Spin-configuration and Electron-interaction Effects on Transport through Doped Nanotube Junctions

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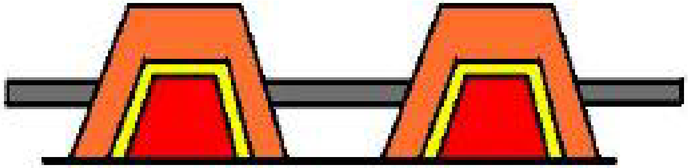
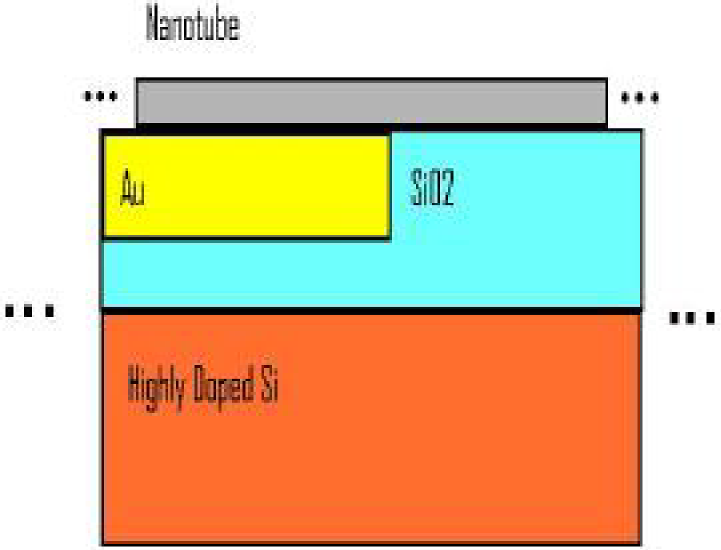
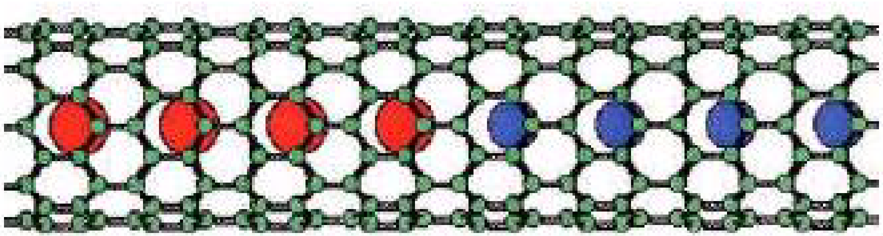
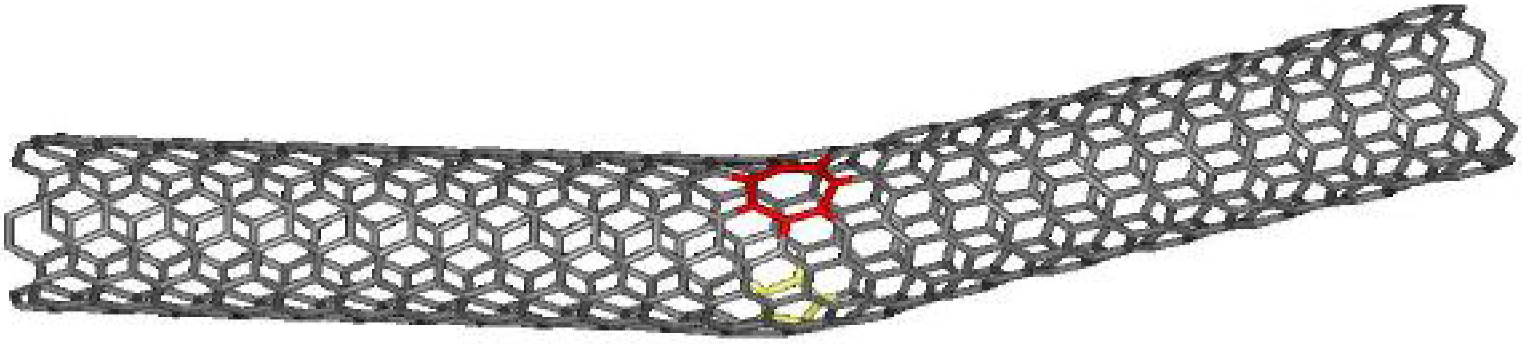
Doped Nanotube Junctions (1)



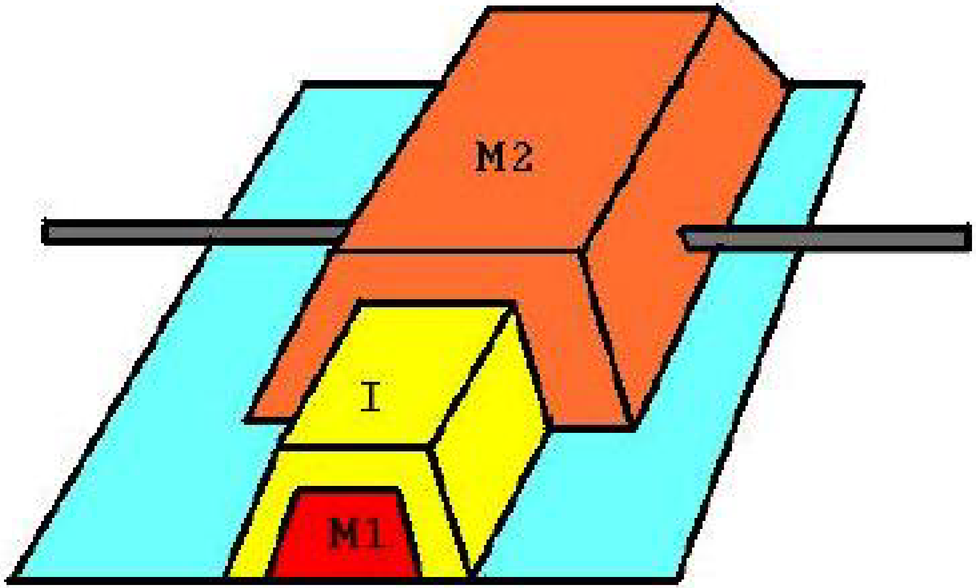


Doped Nanotube Junctions (2)

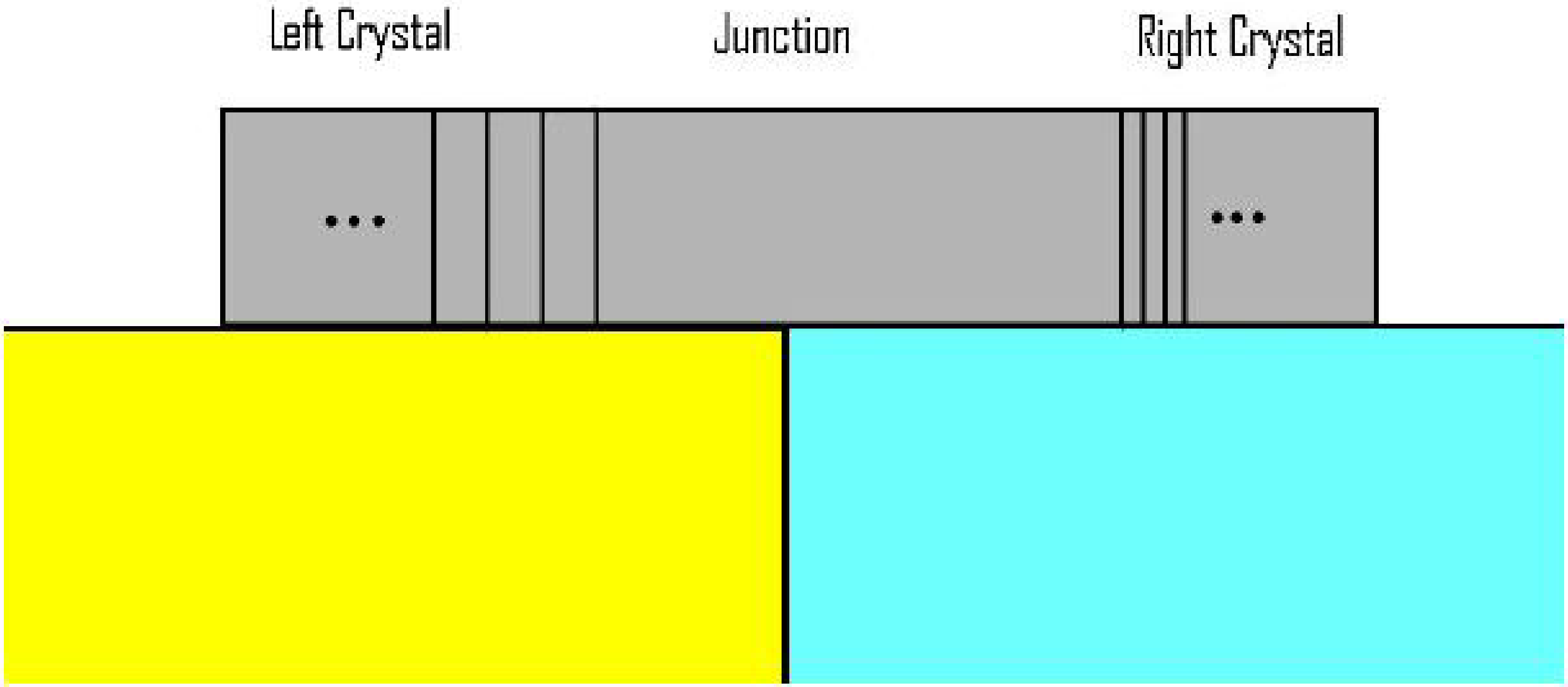




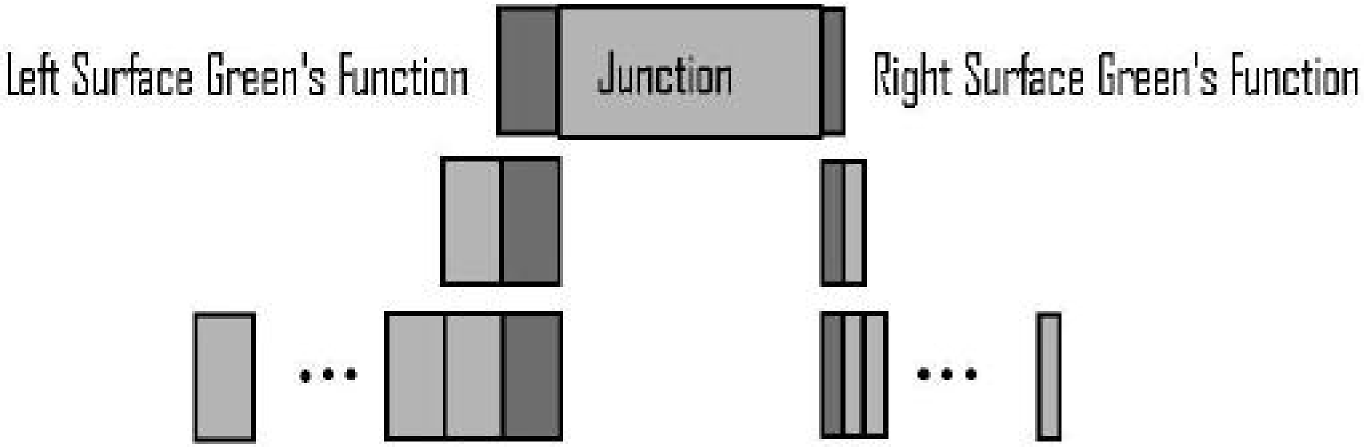
Transport



Junction and Bulk Geometries



Surface Green's Function Matching



Transfer Matrices

$$G_{M;n+1,m} = T_M G_{M;n,m}, (n\ ?\ m)$$

$$G_{M;n-1,m} = \bar{T}_M G_{M;n,m}, (n \le m)$$

$$G_{M;n,m+1} = G_{M;n,m} S_M, (m\ ?\ n)$$

$$G_{M;n,m-1} = G_{M;n,m} \bar{S}_M, (m \le n)$$

Green's Function of the Matched System Projected onto the Junction

$$\mathbf{G} \equiv \mathbf{I}G\mathbf{I} \equiv \begin{pmatrix} \mathbf{G}_{BB} \mathbf{G}_{BA} \\ \mathbf{G}_{AB} \mathbf{G}_{AA} \end{pmatrix}$$

$$= \begin{pmatrix} E - H_{B;1,1} - V_{B;1,2} T_B & -V_{I;1,-1} \\ -V_{I;-1,1} & E - H_{A;-1,-1} - V_{A;-1,-2} \bar{T}_A \end{pmatrix}^{-1}$$

Reflected and Transmitted Amplitudes; Transmission Matrix

$$\Psi_n^r = G_{B;n,1}\mathbf{G}_B^{-1}(\mathbf{G}_{BB} - \mathbf{G}_B)\mathbf{G}_B^{-1}G_{B;1,n'}G_{B;n',n'}^{-1}\Phi_{B;n'}$$

$$\Psi_n^t = G_{B;n,1}\mathbf{G}_B^{-1}\mathbf{G}_{BA}\mathbf{G}_A^{-1}G_{A;-1,n'}G_{A;n',n'}^{-1}\Phi_{A;n'}$$

$$\mathbf{S}_{n,n'}^{BA}(E,V) = T_B^n\mathbf{G}_{BA}\overline{S}_A^{n'}G_{A;n',n'}^{-1}$$

Conductance and Current; Landauer-Buttiker Formulas

$$\Gamma(E,V) = \frac{2e^2}{h}\mathrm{T}(E,V)$$

$$\equiv \frac{2e^2}{h}\sum_{\alpha\beta}\sum_{n,n'}\left(\frac{v_\beta}{v_\alpha}\right)\left|<\Phi^{\beta}_{B;n}\,|\,\mathbf{S}^{BA}_{n,n'}(E,V)\,|\,\Phi^{\alpha}_{A;n'}>\right|^2$$

$$I(V) = \frac{2e^2}{h}\int_{-\infty}^{\infty} dE\,\mathrm{T}(E,V)[f_B(E) - f_A(E)]$$

Simple Tight-binding Model; Mean-field Approximation

$$H=\sum_{i,\sigma}\varepsilon_i n_{i,\sigma}+\sum_{<ij>,\sigma}V_\pi c^+_{i,\sigma}c_{j,\sigma}-\sum_i B(n_{i\uparrow}-n_{i\downarrow})+\sum_i U_H n_{i\uparrow}n_{i\downarrow}$$

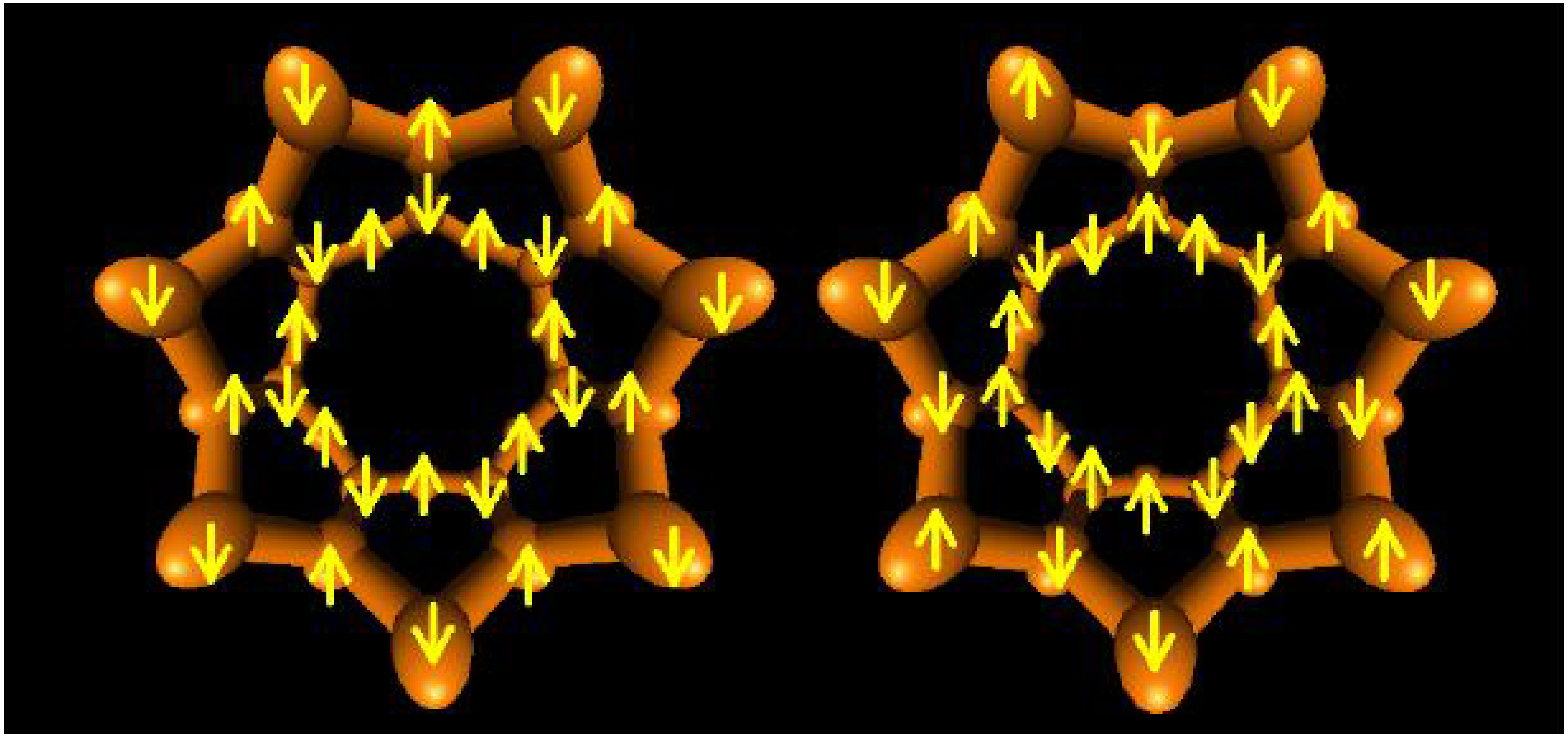
$$U_H\sum_i(n_{i\uparrow}<n_{i\downarrow}>+n_{i\downarrow}<n_{i\uparrow}>-<n_{i\uparrow}><n_{i\downarrow}>)$$

Self-consistency loop

- Initialize occupation numbers
- Calculate the Hamiltonian
- Derive the system Green's function
- Determine the DOS, chemical potential and the occupations
- Repeat to reach convergence

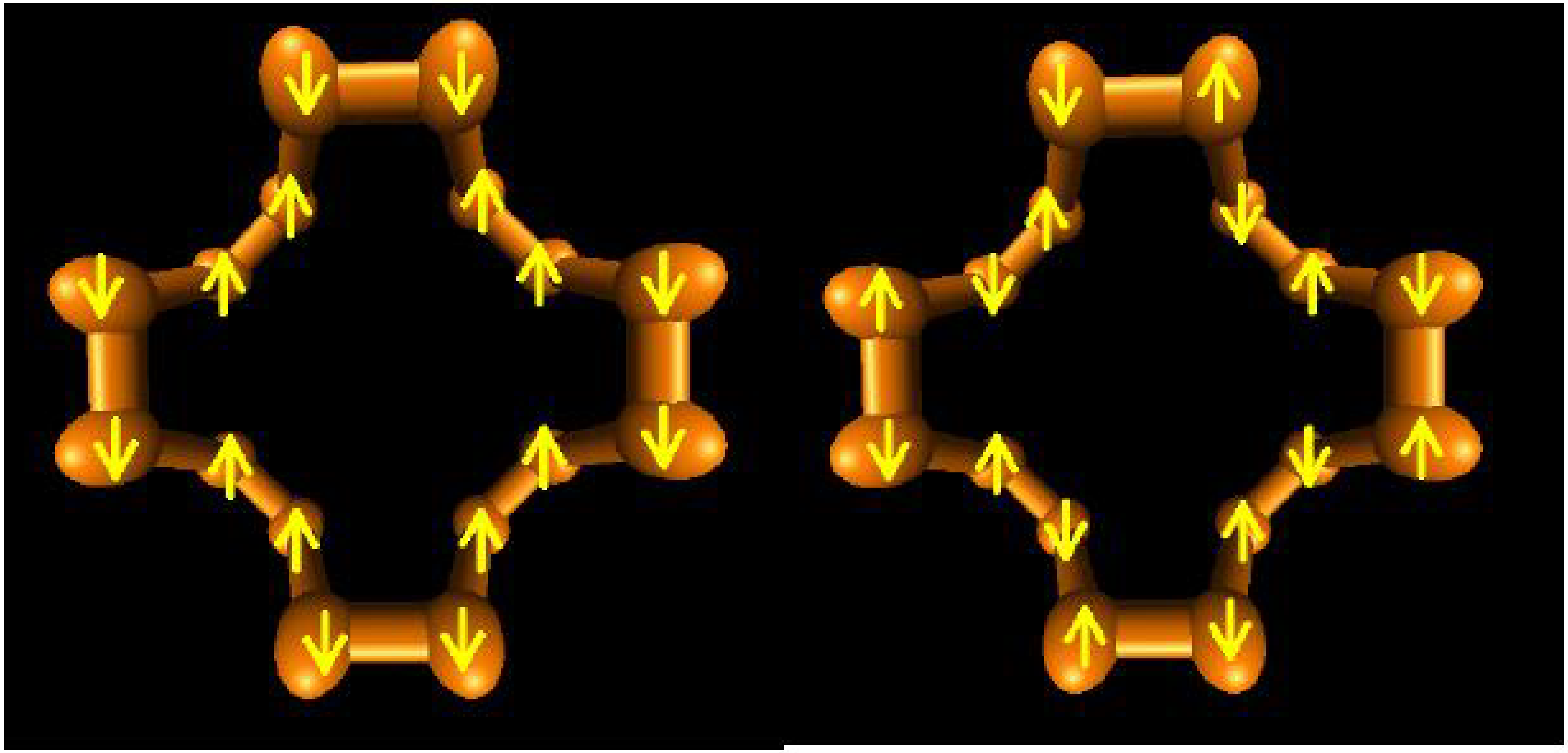
Initial Spin-configurations: (7,0)

SDW-1 SDW-2

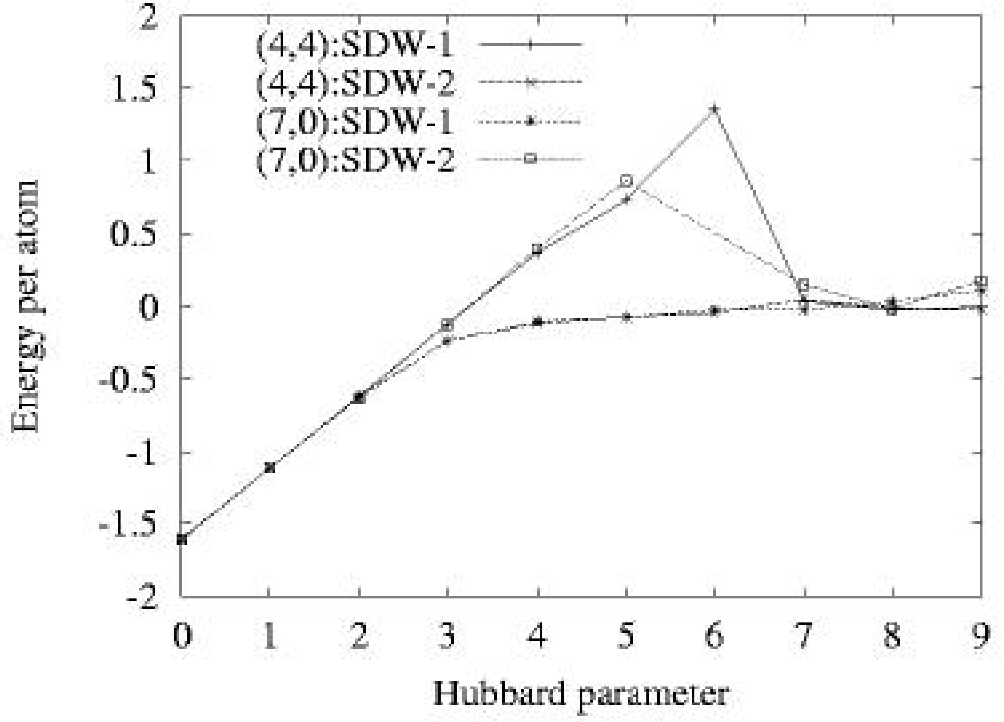


Initial Spin-configurations: (4,4)

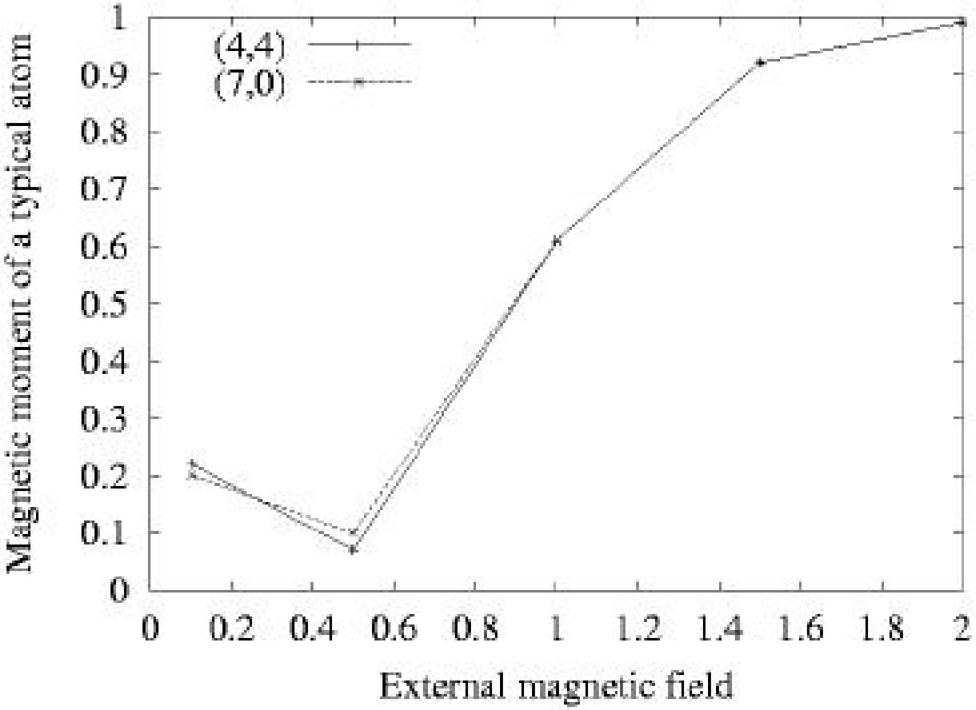
SDW-1 SDW-2



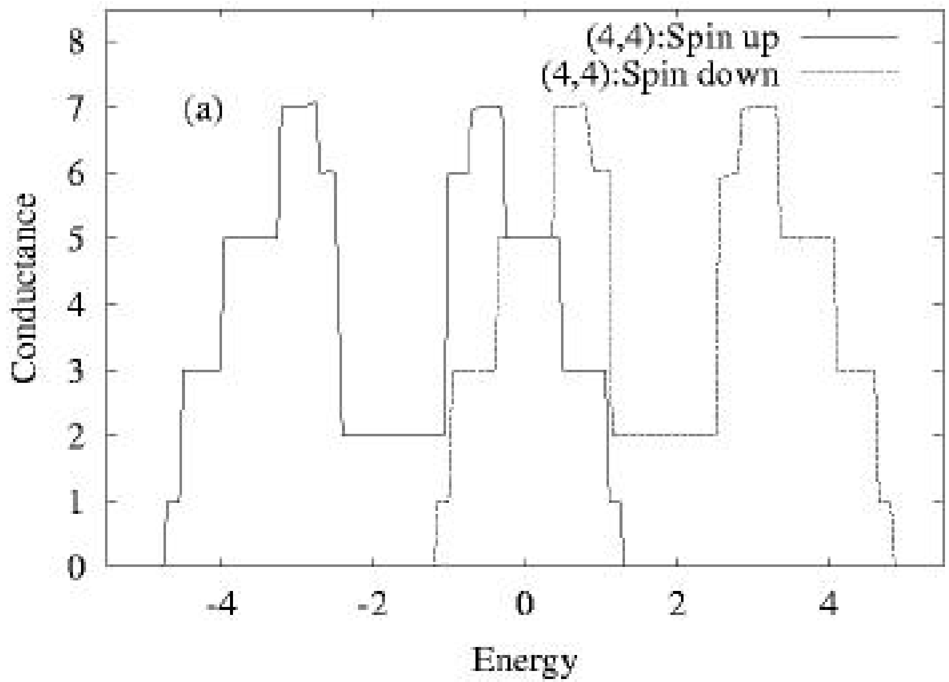
Energy vs. Hubbard coupling



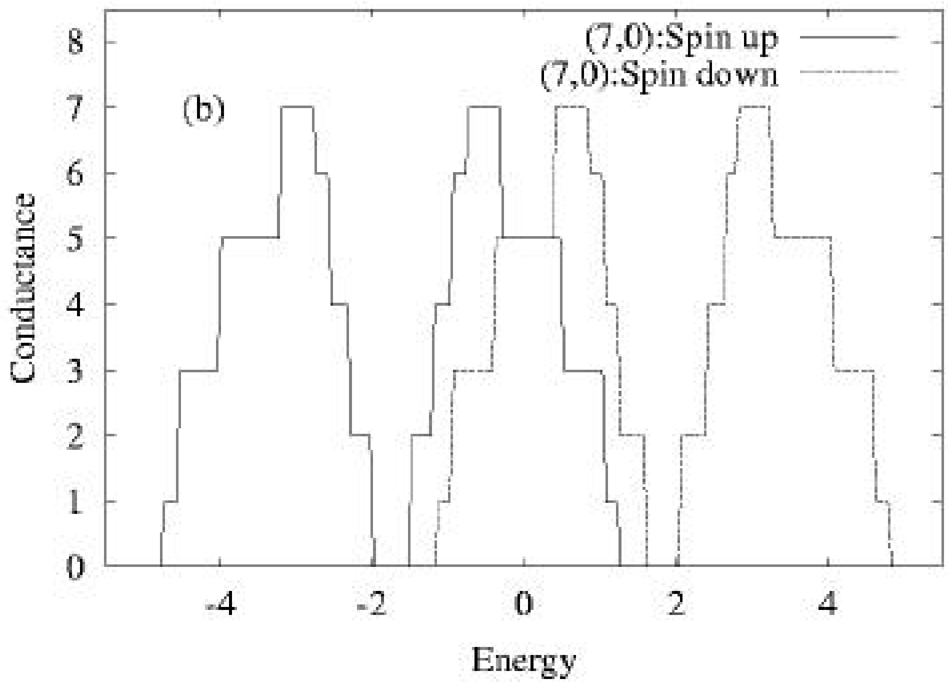
Magnetic moment vs. applied magnetic field



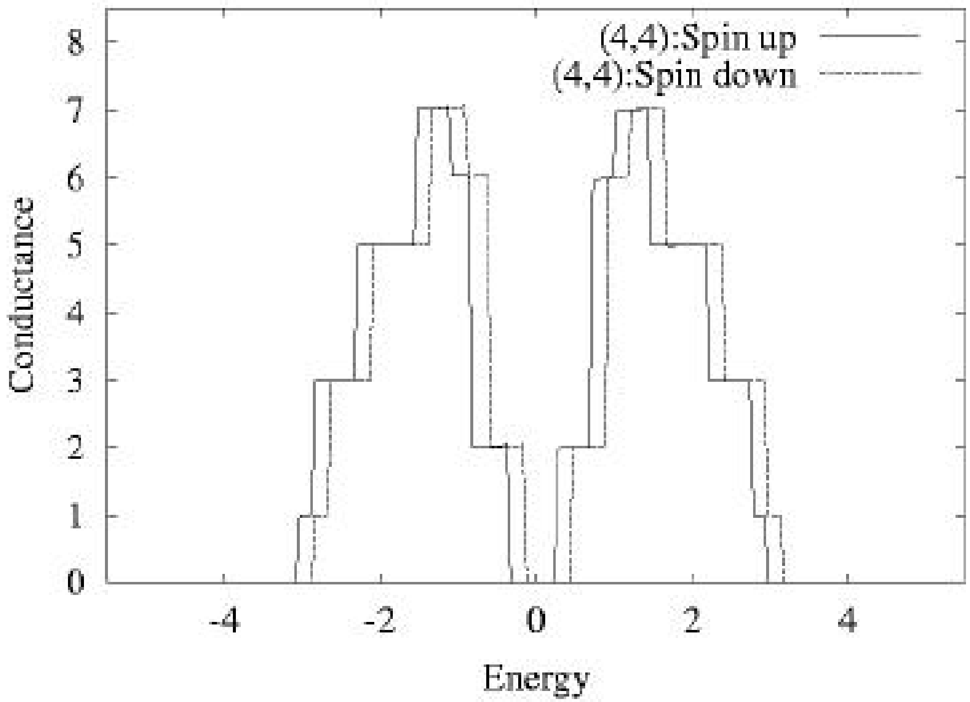
Conductance of the (4,4) tube at B=1.0



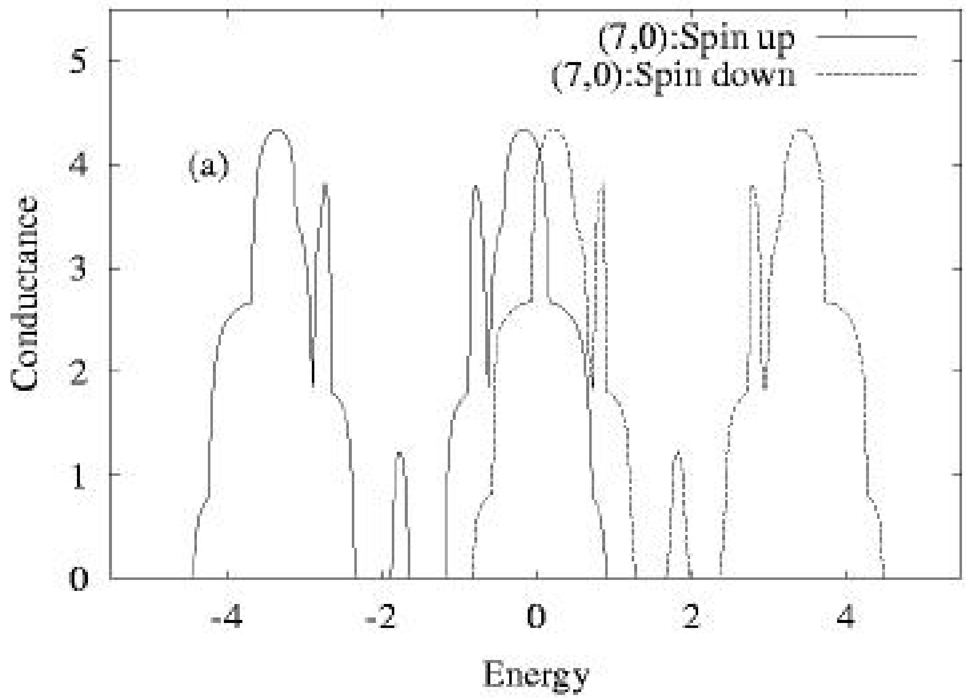
Conductance of the (7,0) tube at B=1.0



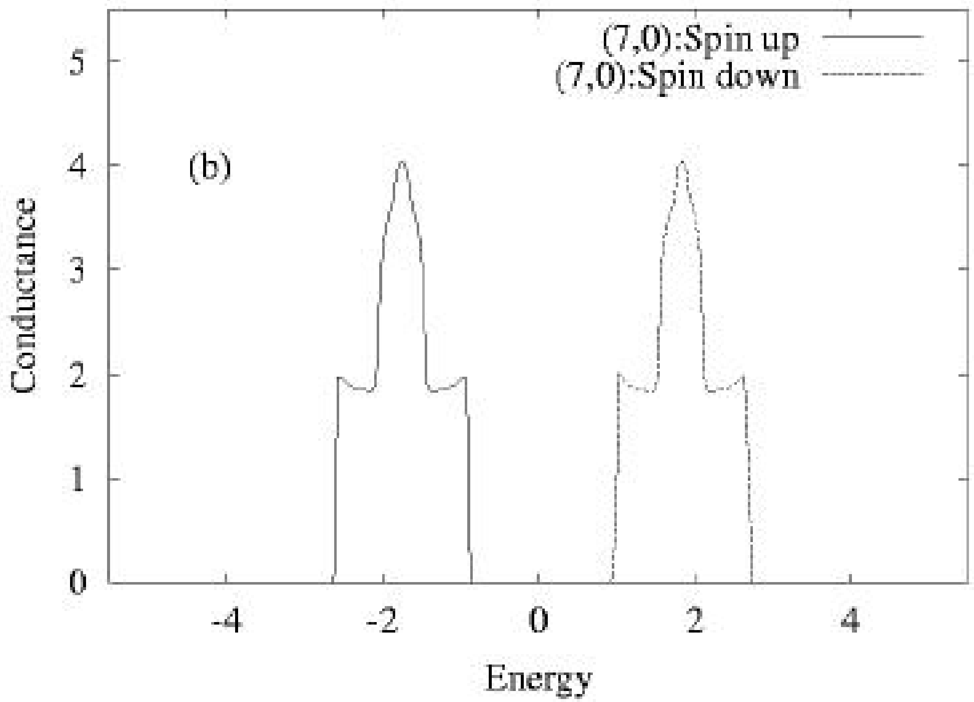
Conductance of the (4,4) tube at B=0.1



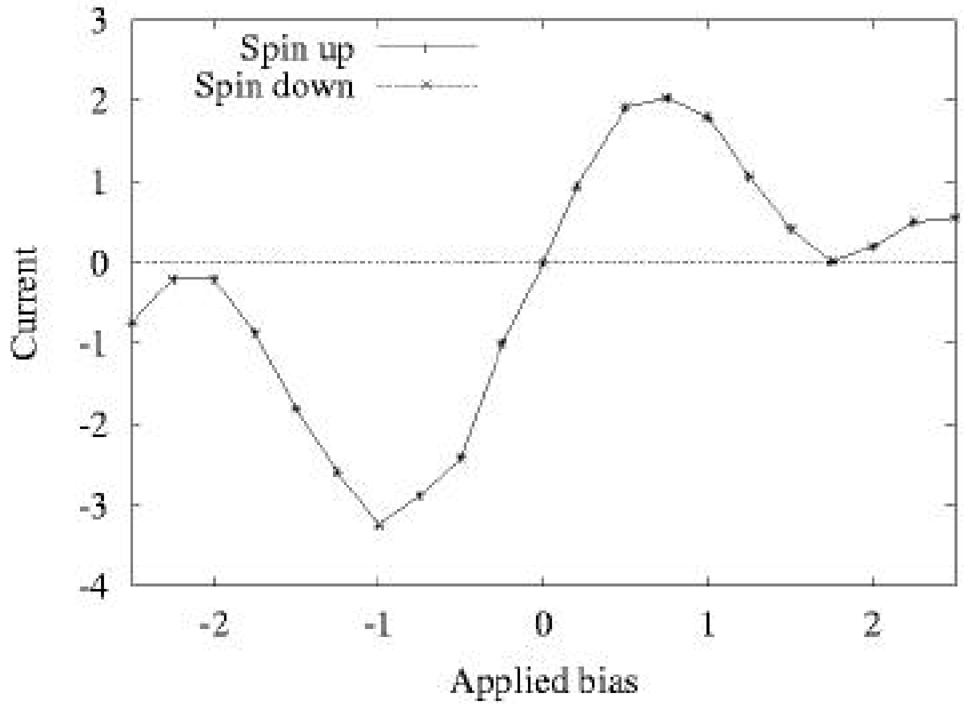
Conductance of the (7,0) tube at B=1.0, V=0.5



Conductance of the (7,0) tube at B=1.0, V=2.0



I-V characteristics for the (7,0) tube at B=1.0



Conclusions

- Mean-field ground states are antiferromagnetic
- A gap opens in the DOS of metallic tubes for weak applied magnetic fields
- For the semiconducting tubes, I-V characteristics of up- and down-carriers are identical. The I-V curves show NDR feature with big peak-to-valley ratio