Lab Exercise I: MolCToy (Understanding the simple models)

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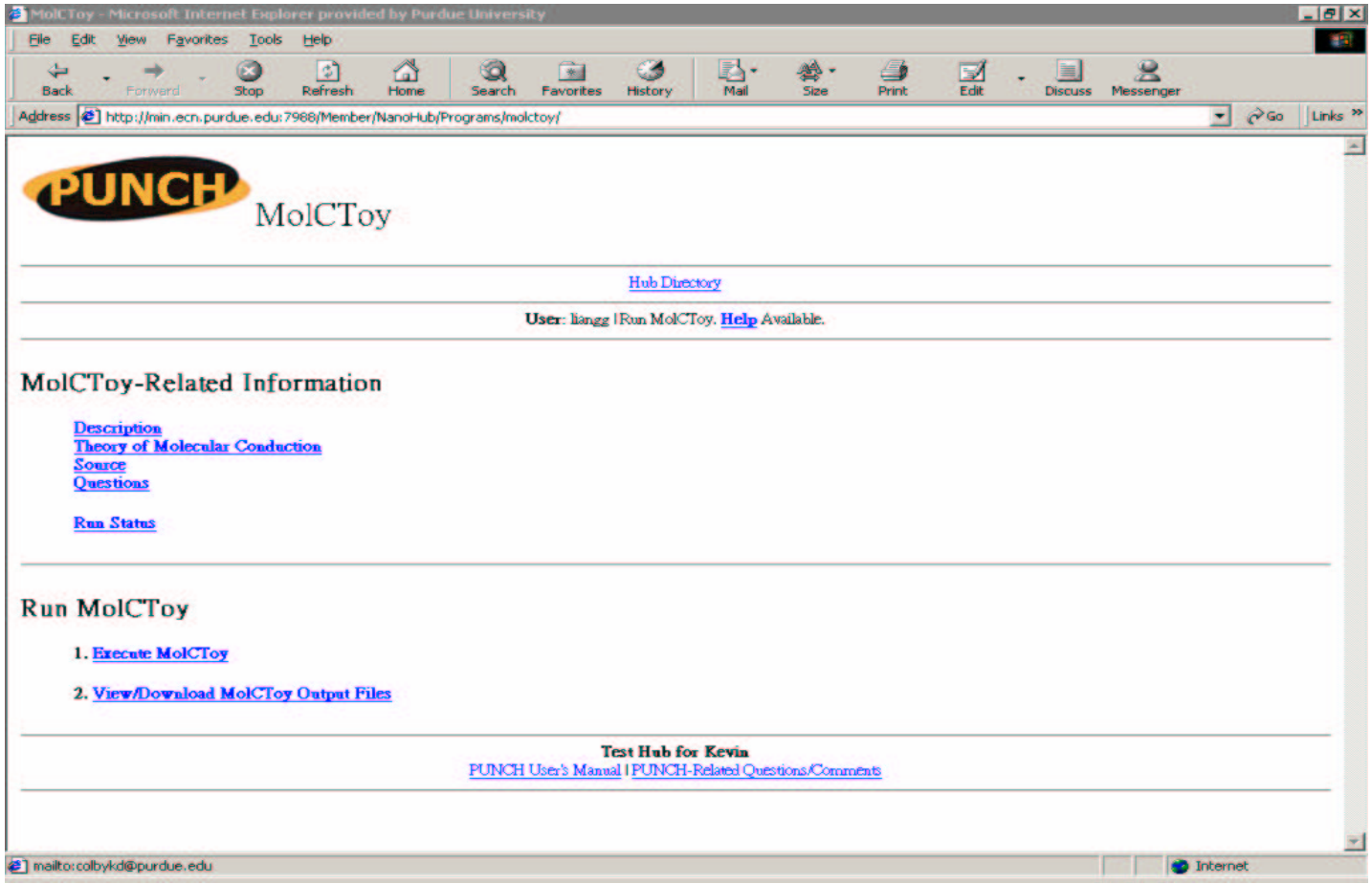
Login

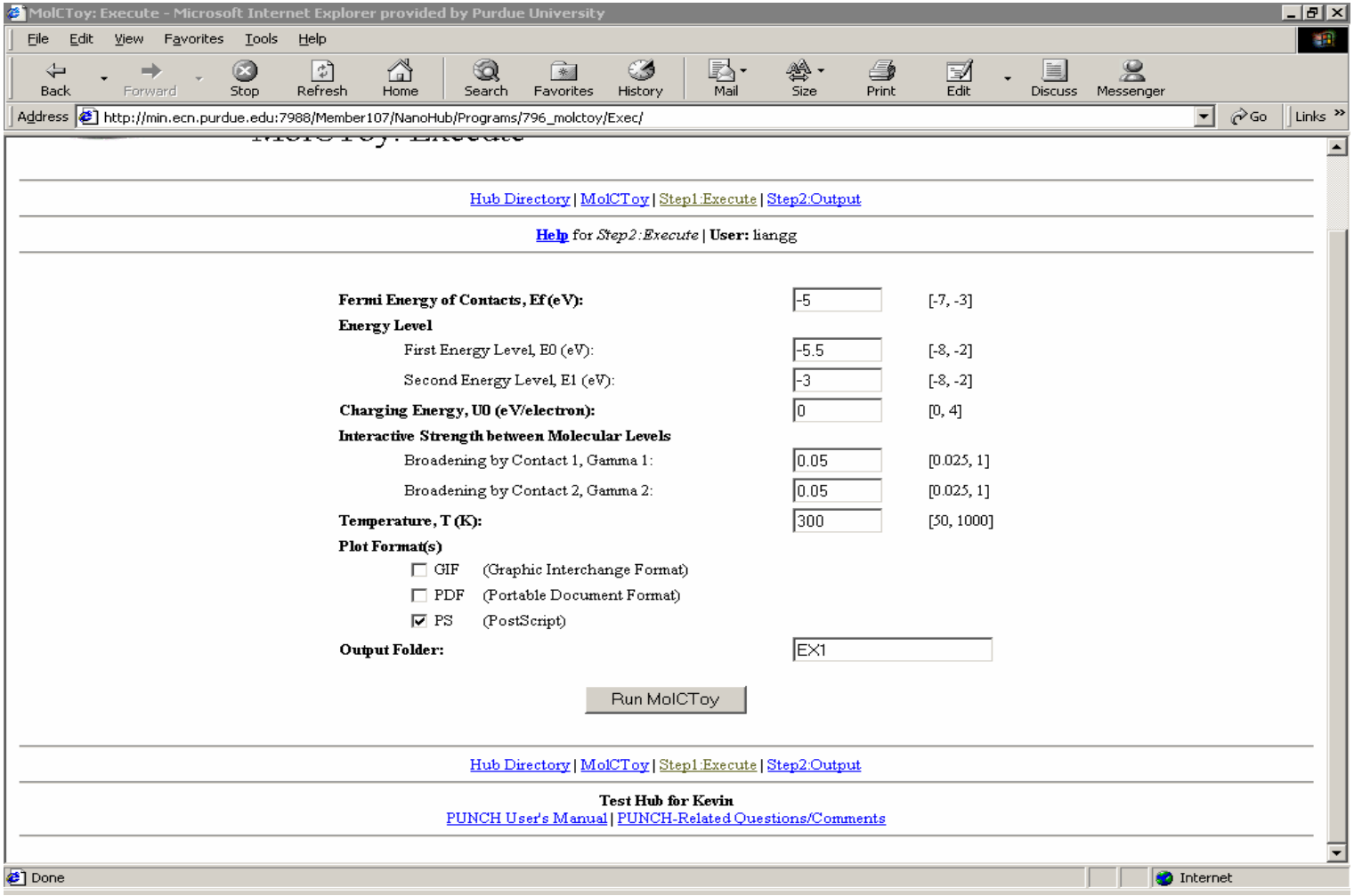
Website: www.nanohub.purdue.edu

MolCToy

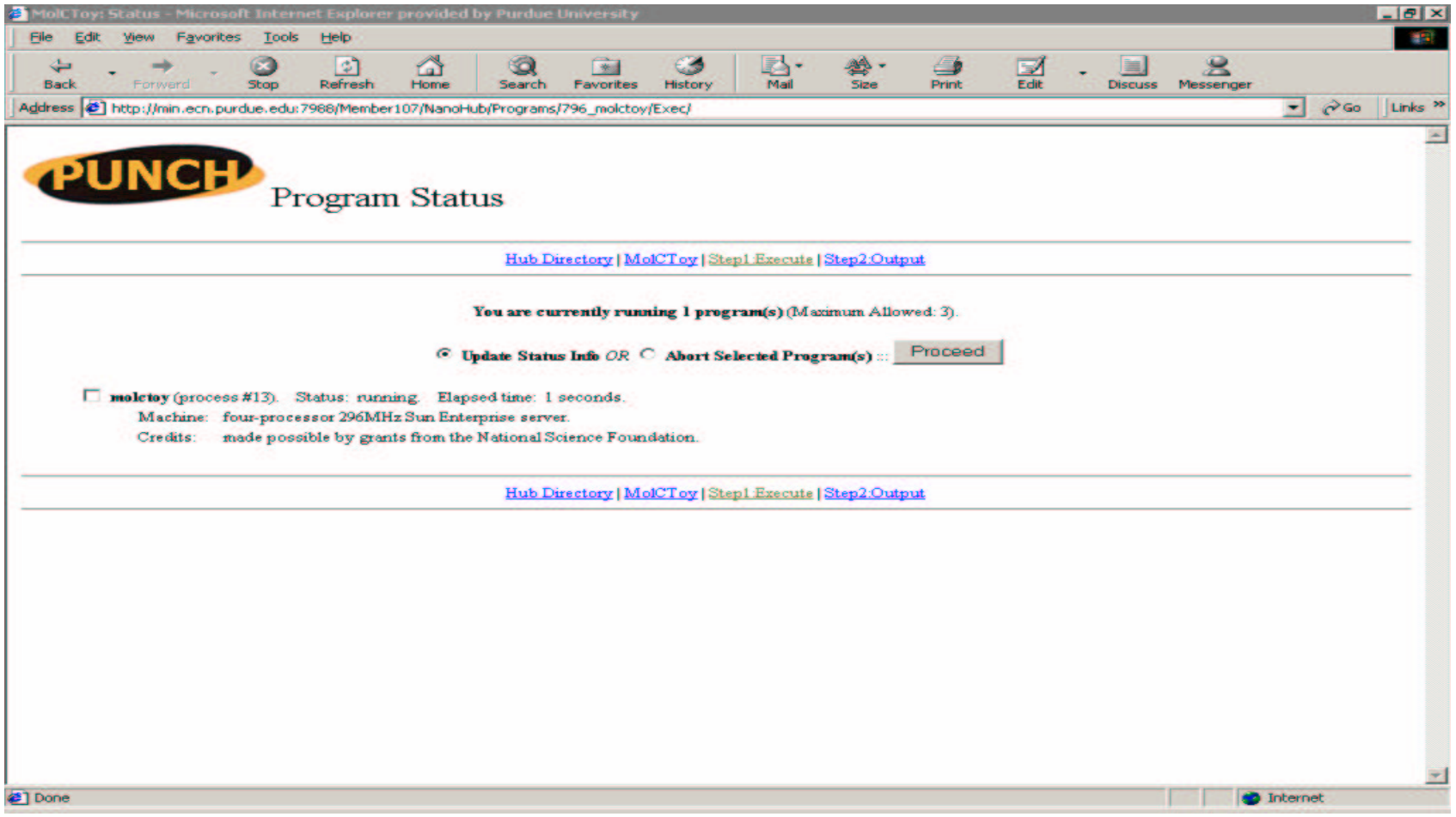
Name/Password



Run MolCToy

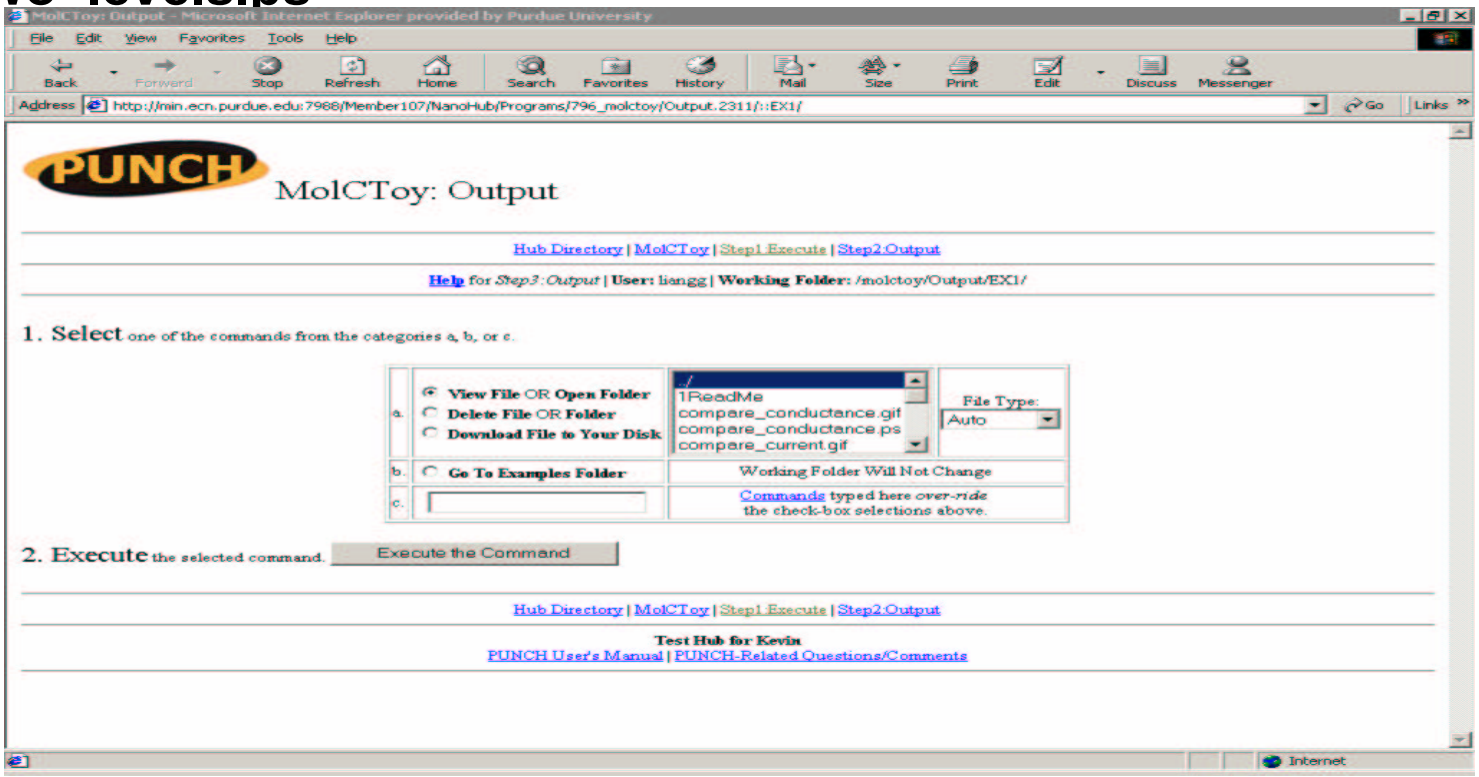

MolCToy: Execute - Microsoft Internet Explorer provided by Purdue University
File Edit View Favorites Tools Help
Back Forward Stop Refresh Home Search Favorites History Mail Size Print Edit Discuss Messenger
Address http://min.ecn.purdue.edu:7988/Member107/NanoHub/Programs/796_molctoy/Exec/
Go Links
Hub Directory | MolCToy | Step1:Execute | Step2:Output
Help for Step2:Execute | User: liangg
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 Levels
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
Run MolCToy
Hub Directory | MolCToy | Step1:Execute | Step2:Output
Test Hub for Kevin
PUNCH User's Manual | PUNCH-Related Questions/Comments
Done
Internet

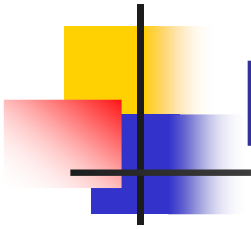
Program Status



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





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?

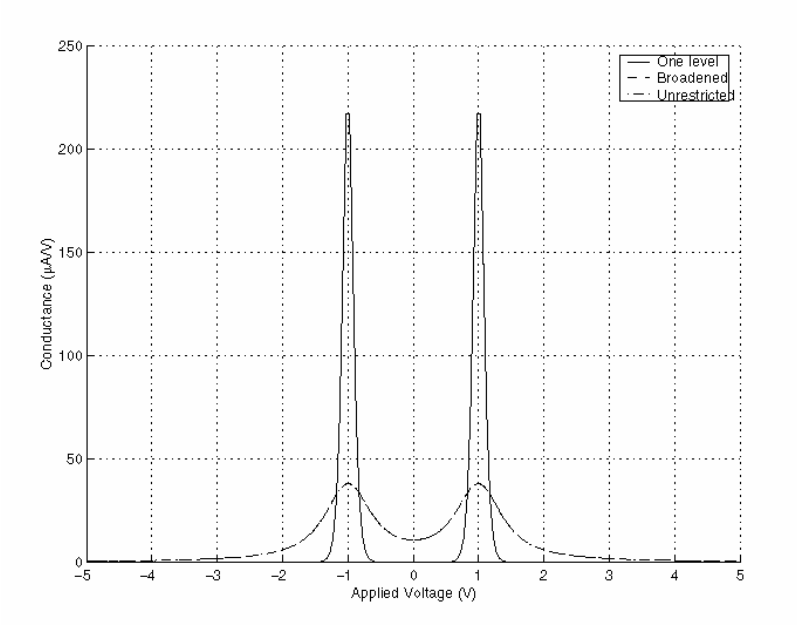
Exercise I:

U0=0

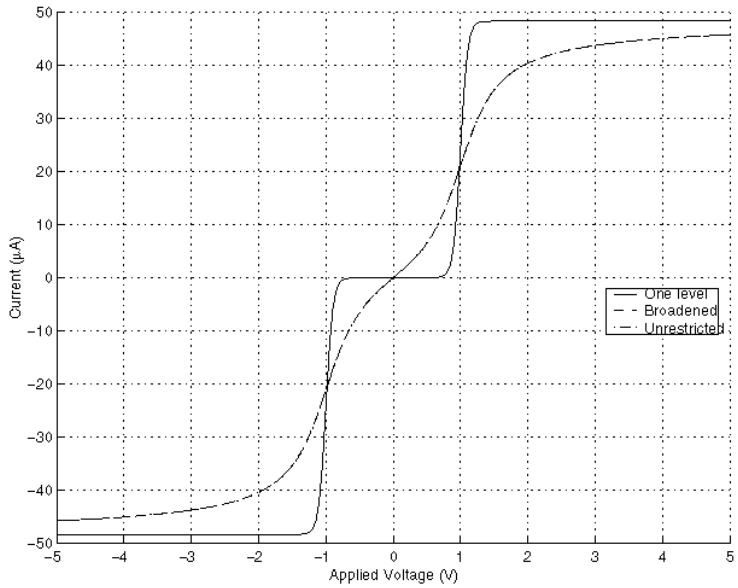
Fermi Energy of Contacts**, Ef (eV):**	**-5**	[-7, -3]
Energy Level		
First Energy Level, E0 (eV):	**-5.5**	[-8, -2]
Second Energy Level, E1 (eV):	**-3**	[-8, -2]
Charging Energy, U0 (eV/electron):	**0**	[0, 4]
Interactive Strength between Molecular Level		
Broadening by Contact 1, Gamma 1:	**0.05**	[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



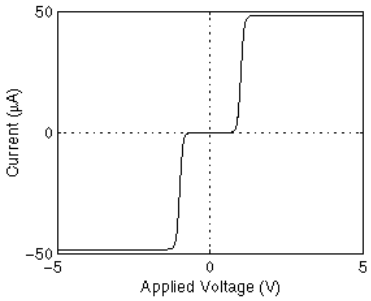
compare_current

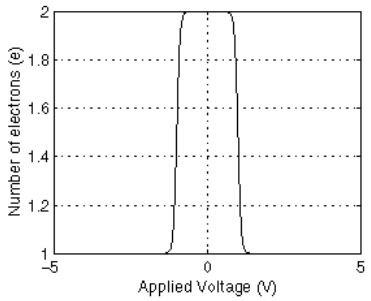


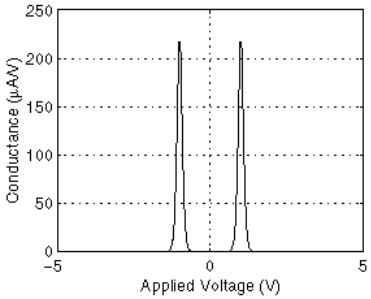
Output I-2

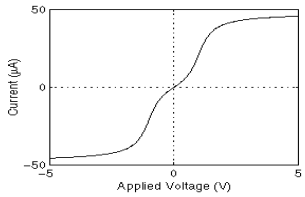
one_level_broadened

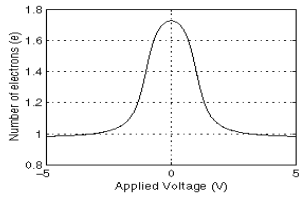
one_level

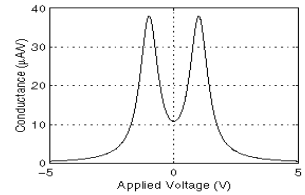




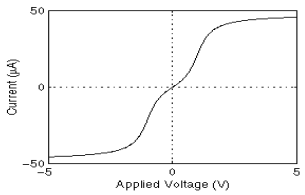


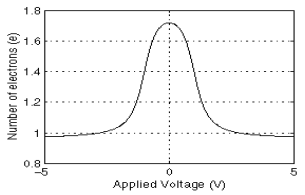


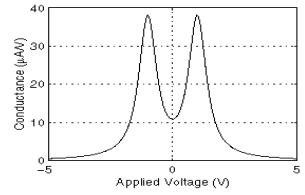




one_level_unrestricted







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?

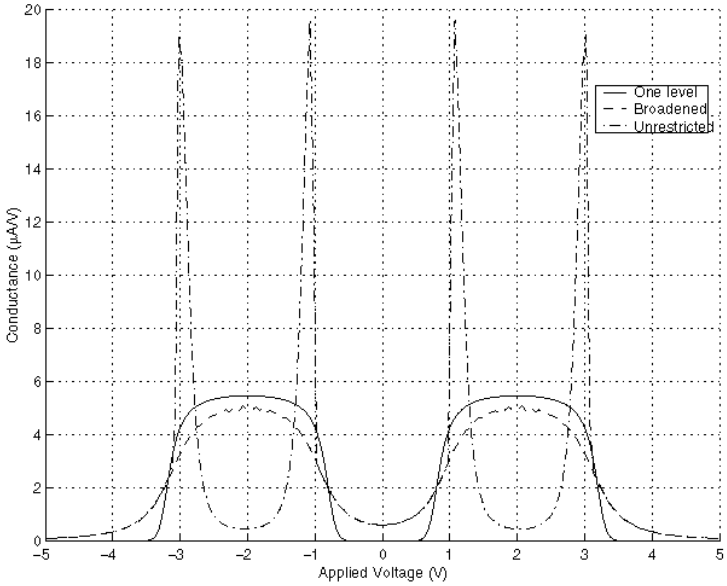
Exercise II

U0=1 eV

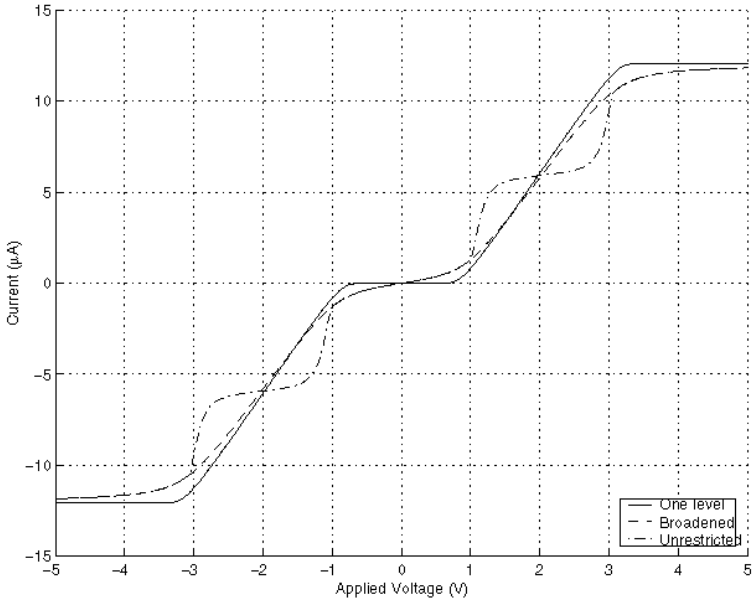
Fermi Energy of Contacts**, Ef (eV):**	**-5**	[-7, -3]
Energy Level		
First Energy Level, E0 (eV):	**-5.5**	[-8, -2]
Second Energy Level, E1 (eV):	**-3**	[-8, -2]
Charging Energy, U0 (eV/electron):	**1**	[0, 4]
Interactive Strength between Molecular Level		
Broadening by Contact 1, Gamma 1:	**0.05**	[0.025, 1]
Broadening by Contact 2, Gamma 2:	**0.05**	[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?

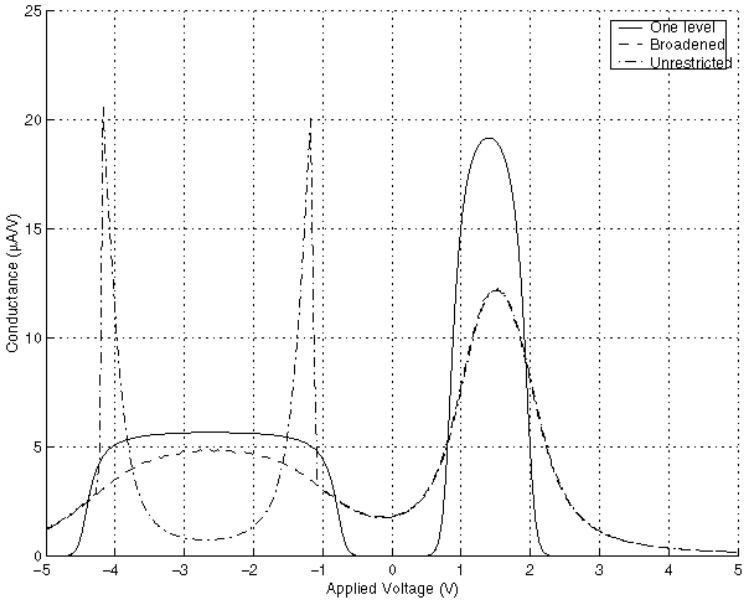
Exercise III

Gamma1=0.05 Gamma2=0.2

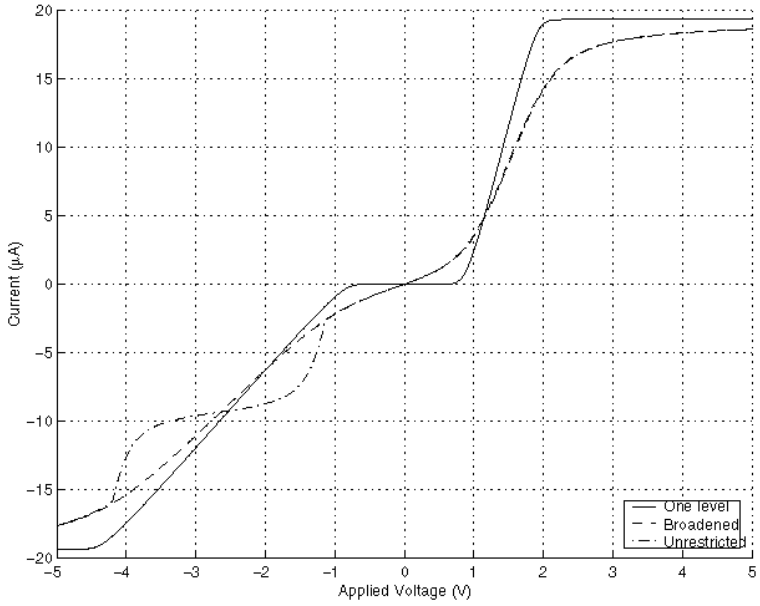
Fermi Energy of Contacts**, Ef (eV):**	**-5**	[-7, -3]
Energy Level		
First Energy Level, E0 (eV):	**-5.5**	[-8, -2]
Second Energy Level, E1 (eV):	**-3**	[-8, -2]
Charging Energy, U0 (eV/electron):	**1**	[0, 4]
Interactive Strength between Molecular Level		
Broadening by Contact 1, Gamma 1:	**0.05**	[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.

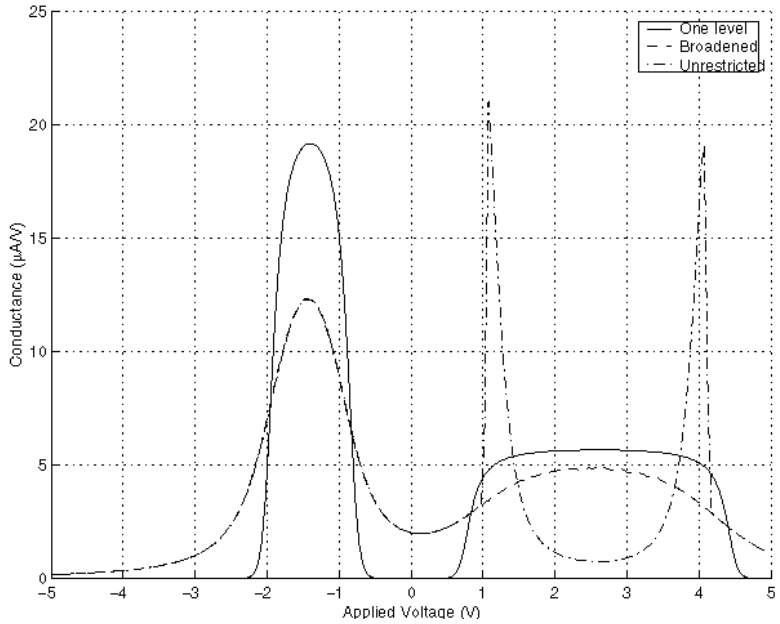
Exercise IV

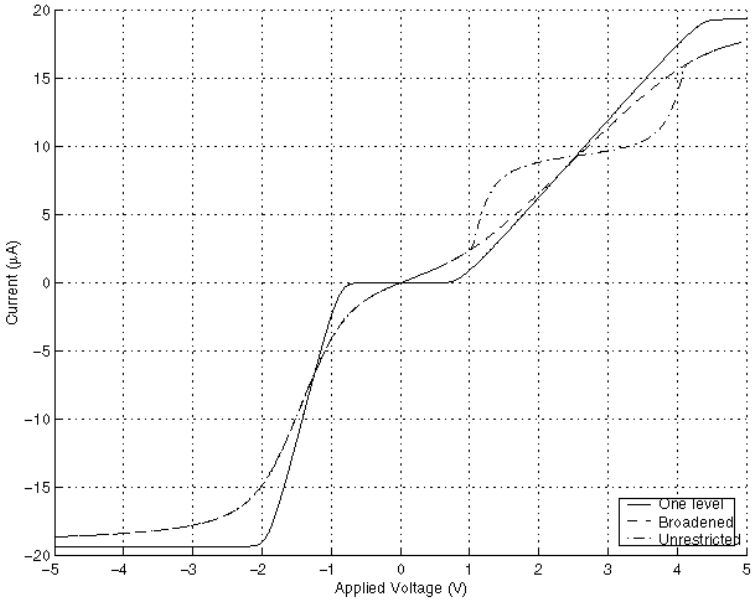
Changing Ef

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?