels: Unrestricted SCF

Unrestricted SCF

\[ U_i = U_0 (N - N_i) \]

Self-interaction Correction

Restricted SCF

\[ U_i = U_0 N \]
2 levels: SCF versus exact

One-electron energy levels

Exact Needs picture in “Fock” space

One-electron energy levels

\[ \frac{\gamma_1}{\hbar} = \frac{\gamma_2}{\hbar} = \frac{\mu_1}{\hbar} = \frac{\mu_2}{\hbar} \]

Needs picture in “Fock” space
1-level: the view from “Fock space”

One-electron picture

\[ E = \varepsilon_1 \]

“Fock space”

\[ E = \varepsilon_1 \]
\[ E = 0 \]

Most of our thinking is based on this picture
2 levels: the view from “Fock space”

2 one-electron levels

$E = \varepsilon_2$

$E = \varepsilon_1$

2^2 many-electron levels

$E = \varepsilon_1 + \varepsilon_2 + U_0$

$E = \varepsilon_2$

$E = \varepsilon_1$

$E = 0$

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1-level: Current flow in “Fock space”

\[ E = \varepsilon_1 \]

\[ P_1 = 0 \]

\[ P_0 = 1 \]

\[ I = \frac{q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \]

\[ P_1 = \frac{\gamma_2}{(\gamma_1 + \gamma_2)} \]

\[ I = \left(\frac{q}{\hbar}\right) \gamma_1 P_1 \]

\[ = \left(\frac{q}{\hbar}\right) \gamma_2 P_0 \]

\[ P_0 = \frac{\gamma_1}{(\gamma_1 + \gamma_2)} \]
2 levels: Current flow in “Fock space”

\[ \mu_1 / h \quad \mu_2 / h \]

\[ \gamma_1 / h \quad \gamma_2 / h \]

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2 levels: Current flow in “Fock space”

\[ I = \frac{q}{\hbar} \frac{2\gamma_1\gamma_2}{\gamma_1 + \gamma_2} \]
\[ \rightarrow (q\gamma_1/\hbar) \]

\[ I = \frac{q}{\hbar} \frac{2\gamma_1\gamma_2}{\gamma_1 + 2\gamma_2} \]
\[ \rightarrow (2/3)(q\gamma_1/\hbar) \]

\[ I = (q/\hbar) \gamma_1 P_1 \]
\[ = (q/\hbar) 2\gamma_2 P_0 \]

\[ P_1 = 2\gamma_2 / (\gamma_1 + 2\gamma_2) \]
\[ P_0 = \gamma_1 / (\gamma_1 + 2\gamma_2) \]
Coulomb blockade and strong correlation

\[ P_{00} = (1 - f^\uparrow) \times (1 - f^\downarrow) \]
\[ P_{10} = f^\uparrow \times (1 - f^\downarrow) \]
\[ P_{01} = (1 - f^\uparrow) \times f^\downarrow \]
\[ P_{11} = f^\uparrow \times f^\downarrow \]

**UNCORRELATED**

\[ P_{11} = 0 \]
\[ P_{10} = P_{01} = \frac{\gamma_2}{\gamma_1 + 2\gamma_2} \]
\[ P_{00} = \frac{\gamma_1}{\gamma_1 + 2\gamma_2} \]

**STRONGLY CORRELATED**
4 levels: USCF versus exact

Unrestricted SCF

\[ U_i = U_0 (N - N_i) \]

Exact Fock space approach

USCF plateaus have wrong width: \( U_0 / 2 \)
wrong height: \( 1/N \)

Restricted SCF

\[ U_i = U_0 N \]
Equilibrium is different ...

\[ \gamma_1 / \hbar \quad \gamma_2 / \hbar \]

\[ \mu_1 \quad \mu_2 \]

Non-equilibrium

Normalized Current

\[ -qV_D \Rightarrow \]

Number of electrons

\[ \mu_1 = \mu_2 \Rightarrow \]

Equilibrium

SCF: Restricted and unrestricted
Being “close” to equilibrium helps too

\[ \gamma_2 = \gamma_1 \]
\[ \gamma_2 = 10 \gamma_1 \]
\[ \gamma_2 = 100 \gamma_1 \]

---> Closer ---> to equilibrium --->

\[ \frac{\gamma_1}{\hbar} \quad \frac{\gamma_2}{\hbar} \]

\[ \mu_1 \quad \mu_2 \]

Exact

SCF: Restricted and unrestricted

Normalized Current

\[ -qV_D \Rightarrow \]
General “Fock space” approach

2 one-electron levels

\[ \frac{\gamma_1}{\hbar} \quad \frac{\gamma_2}{\hbar} \]
\[ \epsilon + U_0 \]
\[ \epsilon \]
\[ \mu_1 \quad \mu_2 \]

2^2 many-electron levels

11 \[ E = 2\epsilon + U_0 \]

01 \[ E = \epsilon \]

10 \[ E = 0 \]

\[ \gamma_1 f_1(\epsilon + U_0) \]

\[ \gamma_1 f_1(\epsilon) \]

\[ \gamma_1 (1 - f_1(\epsilon + U_0)) \]

\[ \gamma_1 (1 - f_1(\epsilon)) \]
Equilibrium in “Fock space”

\[ E = 2\varepsilon + U_0 \]

\[ E = \varepsilon \]

\[ E = 0 \]

\[ \frac{P_{N+1}}{P_N} = \frac{f_1(\Delta E)}{1 - f_1(\Delta E)} = e^{-\left(\Delta E - \mu\right)/k_BT} \]

\[ P_i = \frac{1}{Z} e^{-\left(E_i - \mu N_i\right)/k_BT} \]

No general solution out-of-equilibrium with \( \mu_2 \neq \mu_1 \)

Law of Equilibrium

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Rate equations in “Fock space”

\[
\begin{align*}
E &= 2\varepsilon + U_0 \\
E &= \varepsilon \\
E &= 0
\end{align*}
\]

\[
\begin{align*}
\gamma_1 f_1(\varepsilon + U_0) + \gamma_2 f_2(\varepsilon + U_0) &
\gamma_1 \tilde{f}_1(\varepsilon + U_0) + \gamma_2 \tilde{f}_2(\varepsilon + U_0) \\
\gamma_1 f_1(\varepsilon) + \gamma_2 f_2(\varepsilon) &
\gamma_1 \tilde{f}_1(\varepsilon) + \gamma_2 \tilde{f}_2(\varepsilon)
\end{align*}
\]

\[
\begin{align*}
\frac{d}{dt} \begin{pmatrix} P_{00} \\ P_{01} \\ P_{10} \\ P_{11} \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\
&= \begin{pmatrix} * & \downarrow & \downarrow & 0 \\ \downarrow & * & 0 & \downarrow \\ \uparrow & 0 & * & \downarrow \\ 0 & \uparrow & \uparrow & * \end{pmatrix} \begin{pmatrix} P_{00} \\ P_{01} \\ P_{10} \\ P_{11} \end{pmatrix}
\end{align*}
\]

Each column adds to zero

\[
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}
\]
Solving the rate equations

\[
\begin{align*}
E &= 2\varepsilon + U_0 \\
E &= \varepsilon \\
E &= 0
\end{align*}
\]

All probabilities add to ONE
Calculating current in "Fock space"

\[
\begin{align*}
\gamma_1 f_1(\varepsilon + U_0) + \gamma_2 f_2(\varepsilon + U_0) & \quad \gamma_1 \tilde{f}_1(\varepsilon + U_0) + \gamma_2 \tilde{f}_2(\varepsilon + U_0) \\
\gamma_1 f_1(\varepsilon) + \gamma_2 f_2(\varepsilon) & \quad \gamma_1 \tilde{f}_1(\varepsilon) + \gamma_2 \tilde{f}_2(\varepsilon)
\end{align*}
\]
"Fock space" for 4 one-electron levels

Two problems: *Size

N one-electron levels

γ₁/ℏ γ₂/ℏ

μ₁ μ₂

N=4

N=3

N=2

N=1

N=0

2ᴺ many-electron levels

1111

1110 1101 1011 0111

1100 1010 1001 0110 0101 0011

0001 0010 0100 1000

0000

"Orthodox Theory"
If $k_B T + \text{broadening} \ll \text{charging } U_0$

$U_0 < k_B T, \gamma_1, \gamma_2$

Use SCF method

Assume $\gamma_2 = \gamma_1$

$2\gamma_1 + 4k_B T \Rightarrow \frac{q\gamma_1}{2\hbar}$

$-qV_D \Rightarrow$
Concepts of Quantum Transport (CQT)

Hot \( \Sigma_s \)

\( H+U \)

\( \Sigma_1 \) \( \Sigma_2 \)

\( \mu_1 \) \( \mu_2 \)

Nanowires, nanotubes, molecules ..... Switches, energy conversion ...

Entangled!
Concepts of Quantum Transport

Introduction:
Lecture #1:
Nanodevices and Maxwell’s demon

Lecture #2:
Electrical Resistance: A Simple Model

Lecture #3:
Probabilities, Wavefunctions and Green functions

Lecture #4:
Coulomb blockade and Fock space

No advanced background required. Familiarity with linear algebra may be useful for some topics.

Unified Model for Quantum Transport Far from Equilibrium

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