Electron Transport in Nanostructures

K.A. Al-Hassanieh
The University of Tennessee and ORNL

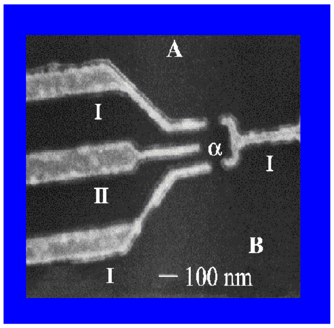
Dr. C.A. Busser, Prof. A.Moreo, and Prof. E.Dagotto
The University of Tennessee and ORNL

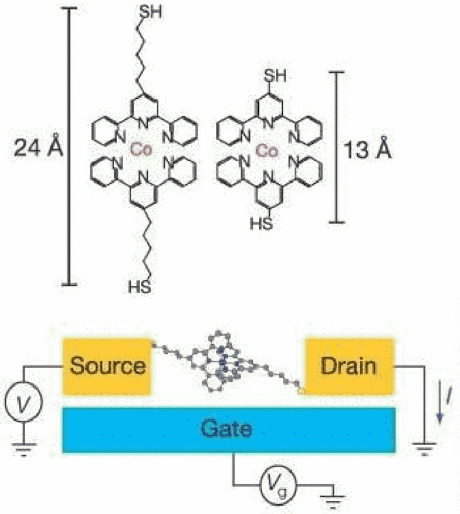
Prof. G.B. Martins
Oakland University

Electron Transport in Nanostructures

- Quantum Dots and Molecular conductors
- Many-Body effects: Coulomb blockade and Kondo effect
- Numerical technique
- Multilevel Quantum Dots
- Electron-phonon coupling effects
- Non-local spin control in QD's

Quantum Dots and Molecular Conductors



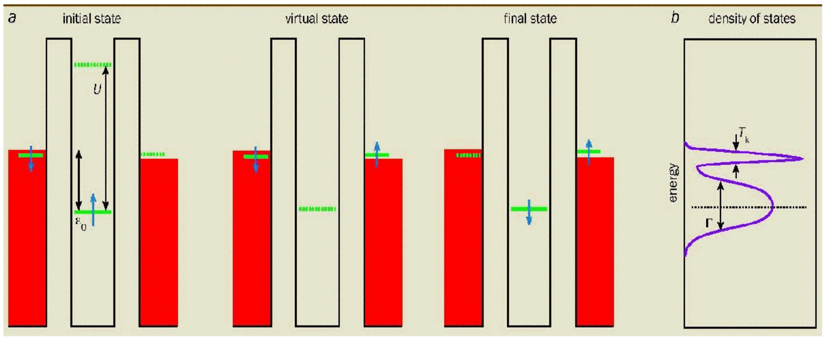


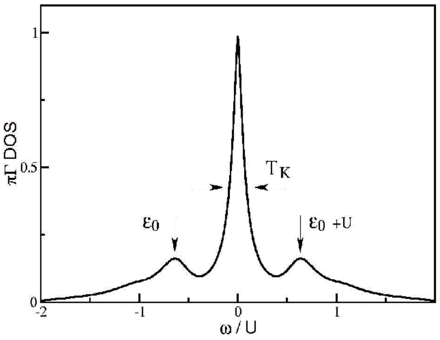
Model: Anderson Impurity

$$H = V_g n_d + U n_{d\nless} n_{d\in} + \sum_{k\sigma} (V_{k\sigma} d^{\infty}_{\sigma} c_{k\sigma} + h.c.) + H_{lead}$$

D. Goldhaber-Gordon et al., Nature (1998).
J. Park et al., Nature (2002).

Kondo Effect





Conduction electrons screen the localized spin. An overall singlet is formed.

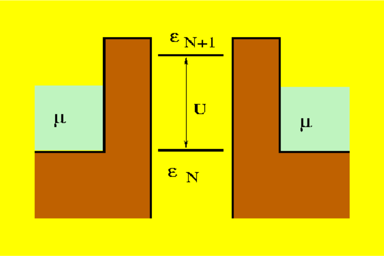
Kondo resonance is formed at the Fermi level.

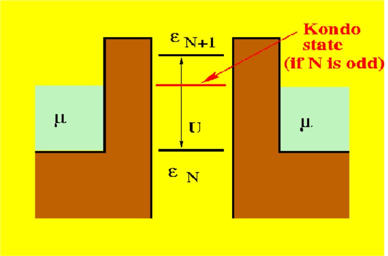
L. Kouwenhoven and L. Glazman, Physics World, January (2001).

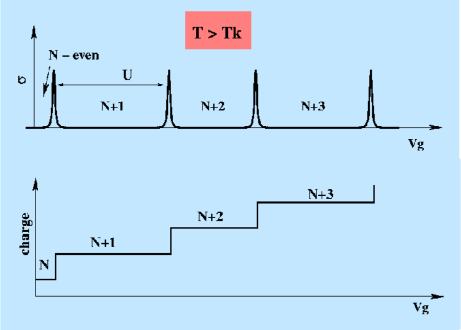
Coulomb Blockade and Kondo Effect

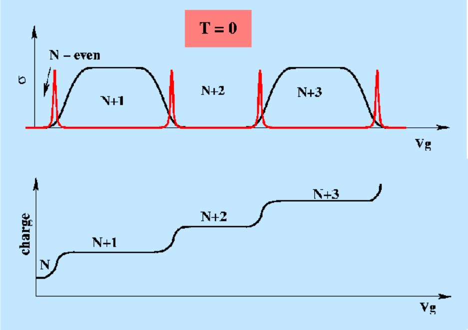
CB Regime (T>Tk)

Kondo Regime (T<Tk)

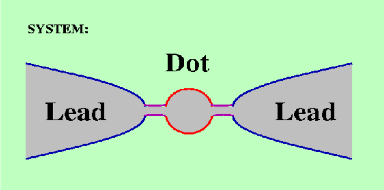


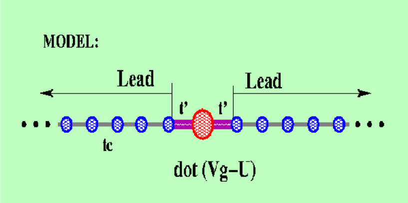


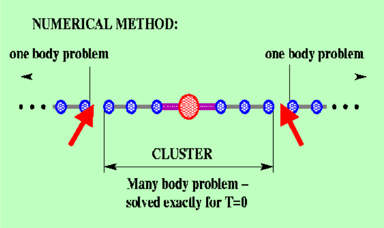




Numerical Method







1) The leads are modeled as semi-infinite tight-binding chains.

2) A cluster consisting of the central interacting region and a few sites of the leads is solved exactly using Lanczos. A matrix of Green's functions is calculated.

3) The cluster is embedded in the rest of the leads using Dyson's equation

$$\hat{G}=\hat{g}+\hat{g}\,\hat{t}\,\hat{G}$$

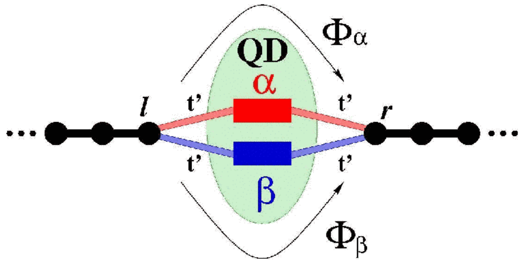
4) The conductance is calculated using

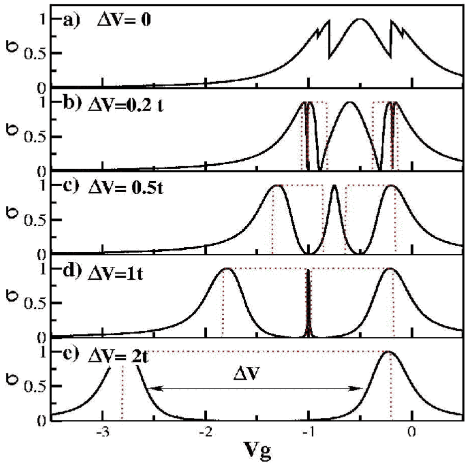
$$G=2\frac{e^2}{h}[t'^2\rho_0]^2 \gg G_{1}$$

Electron Transport in Multilevel QD's Model

$$H_d=\sum_{\sigma}[V_g n_{\alpha\sigma}+(V_g+\Delta V)n_{\beta\sigma}]+U/2\sum_{\lambda=\alpha,\beta\sigma} n_{\lambda\sigma} n_{\lambda\bar{\sigma}}$$

$$+U'/2\sum_{\sigma\sigma'} n_{\alpha\sigma} n_{\beta\sigma'}-J\vec{S}_{\alpha}.\vec{S}_{\beta}$$



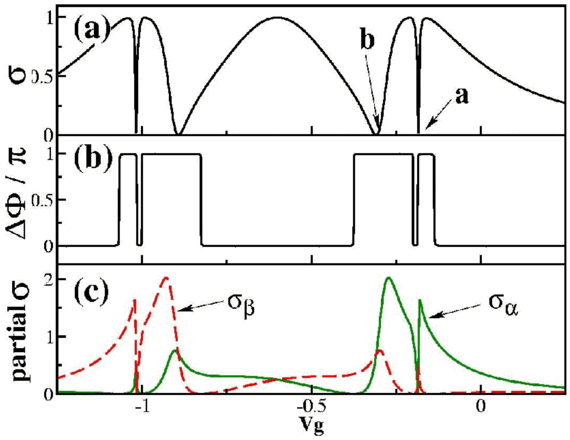


C.A. Busser et al. PRB 70, 245303 (2004)

Electron Transport in Multilevel QD's Interference

Overall conductance is decomposed into the conductance of individual levels with different phases.

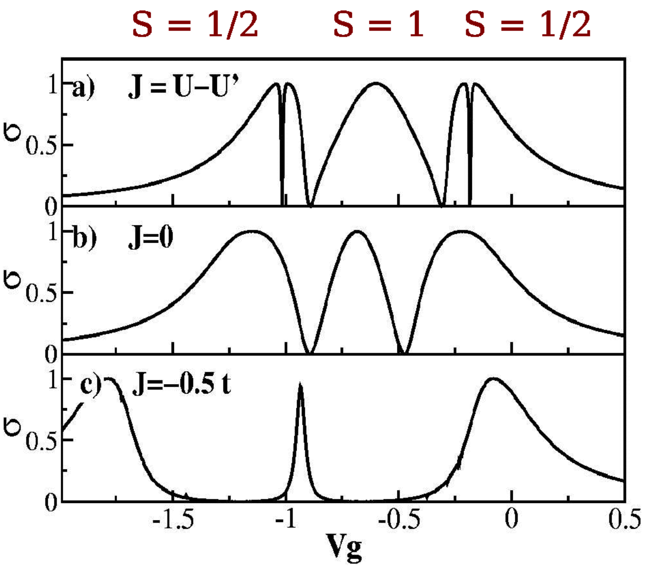
$$\sigma=\sigma_{\alpha}+\sigma_{\beta}+2\sqrt{\sigma_{\alpha}\sigma_{\beta}}\cos(\Delta\Phi)$$



C.A. Busser et al. PRB 70, 245303 (2004)

Electron Transport in Multilevel QD's Integer-Spin Kondo

Spin-1 Kondo resonance when 2 electrons occupy the dot.



C.A. Busser et al. PRB 70, 245303 (2004)

Electron-Phonon Coupling Effects

Anderson-Holstein Model.
Diagonal electron-phonon coupling

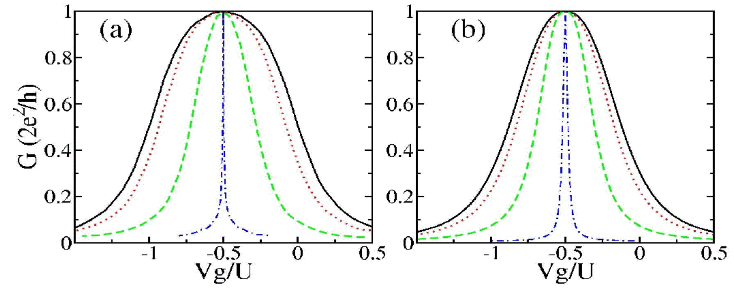
$$H_M = V_g n_d + U n_{d\sphericalangle} n_{d\in} - \lambda (n_d - 1)(a + a^{\infty}) + \omega_0 a^{\circ}$$

$$\hat{U} = e^{-\lambda/\omega_0 (1-n_d)(a^{\infty}-a)}$$

$$U_{eff} = U - 2\lambda^2/\omega_0$$

$$V_{geff} = V_g + \lambda^2/\omega_0$$

$$t'_{eff} = t' e^{-\lambda^2/2\omega_0^2}$$



Weak el-ph coupling: spin Kondo with renormalized parameters.

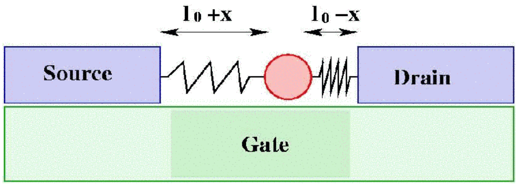
Strong el-ph coupling: charge Kondo.

K.A. Al-Hassanieh et al. Cond-mat/0504528
P.S. Cornaglia et al. PRL 93, 147201 (2004)

Electron-Phonon Coupling Effects

Center-of-Mass Motion.
Asymmetric dynamical tunnel-barrier modulation.

$t'(x)=t'(1\pm\alpha x)=t'[1\pm\alpha(a+a^{\infty})$



$H_M=V_g n_d+U n_{d*} n_{d\in}-\lambda(n_d-1)(a+a^{\infty})+\omega_0 a^{\circ}$

$H_{M-\text{leads}}=t'[1-\alpha(a+a^{\infty})]\sum_{\sigma}(d_{\sigma}^{\infty}c_{l\sigma}+h.c.)+t'[1+\alpha(a+a^{\infty})]\sum_{\sigma}(d_{\sigma}^{\infty}c_{r\sigma}+h.c$

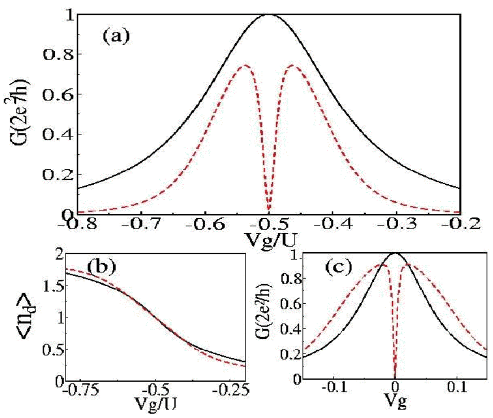
K.A. Al-Hassanieh et al. Cond-mat/0504528

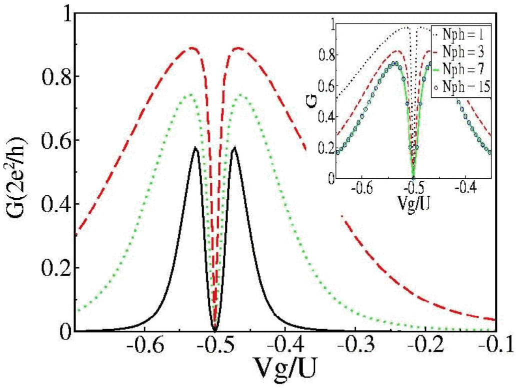
Electron-Phonon Coupling Effects

COM motion leads to conductance
cancellation at the symmetric Vg.

$\alpha=0$, Perfect conductance

$\alpha\neq0$, Conductance cancellation





K.A. Al-Hassanieh et al. Cond-mat/0504528

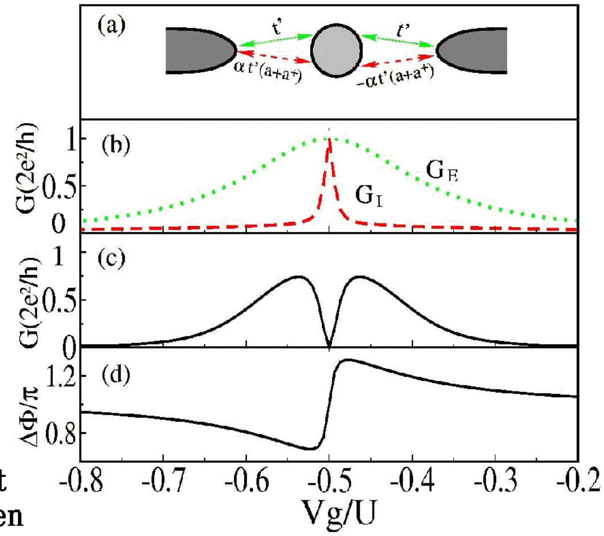
Electron-Phonon Coupling Effects

Molecule-leads connection can be decomposed into two channels:

$t'\sum_{\sigma}(d^{\infty}_{\sigma}c_{l\sigma}+d^{\infty}_{\sigma}c_{r\sigma}+h.c.)$

and

$t'\alpha(a+a^{\infty})\sum_{\sigma}(d^{\infty}_{\sigma}c_{l\sigma}-d^{\infty}_{\sigma}c_{r\sigma}+h.c.$



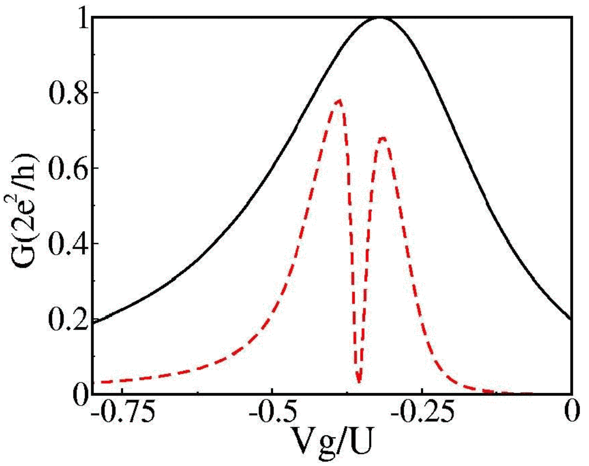
Conductance cancellation is the result of the destructive interference between purely electronic and 'phonon-assisted' tunneling channels

K.A. Al-Hassanieh et al. Cond-mat/0504528

Electron-Phonon Coupling Effects

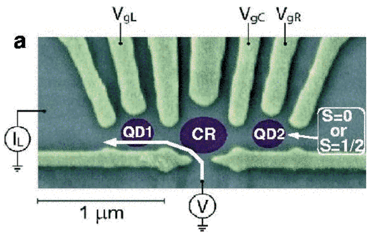
Breathing vibrational mode:
electron-hole asymmetry.

Breathing mode and COM motion:
electron-hole asymmetry but interference is still observed.



K.A. Al-Hassanieh et al. Cond-mat/0504528

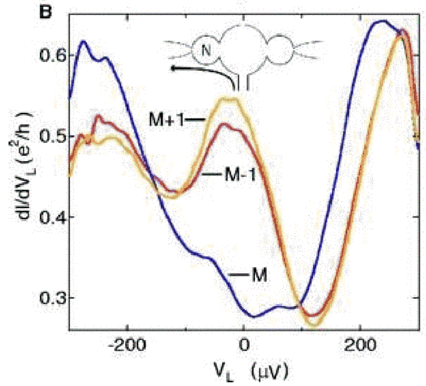
Nonlocal Spin Control in a Coupled QD system Experiment



Conductance of QD1 is measured for:

1)Different QD2 occupations:

2)Different QD2-CR couplings



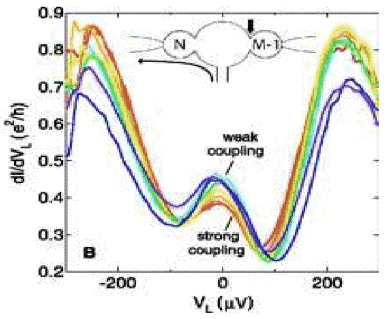
Conductance of QD1 for different QD2 occupations:

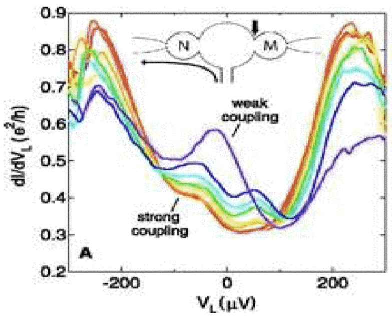
QD2 doubly occupied: Kondo resonance in QD1

QD2 singly occupied: Kondo resonance in QD1 is suppressed

N.J. Craig et al, Science 304, 565 (2004)

Nonlocal Spin Control in a Coupled QD system Experiment





For even QD2 occupation:

Increasing QD2-CR coupling slightly suppresses the conductance.

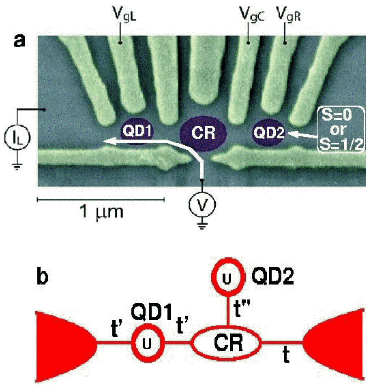
For odd QD2 occupation:

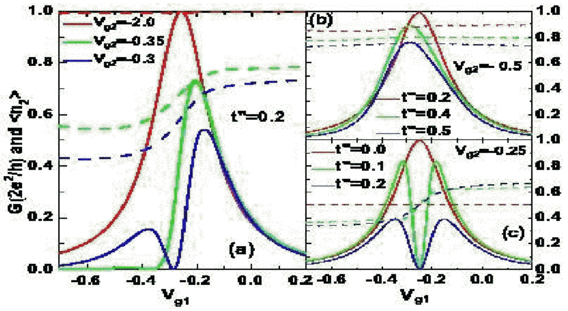
Increasing QD2-CR coupling splits the Kondo peak.

Conclusion: RKKY interaction between the spins on the QD's mediated by the CR electrons.

N.J. Craig et al, Science 304, 565 (2004)

Nonlocal Spin Control in a Coupled QD system Simulations





Numerical simulations reproduce the experimental results.

Alternative explanation to RKKY?

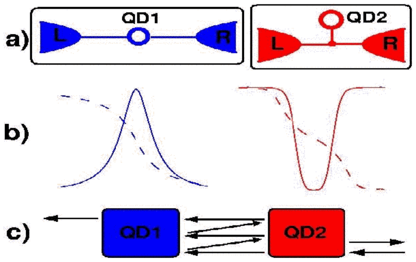
G.B. Martins et al. Cond-mat/0505037

Nonlocal Spin Control in a Coupled QD system Simulations

The experimental setup can also be viewed as a circuit of a serial and a side-connected QD in series.

$$T=\frac{T_1 T_2}{1-R_1 R_2}$$

Input needed: $T_2=T_2[n_2(V_{g1})]$

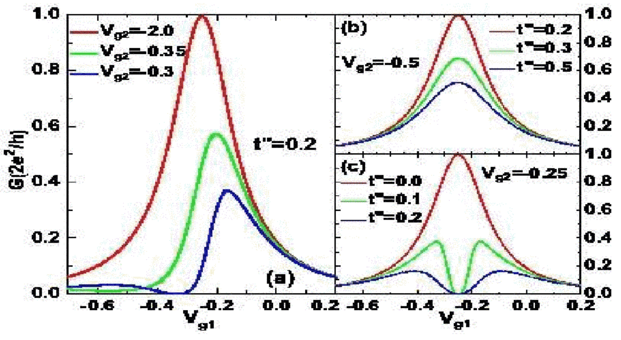


Serial QD1: Kondo resonance

Side-connected QD2: Fano anti-resonance

G.B. Martins et al. Cond-mat/0505037

Nonlocal Spin Control in a Coupled QD system
Simulations



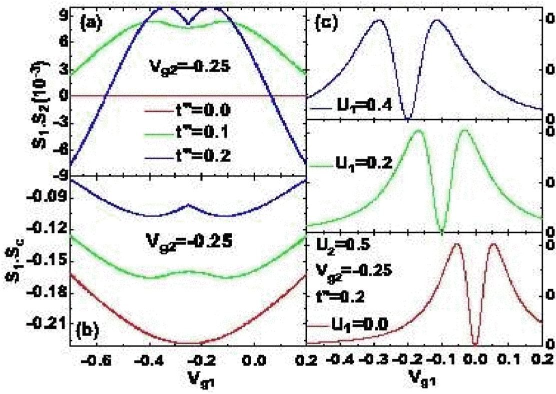
The “Circuit model” results agree qualitatively with the numerical calculations. All the trends are reproduced.

Conclusion: the experimental results can also be explained as the results of Fano anti-resonance.

G.B. Martins et al. Cond-mat/0505037

Summary

- Electron correlations and phase coherence play a key role in nanotransport.
- Interference and integer spin Kondo effects can be observed in multilevel system.
- Electron-phonon coupling causes a rich conductance behavior.


(a)
(b)
(c)
$S_1.S_2(10^{-3})$
$S_1.S_c$
$G(2e^2/h)$
V_{g1}
V_{g1}
V_{g2}=-0.25
V_{g2}=-0.25
t''=0.0
t''=0.1
t''=0.2
U_1=0.4
U_1=0.2
U_2=0.5
V_{g2}=-0.25
t''=0.2
U_1=0.0
9
6
3
0
-3
-6
-9
-0.09
-0.12
-0.15
-0.18
-0.21
-0.6
-0.4
-0.2
0.0
0.2
0.4
0.2
0.0
-0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2