



Lab Exercise I: MolCToy (Understanding the simple models)

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Login



Website: www.nanohub.purdue.edu

A screenshot of the Nanohub website displayed in a Microsoft Internet Explorer browser window. The browser's address bar shows the URL 'http://www.nanohub.purdue.edu/'. The website header features the 'nanohub' logo in a stylized, pixelated font. Below the logo, it states 'Operated by the Purdue Computational Electronics Research Group' and 'The Nanotechnology Simulation Hub Online Computing for Nanotechnology'. The main content area is organized into several sections: 'HOME', 'MY HUB', 'HUB FORUMS', and 'HELP'. The 'HOME' section is further divided into 'NANOTOOLS', 'DEVICES', 'ECAD', 'MATERIALS', and 'GENERAL/PRODUCTIVITY TOOLS'. Each section lists various simulation tools and software, some with 'NEW!' labels. A 'SIGN IN' box on the right side of the page contains links for 'Login', 'Forgot your Password?', and 'Request an Account'. Other sections include 'TRUBLE?', 'SYSTEM LINKS', 'MONITOR', and 'SPONSORS'. The browser's status bar at the bottom indicates 'Internet'.

05/31/2002

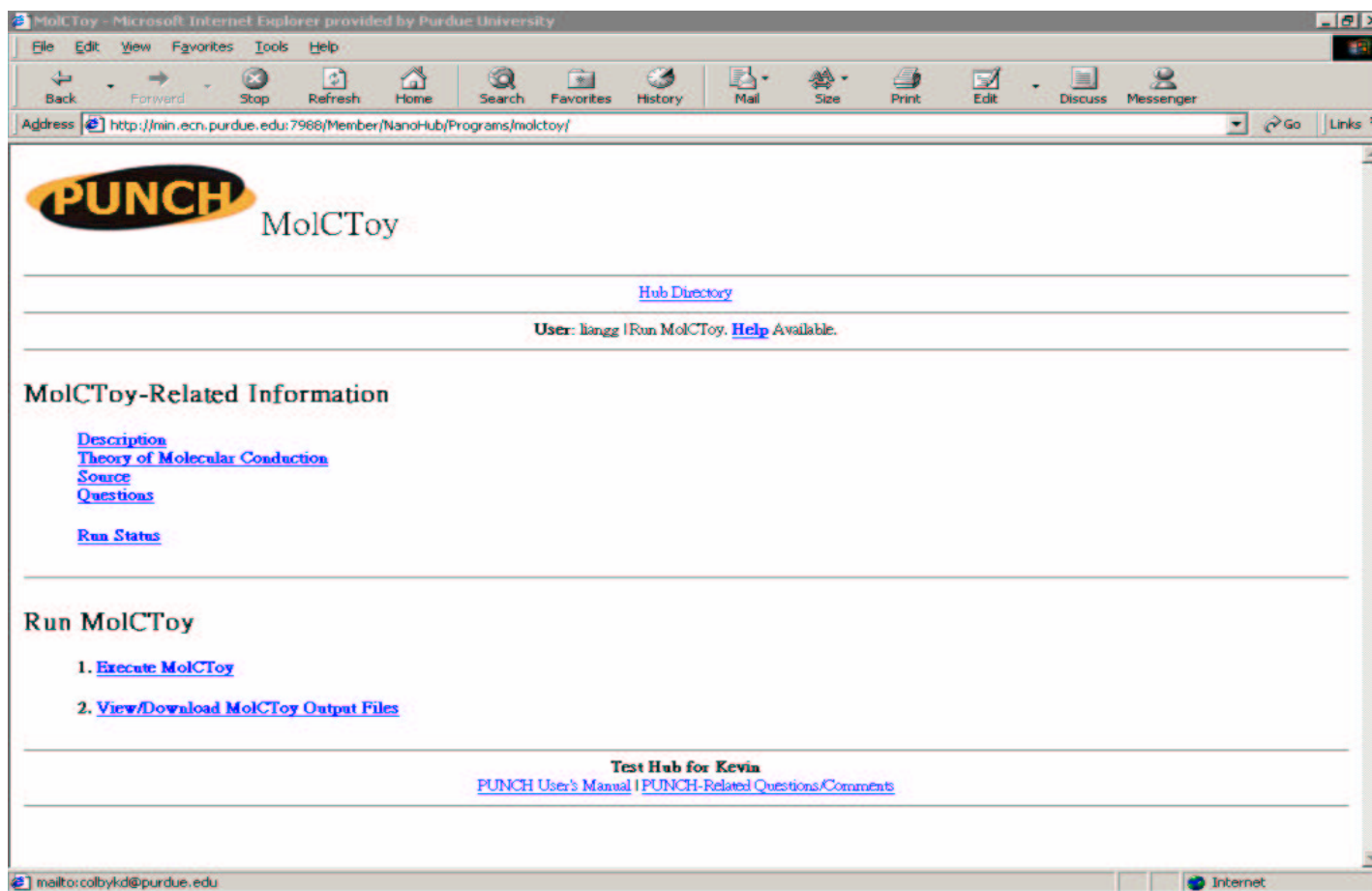
UIUC Summer School May 2002



MolCToy



Name/Password



MolCToy - Microsoft Internet Explorer provided by Purdue University

Address <http://min.ecn.purdue.edu:7988/Member/NanoHub/Programs/molctoy/>

PUNCH MolCToy

[Hub Directory](#)

User: liangg | Run MolCToy. [Help](#) Available.

MolCToy-Related Information

- [Description](#)
- [Theory of Molecular Conduction](#)
- [Source](#)
- [Questions](#)
- [Run Status](#)

Run MolCToy

- [Execute MolCToy](#)
- [View/Download MolCToy Output Files](#)

Test Hub for Kevin

[PUNCH User's Manual](#) | [PUNCH-Related Questions/Comments](#)

mailto:colbykd@purdue.edu

Run MolCToy



The screenshot shows a web browser window titled "MolCToy: Execute - Microsoft Internet Explorer provided by Purdue University". The address bar contains the URL: http://min.ecn.purdue.edu:7988/Member107/NanoHub/Programs/796_molctoy/Exec/. The page content includes navigation links: [Hub Directory](#), [MolCToy](#), [Step1:Execute](#), and [Step2:Output](#). Below these is a "Help" link for Step 2:Execute and the user name "liangg".

The main form contains the following parameters and controls:

- Fermi Energy of Contacts, E_f (eV):** Input field: -5, Range: [-7, -3]
- Energy Level**
 - First Energy Level, E_0 (eV):** Input field: -5.5, Range: [-8, -2]
 - Second Energy Level, E_1 (eV):** Input field: -3, Range: [-8, -2]
- Charging Energy, U_0 (eV/electron):** Input field: 0, Range: [0, 4]
- Interactive Strength between Molecular Levels**
 - Broadening by Contact 1, Gamma 1:** Input field: 0.05, Range: [0.025, 1]
 - Broadening by Contact 2, Gamma 2:** Input field: 0.05, Range: [0.025, 1]
- Temperature, T (K):** Input field: 300, Range: [50, 1000]
- Plot Format(s)**
 - GIF (Graphic Interchange Format)
 - PDF (Portable Document Format)
 - PS (PostScript)
- Output Folder:** Input field: EX1

A "Run MolCToy" button is located below the form.

At the bottom of the page, there are additional navigation links: [Hub Directory](#), [MolCToy](#), [Step1:Execute](#), and [Step2:Output](#). Below these is the text "Test Hub for Kevin" and links to [PUNCH User's Manual](#) and [PUNCH-Related Questions/Comments](#).

Program Status



The screenshot shows a web browser window titled "MolCToy: Status - Microsoft Internet Explorer provided by Purdue University". The address bar shows the URL: http://min.ecn.purdue.edu:7988/Member107/NanoHub/Programs/796_molctoy/Exec/. The page content includes the "PUNCH" logo and the heading "Program Status". Below the heading are navigation links: [Hub Directory](#) | [MolCToy](#) | [Step1.Execute](#) | [Step2.Output](#). A message states: "You are currently running 1 program(s) (Maximum Allowed: 3).". Below this is a control panel with radio buttons for "Update Status Info" (selected) and "Abort Selected Program(s)", followed by a "Proceed" button. A list of running programs is shown, with one entry: **molctoy** (process #13). Status: running. Elapsed time: 1 seconds. Machine: four-processor 296MHz Sun Enterprise server. Credits: made possible by grants from the National Science Foundation. At the bottom of the page, there are more navigation links: [Hub Directory](#) | [MolCToy](#) | [Step1.Execute](#) | [Step2.Output](#). The browser status bar at the bottom shows "Done" and "Internet".

Output



Files: 1ReadMe, compare_conductance.ps, compare_current.ps, one_level.ps, one_level_broadened.ps, one_level_unrestricted.ps, output, punch-run.log and two_levels.ps

A screenshot of a Microsoft Internet Explorer browser window displaying the "MolCToy: Output" web page. The browser's address bar shows the URL: http://main.ecn.purdue.edu:7966/Member107/NanoHub/Programs/796_molctoy/Output.2311/:EX1/. The page features the "PUNCH" logo and the title "MolCToy: Output". Below the title, there are navigation links: "Hub Directory", "MolCToy", "Step1_Execute", and "Step2_Output". A "Help" link is also present, along with user and folder information: "User: liangg" and "Working Folder: /molctoy/Output/EX1/". The main content area is titled "1. Select one of the commands from the categories a, b, or c." and contains a form with three sections: a. "View File OR Open Folder", "Delete File OR Folder", and "Download File to Your Disk"; b. "Go To Examples Folder"; and c. a text input field. A list of files is shown in a dropdown menu: "1ReadMe", "compare_conductance.gif", "compare_conductance.ps", and "compare_current.gif". A "File Type" dropdown is set to "Auto". Below the form is a button labeled "Execute the Command". At the bottom of the page, there are links for "Test Hub for Kevin" and "PUNCH User's Manual | PUNCH-Related Questions/Comments".



Exercises

1. **Resonant tunneling without charging**
Understanding the energy diagrams and why the levels are broadened.
2. **Charging effects in molecular devices**
How does the charging energy affect the I-V?
3. **Asymmetric coupling to the molecule**
How can we make the I-V asymmetric?
4. **LUMO conduction**
Which level (HOMO or LUMO) is the current going through?



Exercise I:



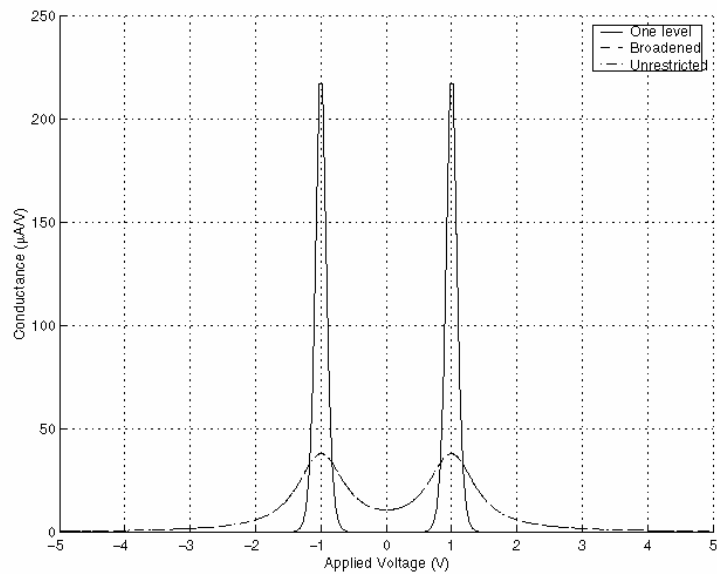
U0=0

Fermi Energy of Contacts, Ef (eV):	-5	[-7, -3]
Energy Level		
First Energy Level, E0 (eV):	-5.5	[-8, -2]
Second Energy Level, E1 (eV):	-3	[-8, -2]
Charging Energy, U0 (eV/electron):	0	[0, 4]
Interactive Strength between Molecular Level		
Broadening by Contact 1, Gamma 1:	0.05	[0.025, 1]
Broadening by Contact 2, Gamma 2:	0.05	[0.025, 1]
Temperature, T (K):	300	[50, 1000]
Plot Format(s)		
GIF (Graphic Interchange Format)		
PDF (Portable Document Format)		
PS (PostScript)		
Output Folder:	EX1	

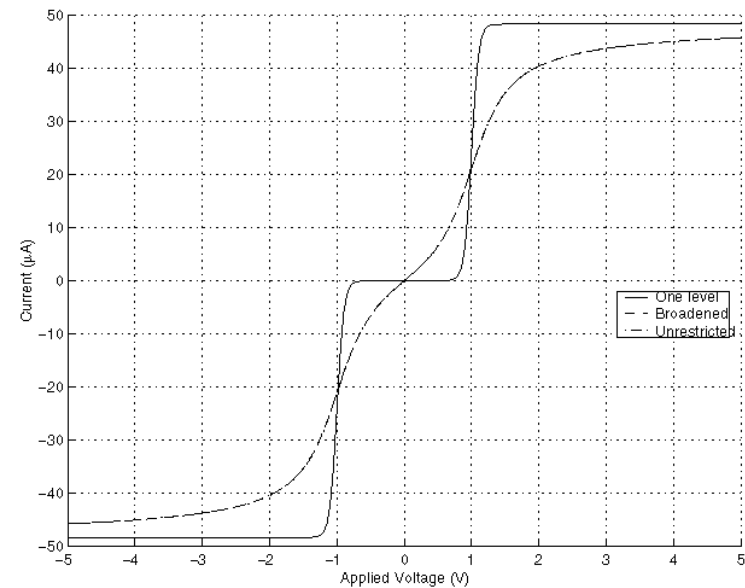
Output I-1



compare_conductance



compare_current

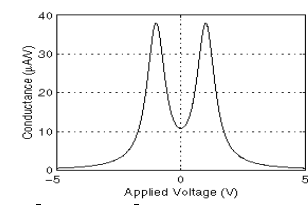
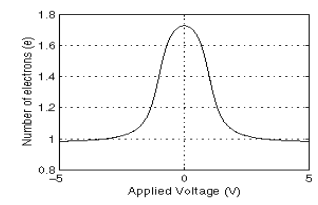
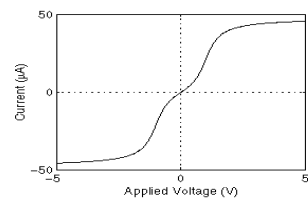
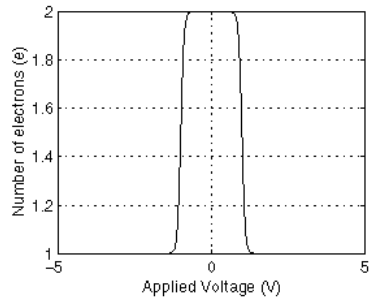
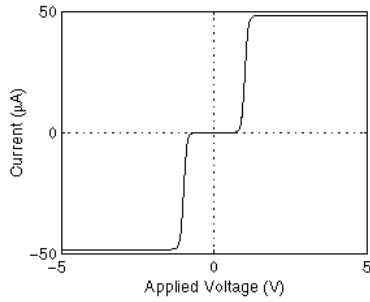


Output I-2

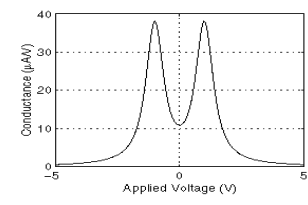
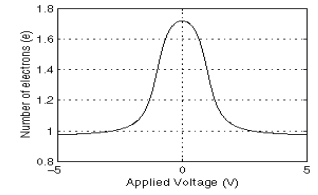
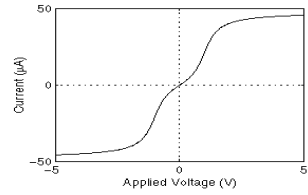
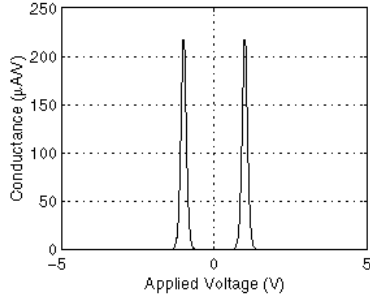


one_level_broadened

one_level



one_level_unrestricted





Questions I



1. What factors influence the “conductance gap”?
2. Explain the broadening of the conductance peaks. Why is the broadening different for the different models? Which factors determine the broadening?
3. Explain the shape of the IV.
4. Why do the one_level_broadened and one_level_unrestricted look similar?



Exercise II



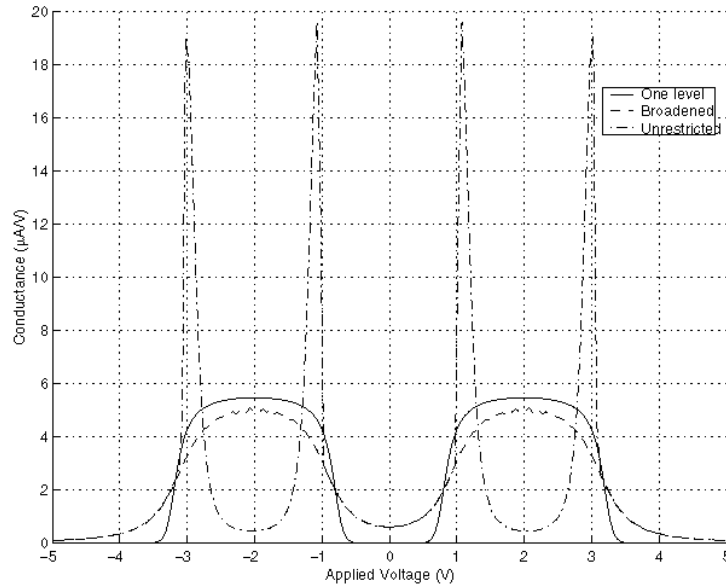
$U_0=1$ eV

Fermi Energy of Contacts, E_f (eV):	-5	[-7, -3]
Energy Level		
First Energy Level, E_0 (eV):	-5.5	[-8, -2]
Second Energy Level, E_1 (eV):	-3	[-8, -2]
Charging Energy, U_0 (eV/electron):	1	[0, 4]
Interactive Strength between Molecular Level		
Broadening by Contact 1, Γ_1 :	0.05	[0.025, 1]
Broadening by Contact 2, Γ_2 :	0.05	[0.025, 1]
Temperature, T (K):	300	[50, 1000]
Plot Format(s)		
GIF (Graphic Interchange Format)		
PDF (Portable Document Format)		
PS (PostScript)		
Output Folder:	EX2	

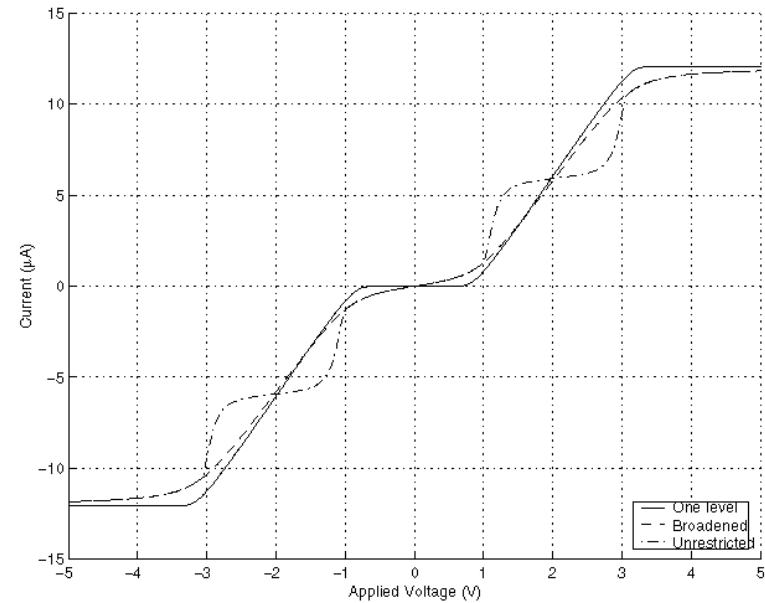
Output II-1



compare_conductance



compare_current





Questions II



1. Why has the broadening of the conductance peaks increased (compared to question I)?
2. How does this change the I-V?
3. Comparing these results with those of Exercise 1, what is different and why?
4. Explain the shape of the I-V for the unrestricted model. Why are there extra steps?



Exercise III



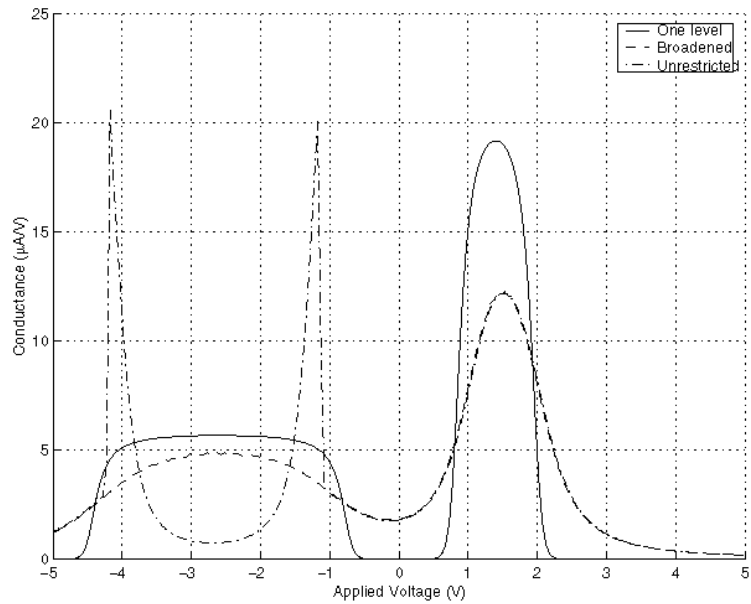
Gamma1=0.05 Gamma2=0.2

Fermi Energy of Contacts, E_f (eV):	-5	[-7, -3]
Energy Level		
First Energy Level, E_0 (eV):	-5.5	[-8, -2]
Second Energy Level, E_1 (eV):	-3	[-8, -2]
Charging Energy, U_0 (eV/electron):	1	[0, 4]
Interactive Strength between Molecular Level		
Broadening by Contact 1, Gamma 1:	0.05	[0.025, 1]
Broadening by Contact 2, Gamma 2:	0.2	[0.025, 1]
Temperature, T (K):	300	[50, 1000]
Plot Format(s)		
GIF (Graphic Interchange Format)		
PDF (Portable Document Format)		
PS (PostScript)		
Output Folder:	EX3	

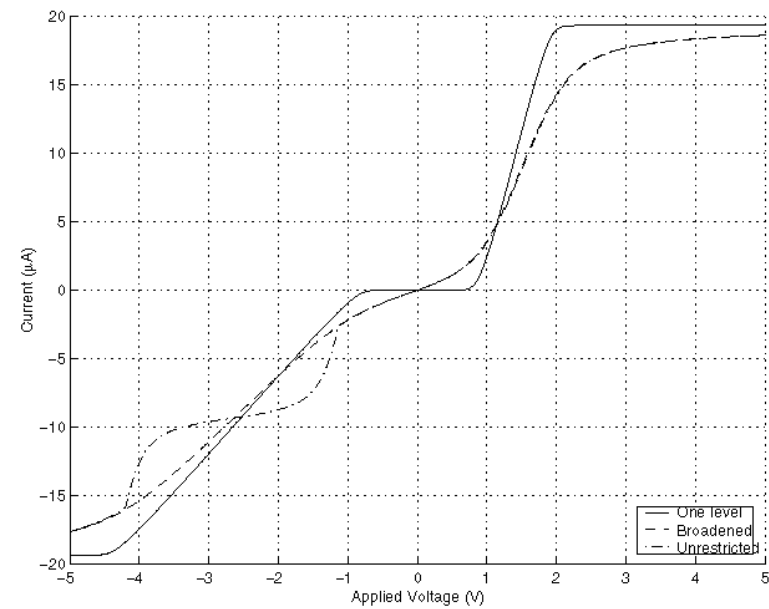
Output III-1



compare_conductance



compare_current





Questions III



1. Why is the I-V asymmetric?
2. Is the charging important for the asymmetry?
3. Explain why the number of electrons is different for positive and negative bias.



Exercise IV



Changing Ef

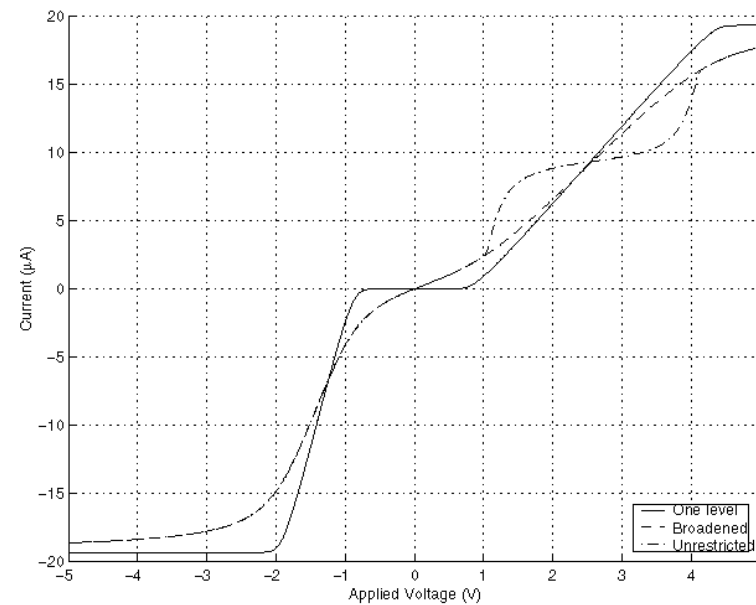
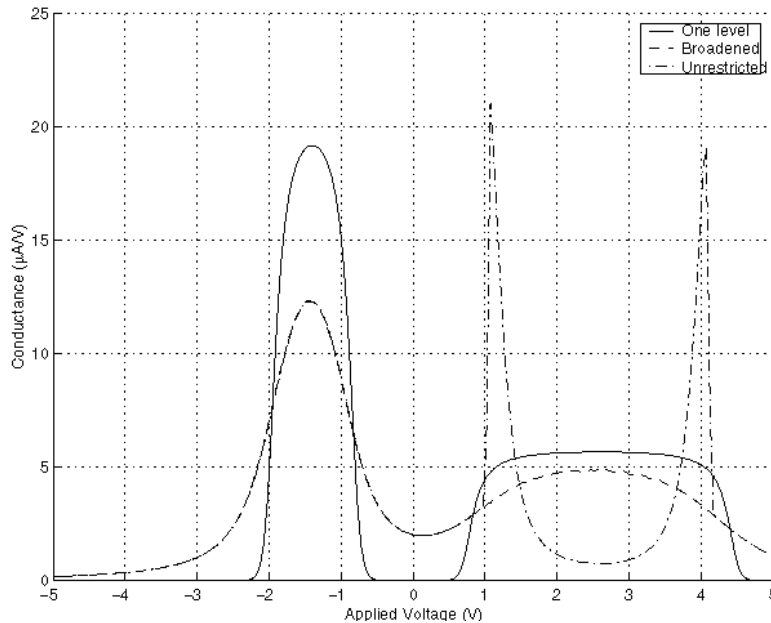
Fermi Energy of Contacts, Ef (eV):	-6	[-7, -3]
Energy Level		
First Energy Level, E0 (eV):	-5.5	[-8, -2]
Second Energy Level, E1 (eV):	-3	[-8, -2]
Charging Energy, U0 (eV/electron):	1	[0, 4]
Interactive Strength between Molecular Level		
Broadening by Contact 1, Gamma 1:	0.05	[0.025, 1]
Broadening by Contact 2, Gamma 2:	0.2	[0.025, 1]
Temperature, T (K):	300	[50, 1000]
Plot Format(s)		
GIF (Graphic Interchange Format)		
PDF (Portable Document Format)		
PS (PostScript)		
Output Folder:	EX4	

Output IV-1



compare_conductance

compare_current





Questions IV



1. Has the asymmetry changed?
2. Is this useful? (Where is the Fermi-energy?)
3. If you have time:
 - Does the temperature affect the results?
 - What new effects can you see in the two level model?