Transport and thermoelectric properties of a semiconductor quantum dot chain connected to metallic electrodes

[1]David M T Kuo ,[2,3]Yia-Chung Chang
[3] Shiue Yuan Shiau and [4] C. C Chen

1:Department of Electrical Engineering, National Central University, Taiwan
2:Research Center for Applied Science, Academic Sinica, Taiwan
3:National Cheng Kung University,Taiwan
4:UIUC

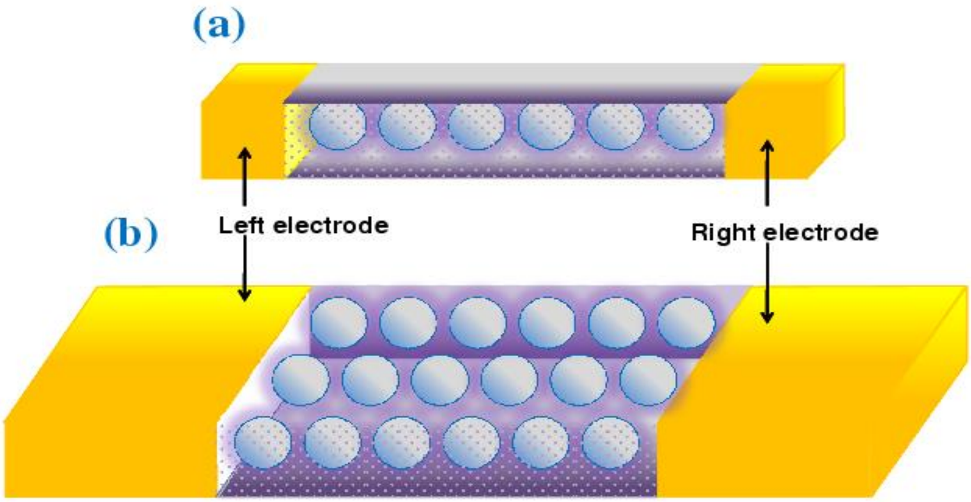
[1] DMT Kuo and Y. C. Chang, PRB 81, 205321 (2010).
[2] DMT Kuo, S. Y. Shiau and Y. C. Chang, PRB 84 245303 (2011)
[3] DMT Kuo and Y. C. Chang, Nanoscale Research Letters 7, 257 (2012)
[4] DMT Kuo and Y. C. Chang, Nanotechnology 24, 175403 (2013)
[5] DMT kuo and Y. C. Chang, PRB 89,115416 (2014)
[6]C. C. Chen, Y. C. Chang and DMT Kuo, Phys. Chem. Chem. Phys. 17, 6606 (2015)

Urbana-Champaign (2003-July)

1997/9/9 to 2003/7/30 at UIUC

1:QD molecule junction system

Strong correlation system



Electron hopping strengths and electron Coulomb interactions

The simple, the better !

1-0:Applications

- Single electron transistors
- Single photon generators
- QD lasers and detectors
- Solid state coolers
- Quantum registers
- Quantum interference transistors

1-0-1: How to study QD chain junction system

(1) Electronic structures of a single QD.

(2) Intradot and interdot Coulomb interactions.

(3) Electron hopping strengths between QDs and tunneling rates coming from the coupling between electrodes and outer QDs.

(4) Interactions between electrons and phonons. (ignored in BP)

(5) Extended Hurbbard and Anderson model

(6) Equation of motion method (nonequilibrium Green's functions)

*One energy level for each QD

1-1:References (Thermoelectric effects)

- [R1]A. J. Minnich, M. S. Dresselhaus, Z. F. Ren and G. Chen, Energy Environ Science, **2**, 466 (2009)
- [R2]G. Mahan, B. Sales and J. Sharp, Physics Today,**50**, 42 (1997).
- [R3]R. Venkatasubramanian, E. Siivola,T. Colpitts,B. O'Quinn, Nature **413**,597 (2001**).”BiTe/SbTe quantum well superlattice”**
- [R4]A. I. Boukai, Y. Bunimovich, J. Tahir-Kheli, J. K.Yu, W. A. Goddard III and J. R. Heath, Nature, **451**, 168(2008**).”Silicon quantum wire”**
- [R5]T. C. Harman, P. J. Taylor, M. P. Walsh, B. E.LaForge, Science **297**, 2229 (2002).”**PbSeTe Quantum dot superlattice** “
- [R6]K. F. Hsu,S. Loo,F. Guo,W. Chen,J. S. Dyck,C. Uher, T. Hogan,E. K. Polychroniadis,M. G. Kanatzidis, Science **303**, 818(2004)
- .[R7]A. Majumdar, Science **303**, 777 (2004).
- [R8]G. Chen, M. S. Dresselhaus, G. Dresselhaus, J. P.Fleurial and T. Caillat, International Materials Reviews,**48**, 45 (2003)
- [R9]Y. M. Lin and M. S. Dresselhaus, Phys. Rev. B **68**, 075304 (2003).

1-2: Simple realistic systems

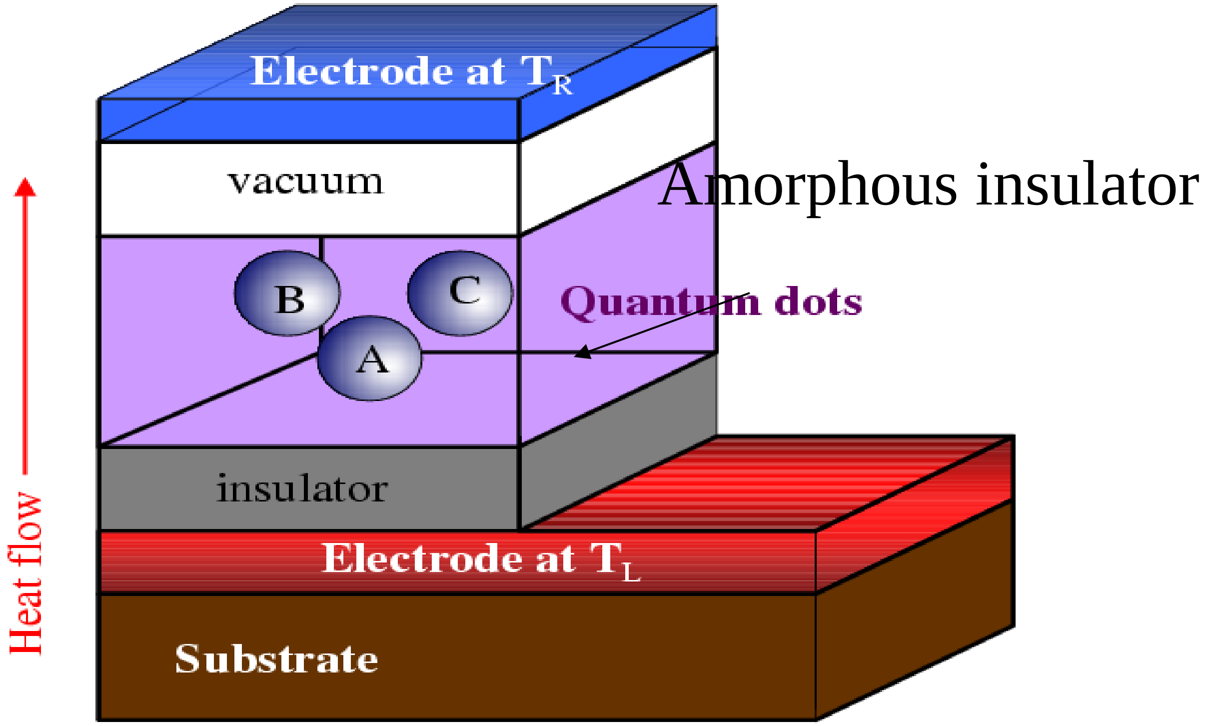


Fig. 1

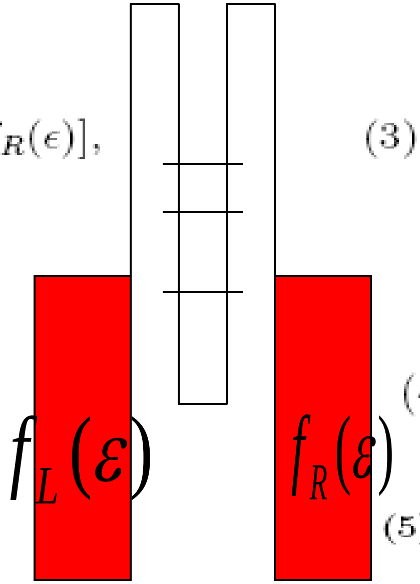
Large intradot and interdot Coulomb interactions,
But weak electron hopping strengths.

[1] DMT Kuo and Y. C. Chang, PRB. 81, 205321 (2010).

1-3:Nonequilibrium Green's function technique

$$J_e = \frac{-2e}{h}\sum_{\ell}\int d\epsilon \gamma_{\ell}(\epsilon) Im G^r_{\ell,\sigma}(\epsilon)[f_L(\epsilon) - f_R(\epsilon)], \quad (2)$$

$$Q = \frac{-2}{h}\sum_{\ell}\int d\epsilon \gamma_{\ell}(\epsilon) Im G^r_{\ell,\sigma}(\epsilon)(\epsilon - E_F - e\Delta V)[f_L(\epsilon) - f_R(\epsilon)], \quad (3)$$



$$G^r_{\ell,\sigma}(\epsilon) = (1 - N_{\ell,-\sigma})\sum_{m=1}^{3^{n-1}} \frac{p_m}{\epsilon - E_\ell - \Pi_m + i\Gamma_\ell} + N_{\ell,-\sigma}\sum_{m=1}^{3^{n-1}} \frac{p_m}{\epsilon - E_\ell - U_\ell - \Pi_m + i\Gamma_\ell}, \quad (4)$$

$$N_{\ell,\sigma} = -\int \frac{d\epsilon}{\pi}\frac{\Gamma_{\ell,L} f_L(\epsilon) + \Gamma_{\ell,R} f_R(\epsilon)}{\Gamma_{\ell,L} + \Gamma_{\ell,R}} Im G^r_{\ell,\sigma}(\epsilon), \quad (5)$$

$$c_\ell = -\int \frac{d\epsilon}{\pi}\frac{\Gamma_{\ell,L} f_L(\epsilon) + \Gamma_{\ell,R} f_R(\epsilon)}{\Gamma_{\ell,L} + \Gamma_{\ell,R}} Im G^r_{\ell,\ell}(\epsilon). \quad (6)$$

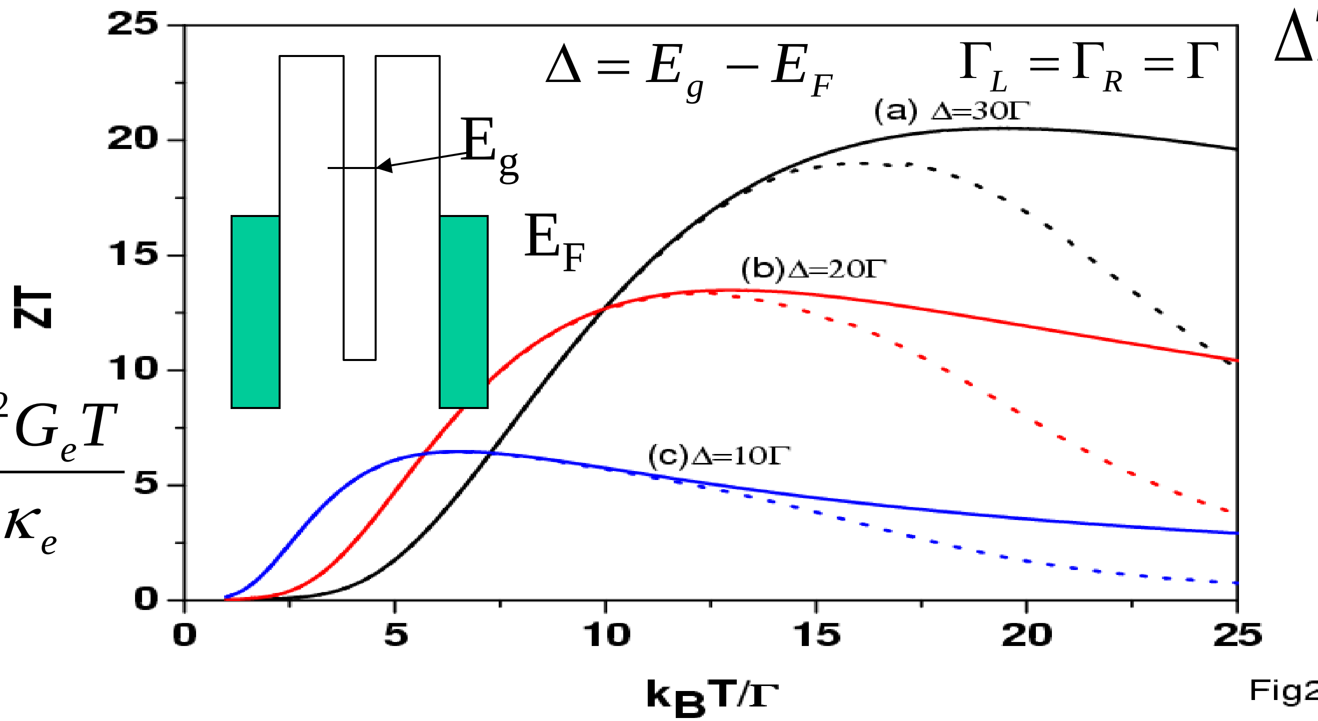
[7]D. M. T. Kuo and Y. C. Chang, Phys. Rev. Lett. 99,086803(2007)

[8]Y. C. Chang and D. M. T Kuo, Phys. Rev. B 77,245412 (2008)

1-4:Linear response

Homogenous QD size, dilute QD density

$$\Delta T / T_0 << 1$$



$$ZT = \frac{S^2 G_e T}{\kappa_e}$$

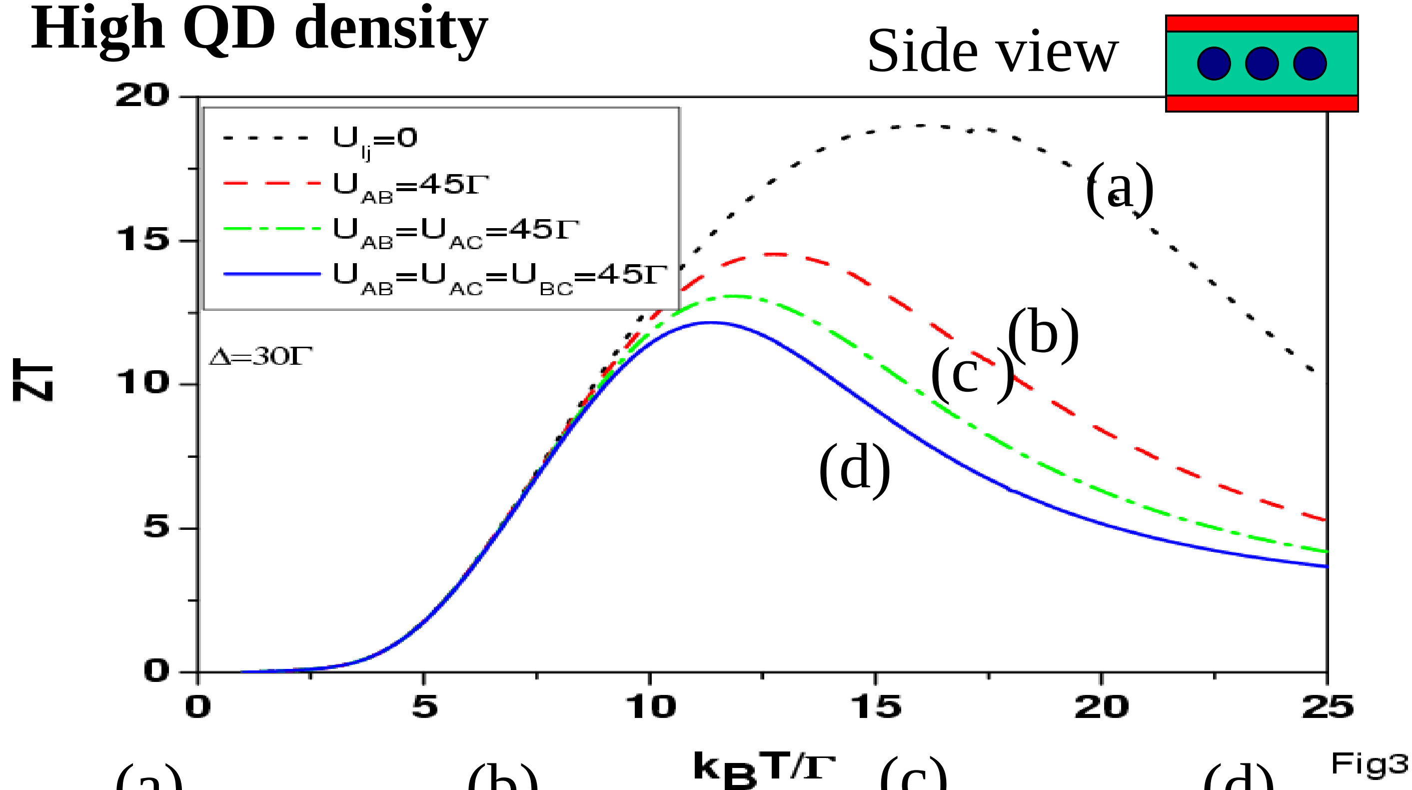
ZT as a function of T for different detuning energies. Solid and dash lines correspond, respectively, without and with intradot Coulomb interactions .

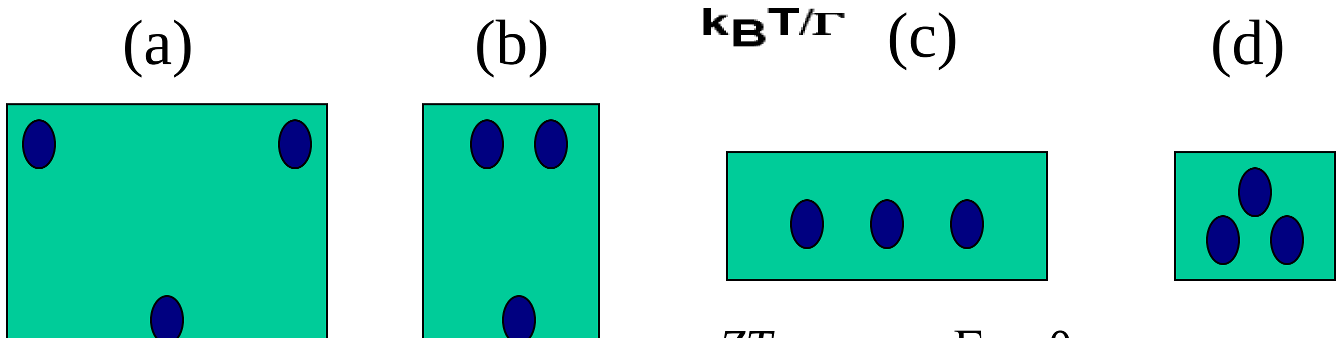
[R10]P. Murphy, S. Mukerjee, J. Morre, Phys. Rev. B 78, 161406 (2008).

$$ZT \to \infty, \qquad \Gamma \to 0$$

1-5:Interdot Coulomb interactions

High QD density





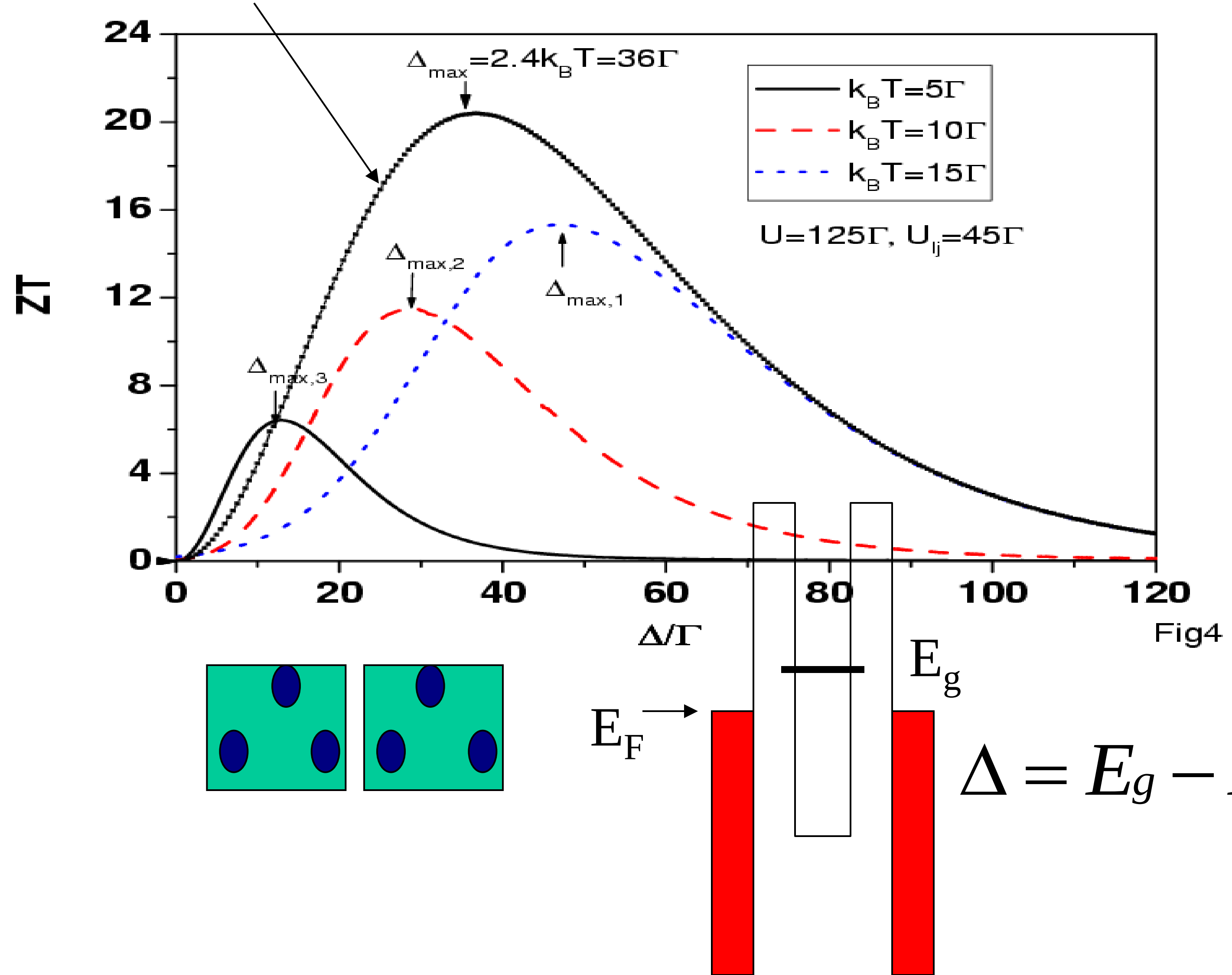
$ZT \to \infty, \quad \Gamma \to 0$

Top view

1-6: ZT detuned by E_g

Noninteraction case

High QD density



$$\Delta = E_g - E_F$$

2-1: Pauli-spin blockade

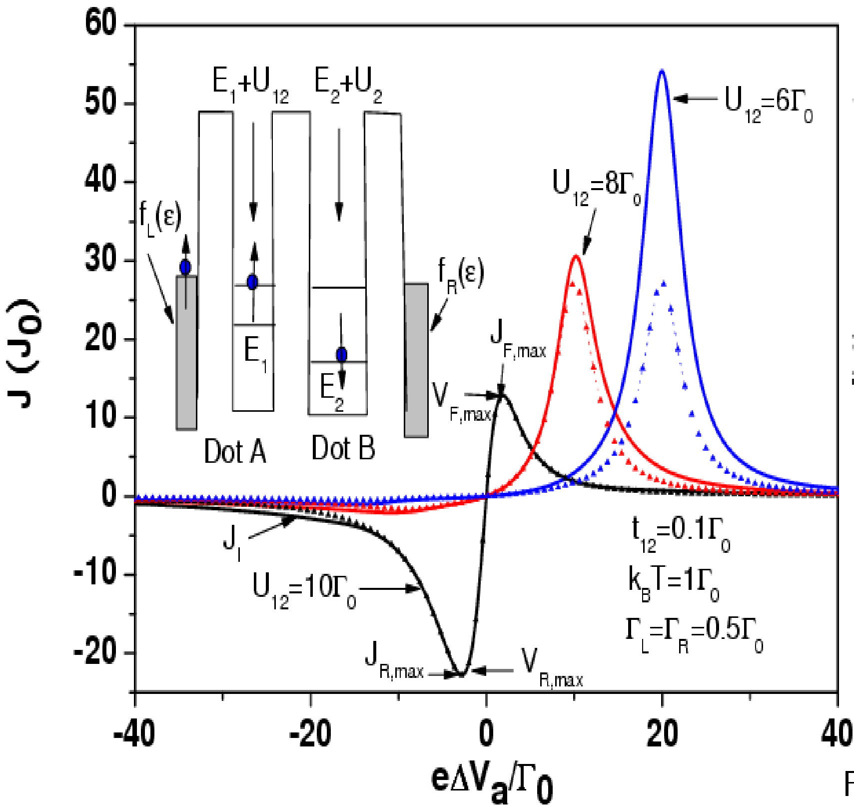
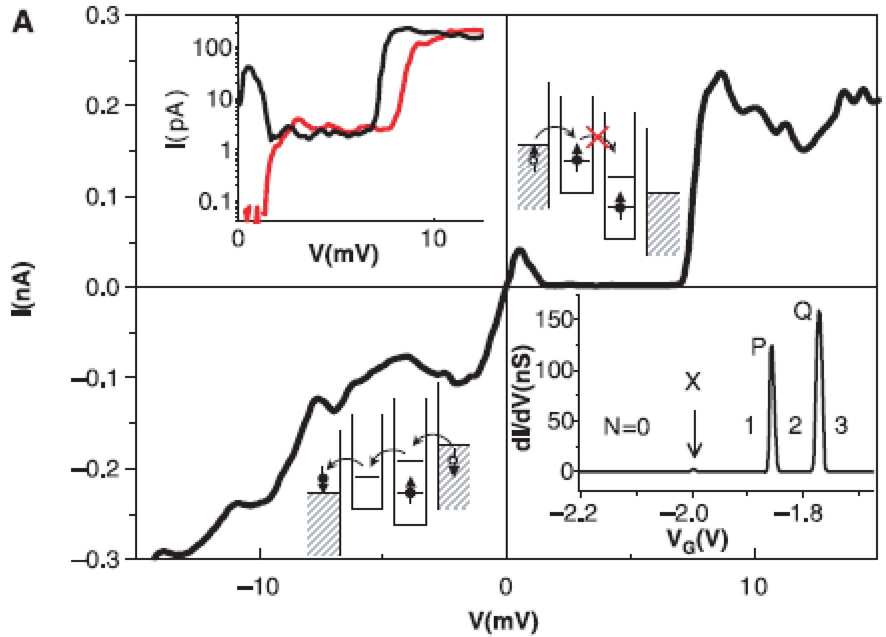
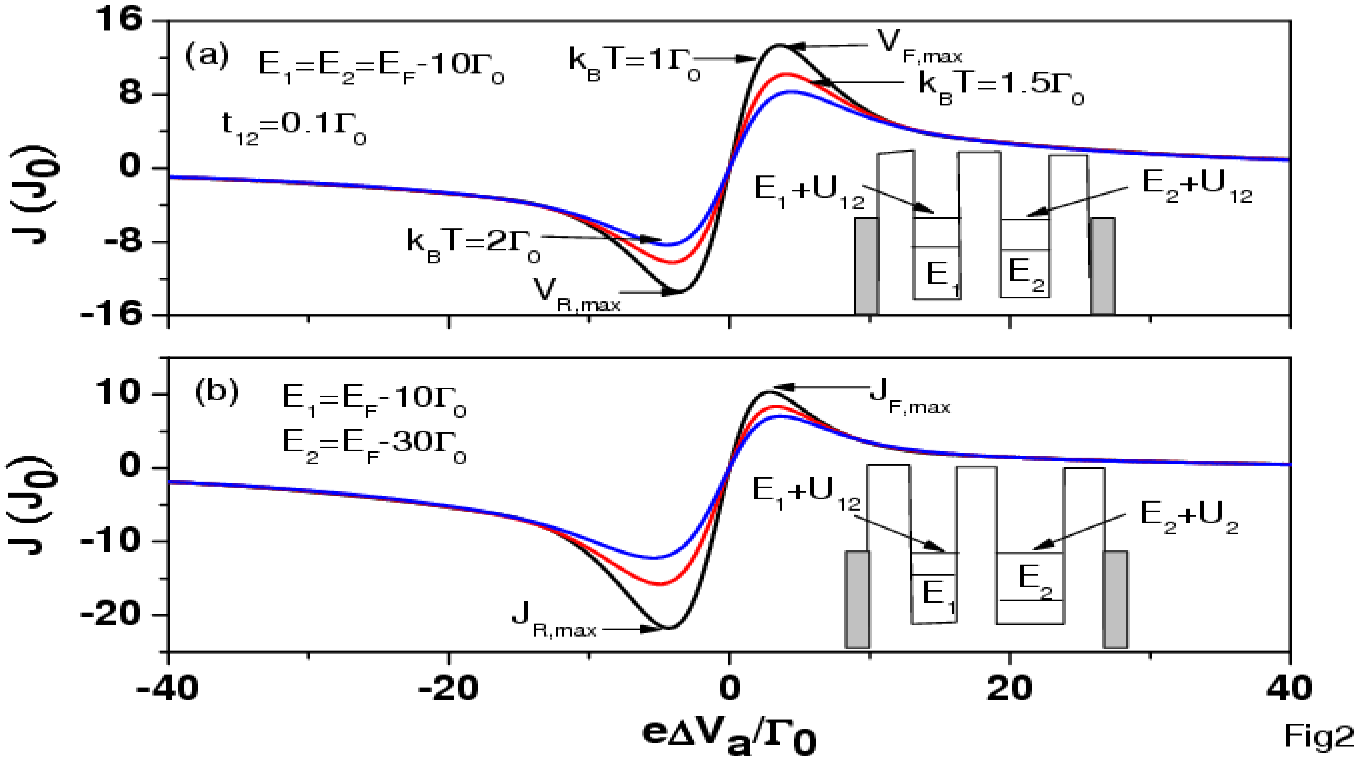


Fig1



[R11] K. Ono , D. G. Austing, Y. Tokura and S. tarucha, science 297, 1313 (2002). Current rectification

2-2: Temperature effect (PSB)



$$E_1 + U_{12} = E_2 + U_2 \qquad t_{12} < \Gamma$$

$$FB:(1-N_{1,-\sigma})*(N_{2,-\sigma}-C_2) \quad RB:N_{2,-\sigma}*(1-N_{1\sigma}-N_{1-\sigma}-C_1)$$

2-3:PSB (three levels)

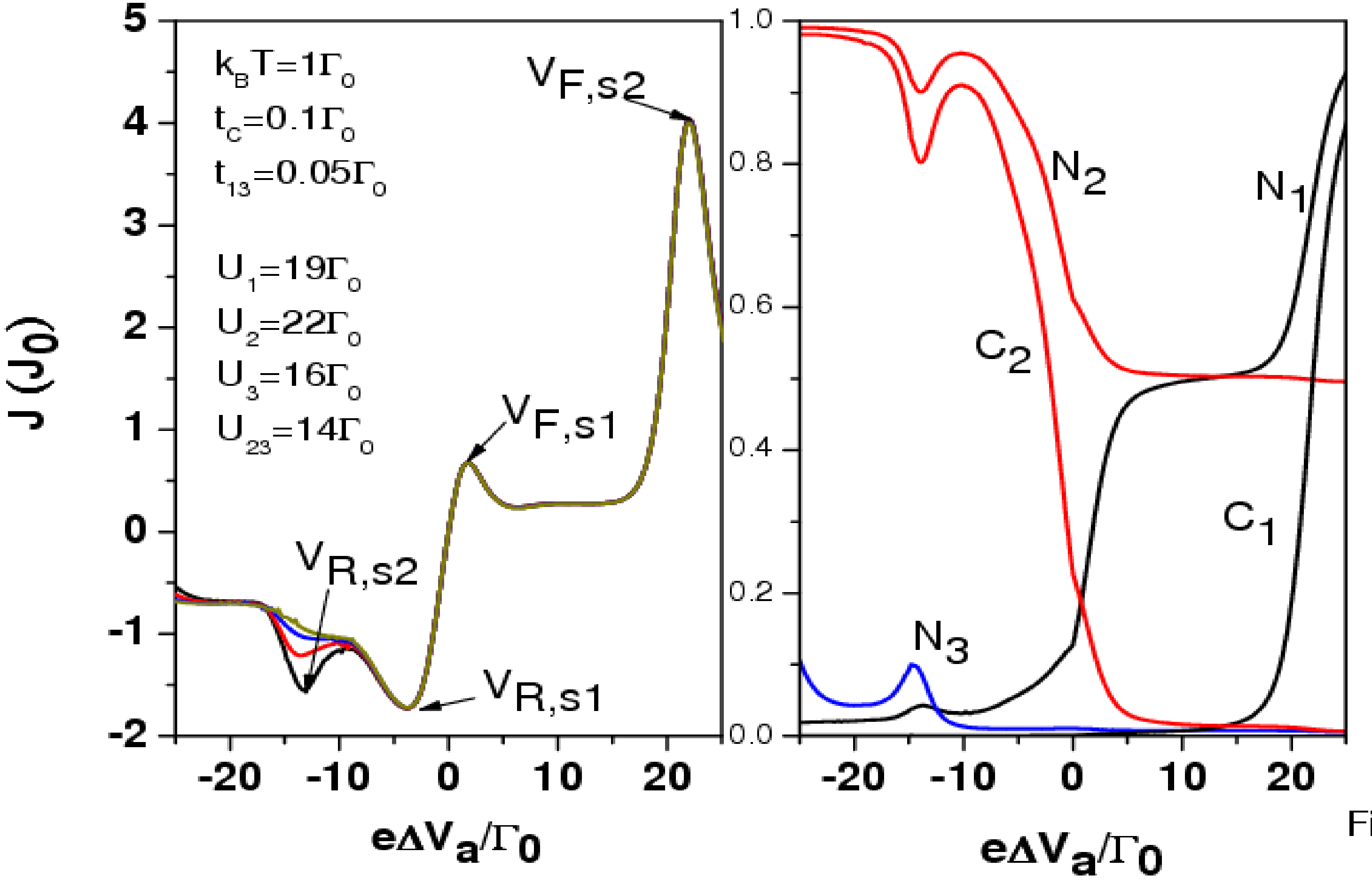
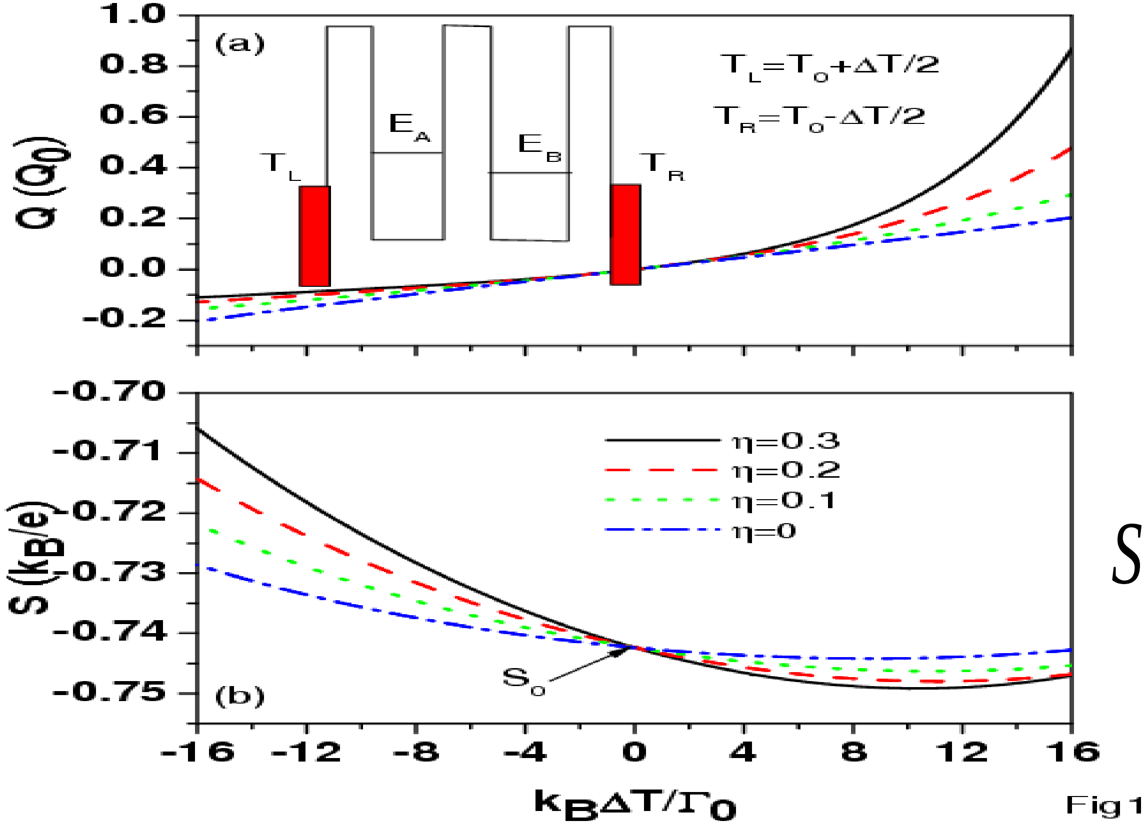


Fig4

3-1: Thermal retification (DQDs)

$$\varepsilon_j = E_j - \eta_j e\Delta V_{th}$$



$$S = \Delta V_{th} / \Delta T$$

$$\Delta T = T_L - T_R < 0$$

$$\Delta T = T_L - T_R > 0$$

3-2:Interdot Coulomb interactions (TR)

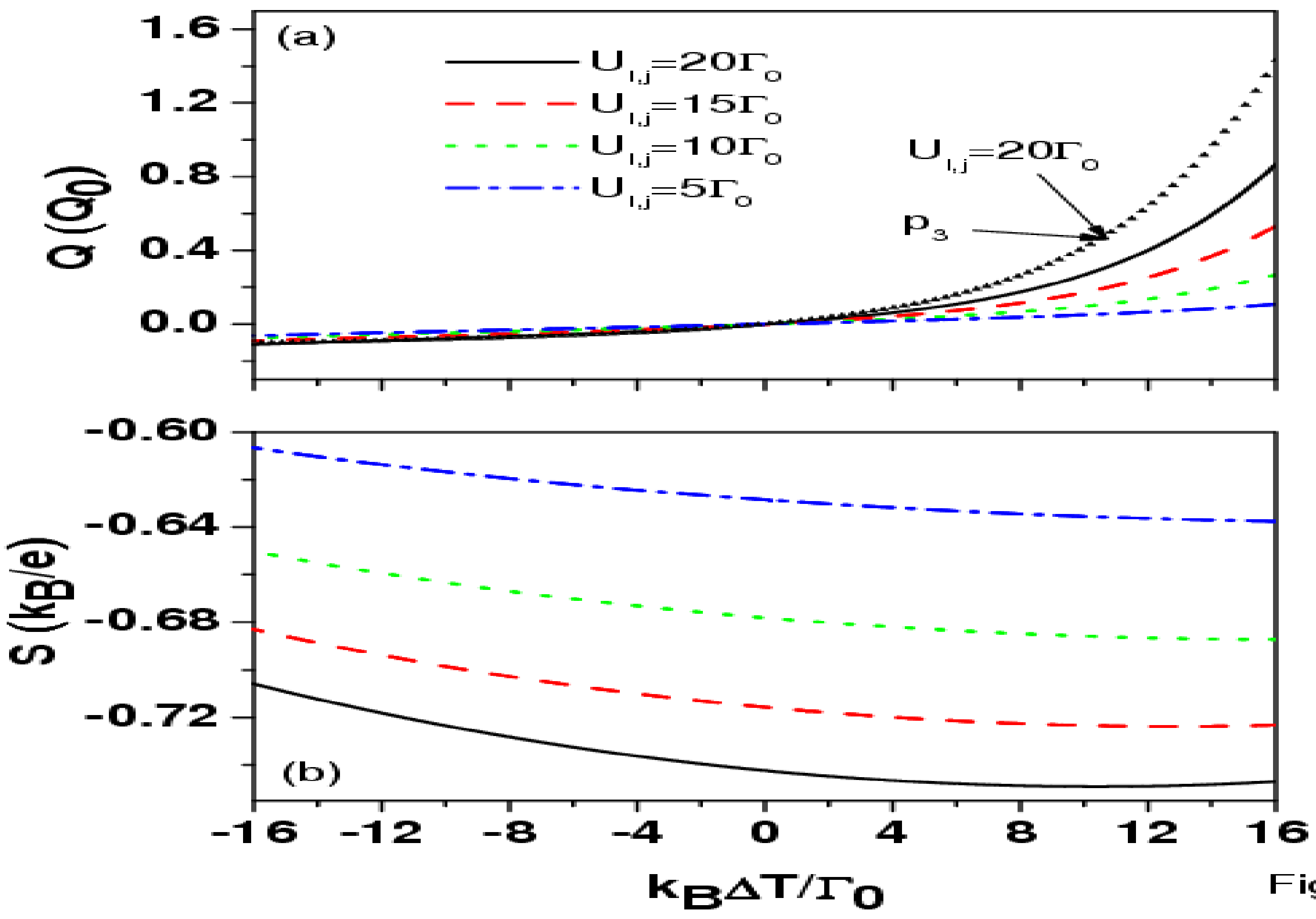
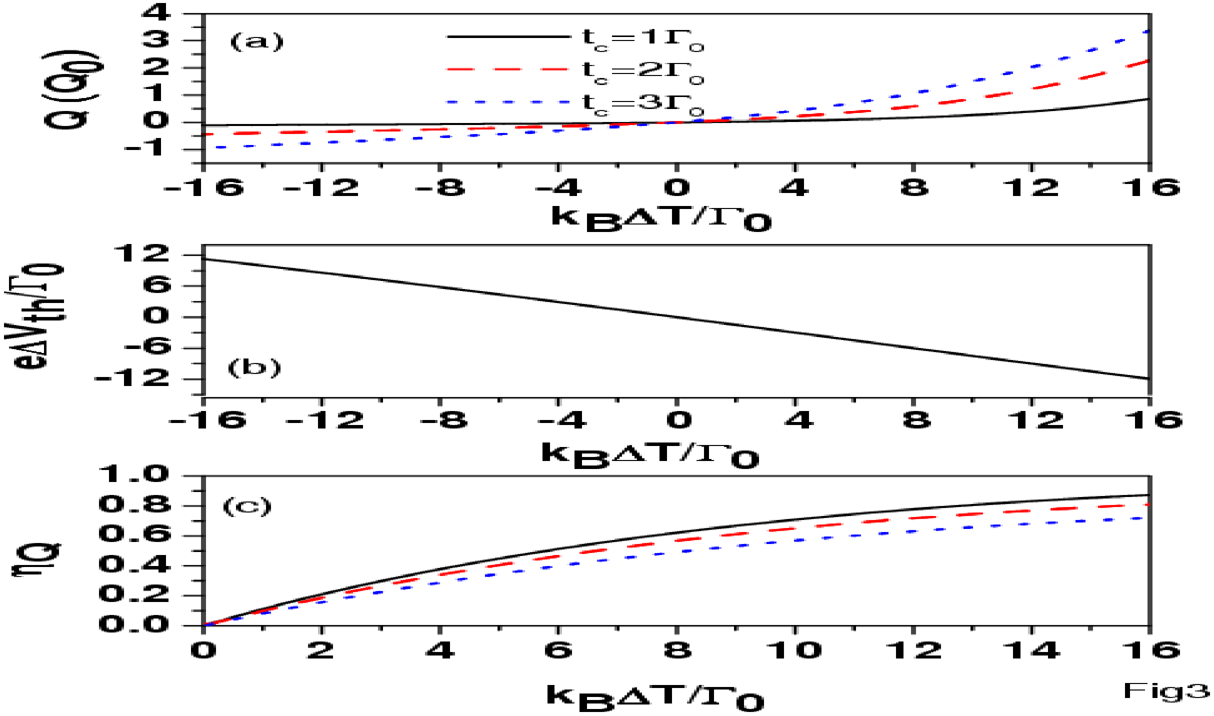
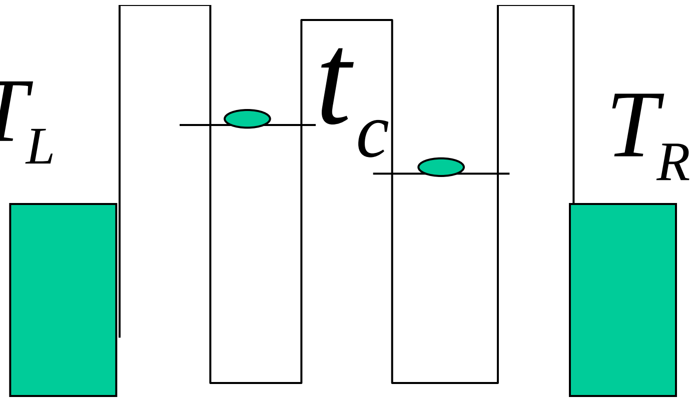


Fig2

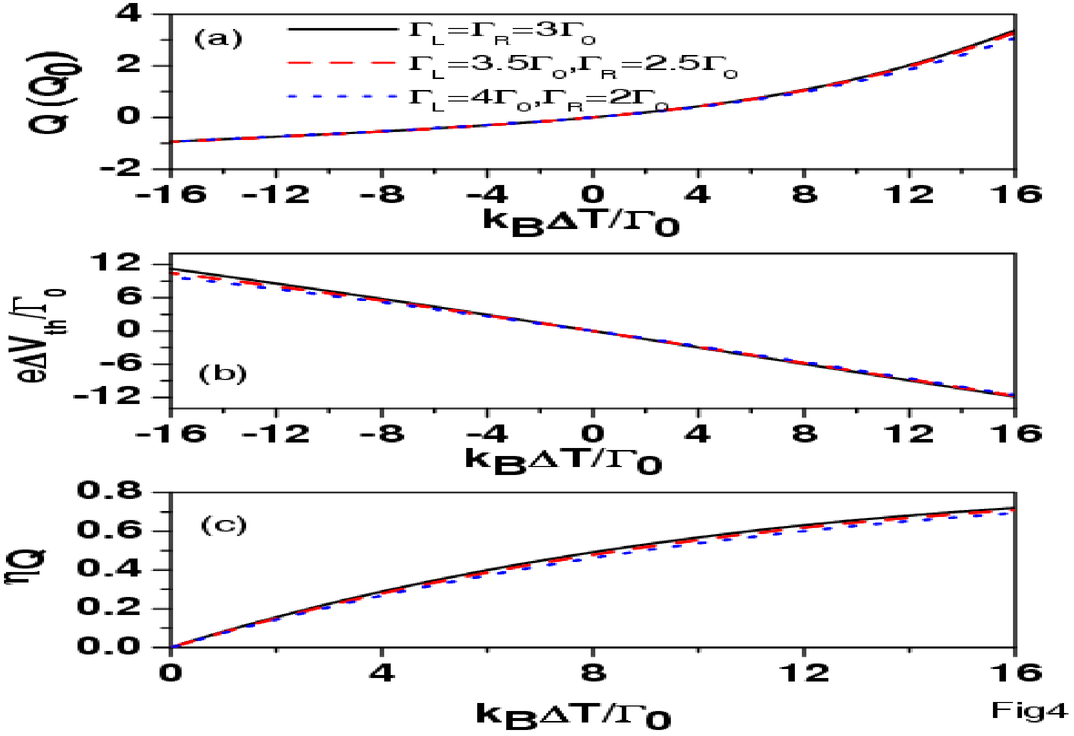
3-3: Electron hopping (TR)



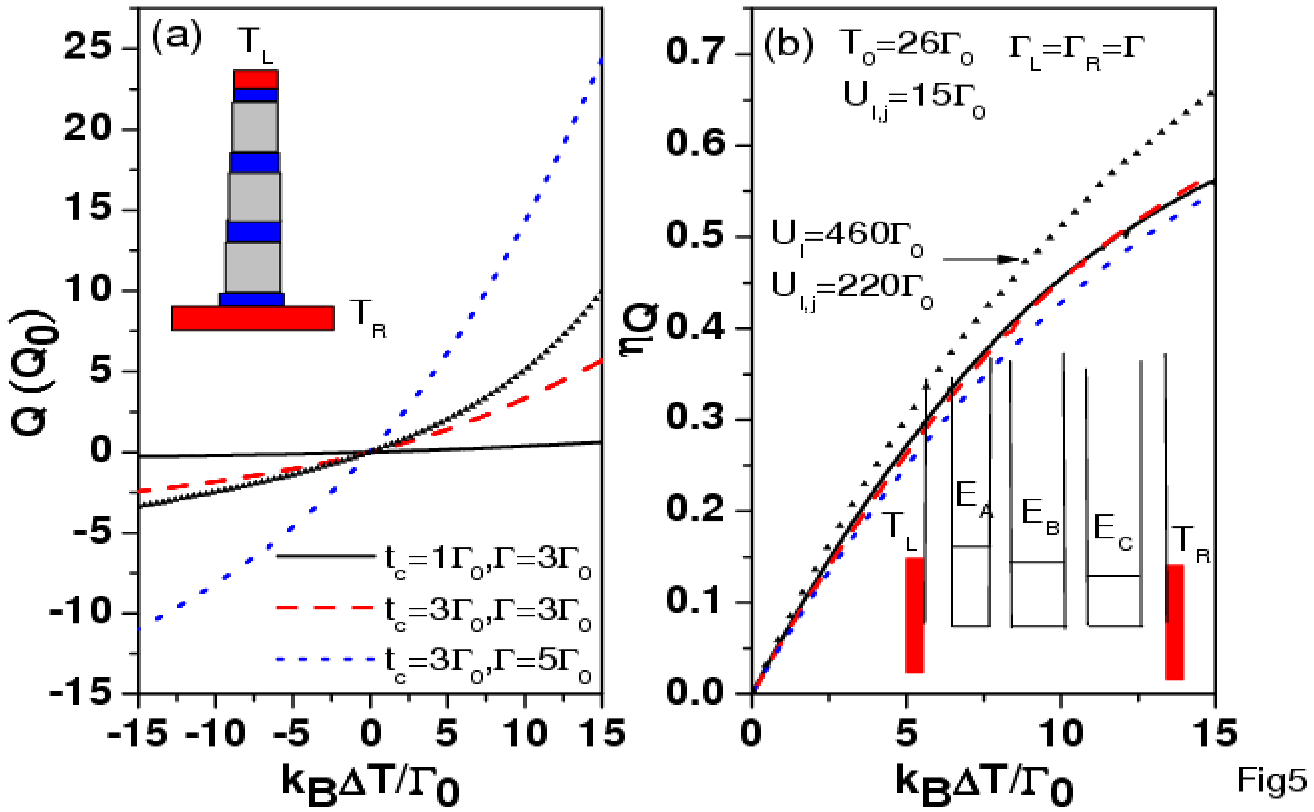


$$\eta_Q = \frac{Q(\Delta T > 0) - |Q(\Delta T < 0)|}{Q(\Delta T > 0)}$$

3-3:Tunneling rates (TR)



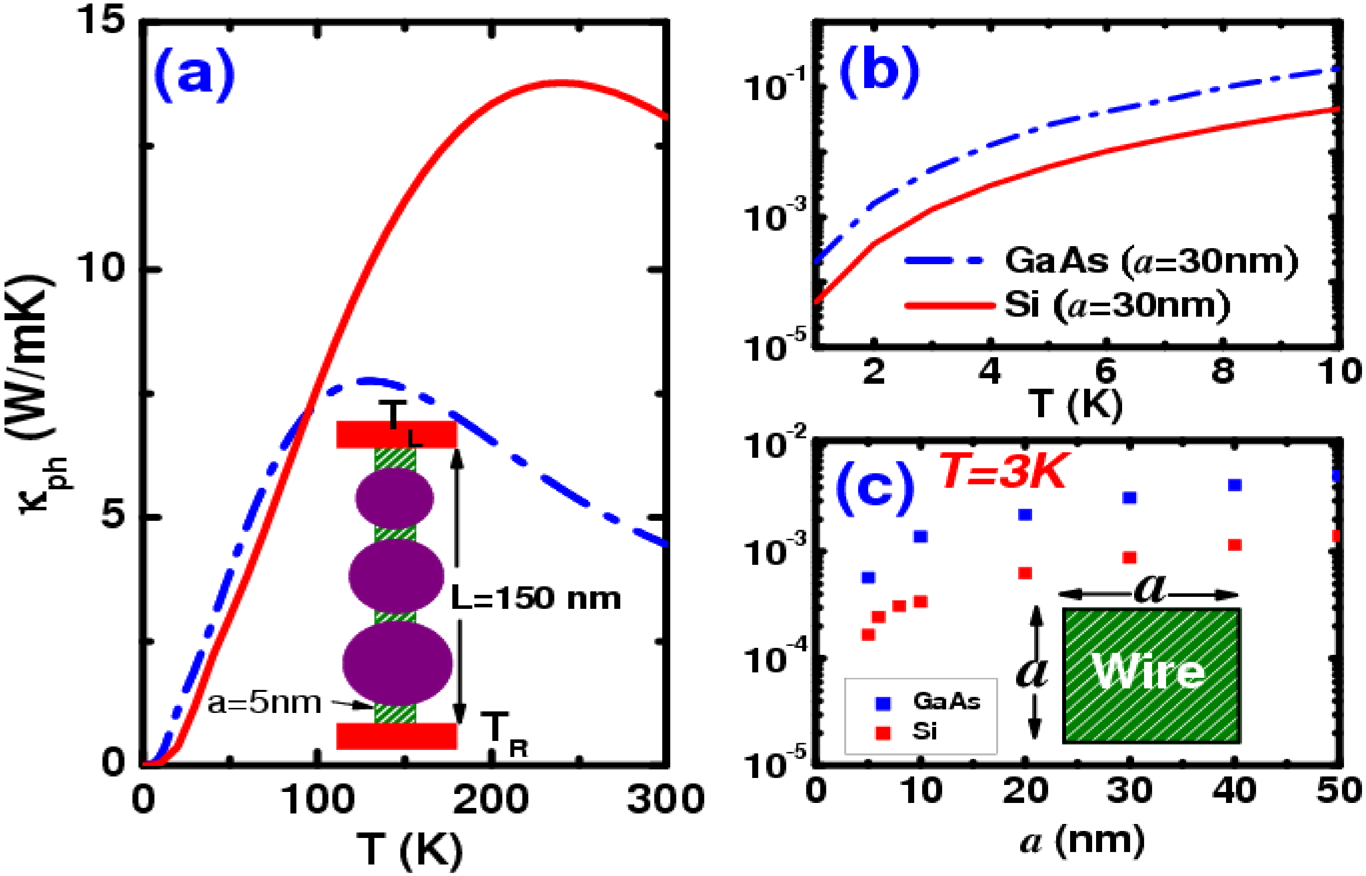
3-4:TR (TQDs)



[R11] R. Scheiber et al, New. J. Phys. 10, 083016 (2008)

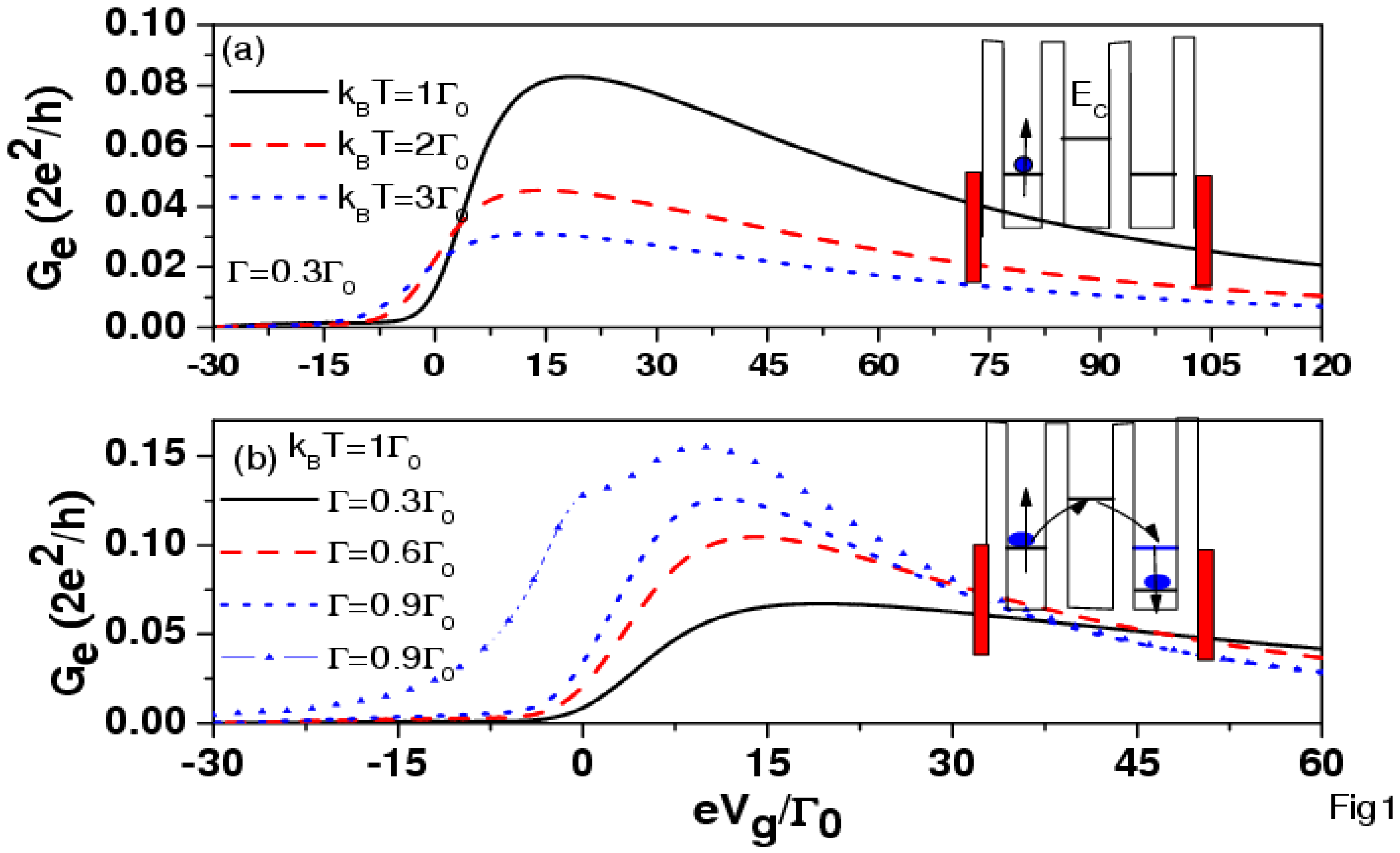
3-5:Thermal rectification at 3k

T



[7]Y C Tsen, D M T Kuo, and Y. C. Chang; APL 103, 053108 (2013)

4-1: LDCT effect (TODs)

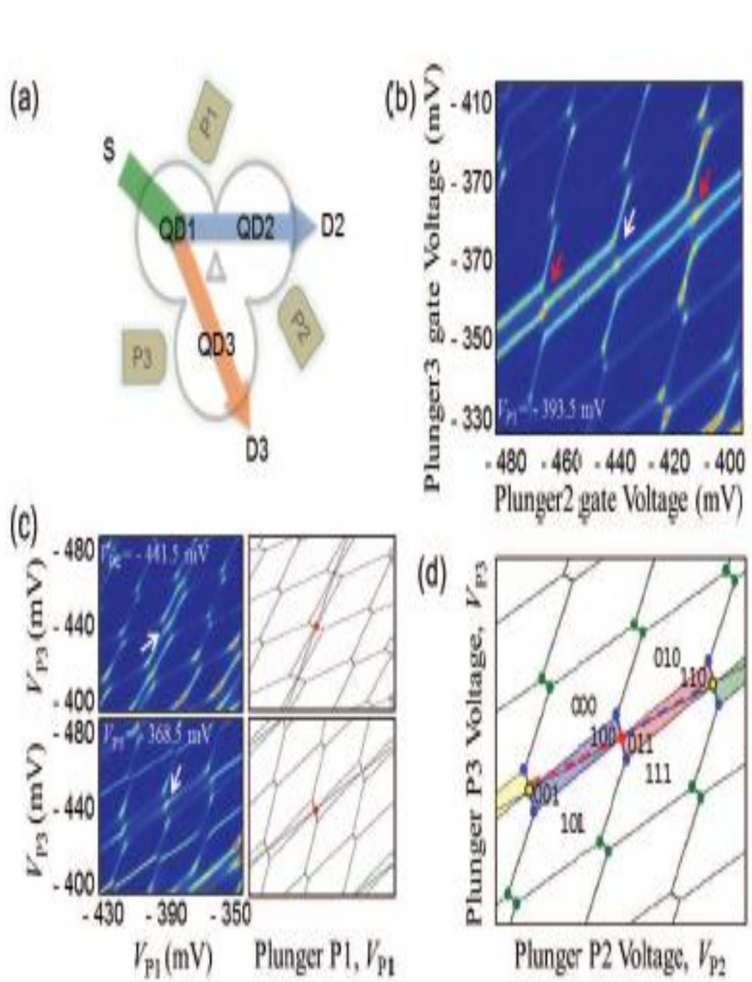


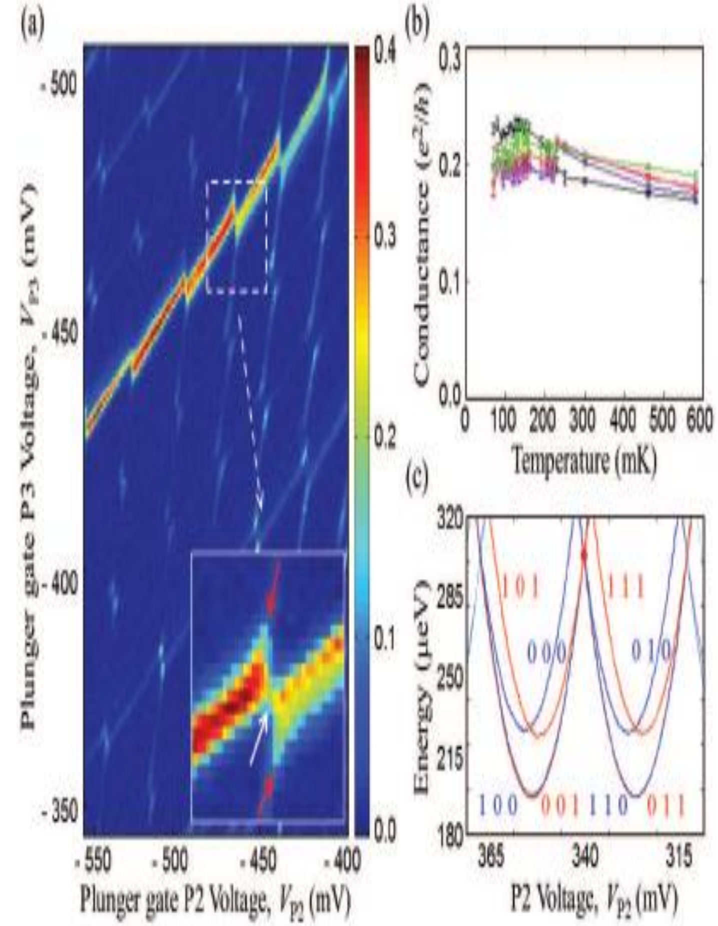
[R12]M. Busl et al Nature Nanotech 8, 261(2013).

[R13]F. R. Braakman et al, Nature Nanotech 8, 432 (2013).

4-2:Experiment of TTQDs

[R14]M. Seo et al , Phys. Rev. Lett. 110,046803 (2013).





4-3:DQD (strong coupling)

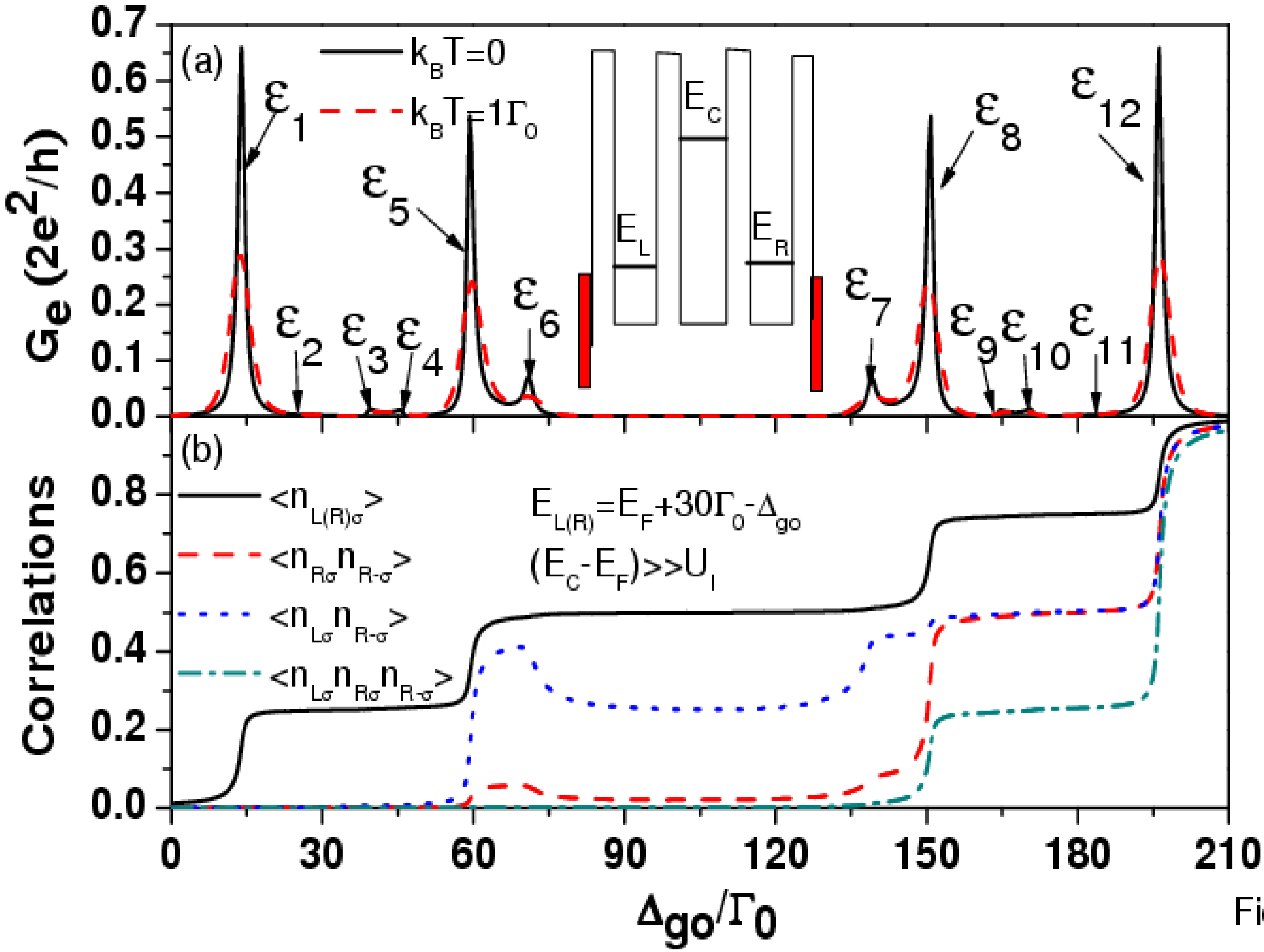


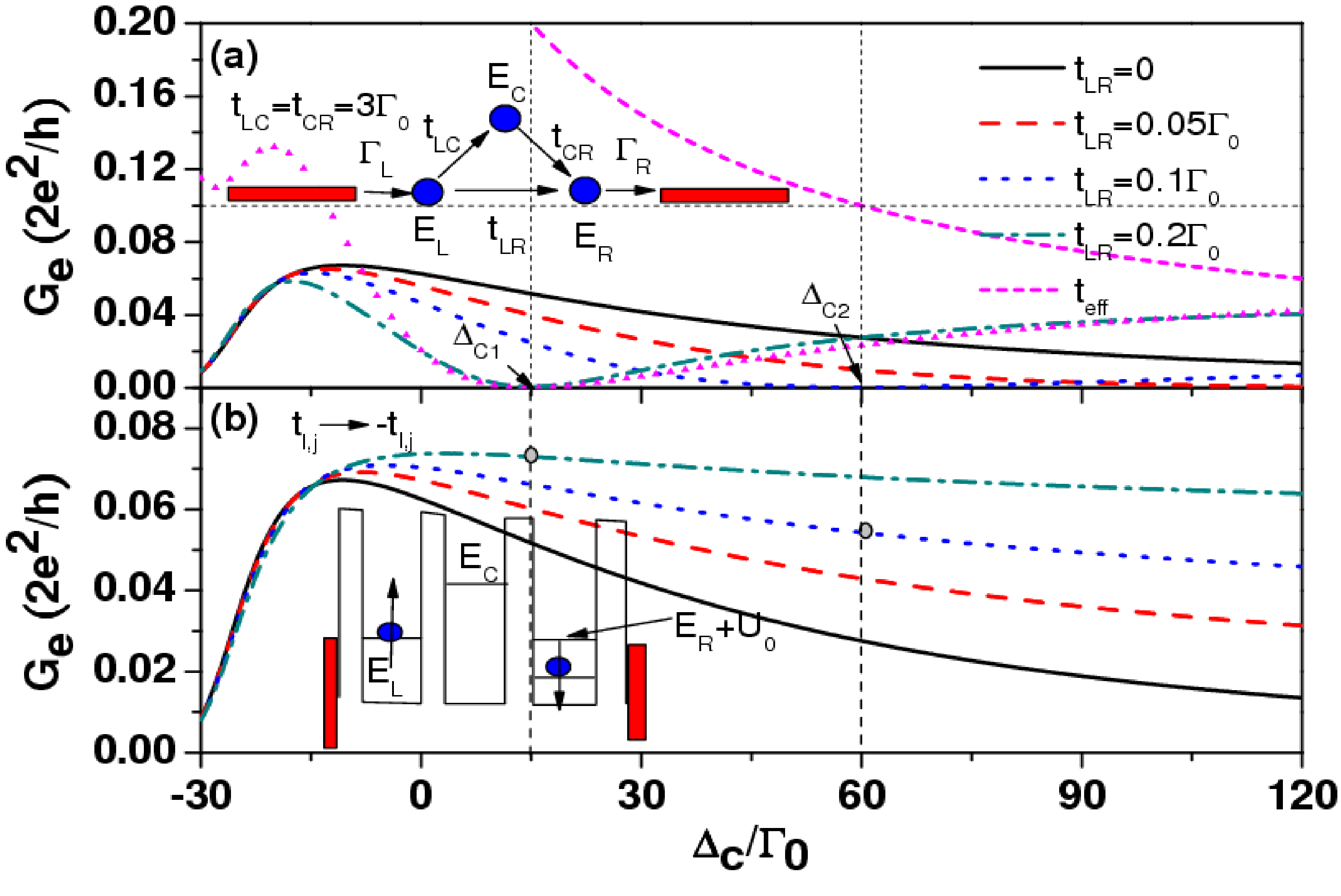
Fig1

4-3-1:Spectra of DQD

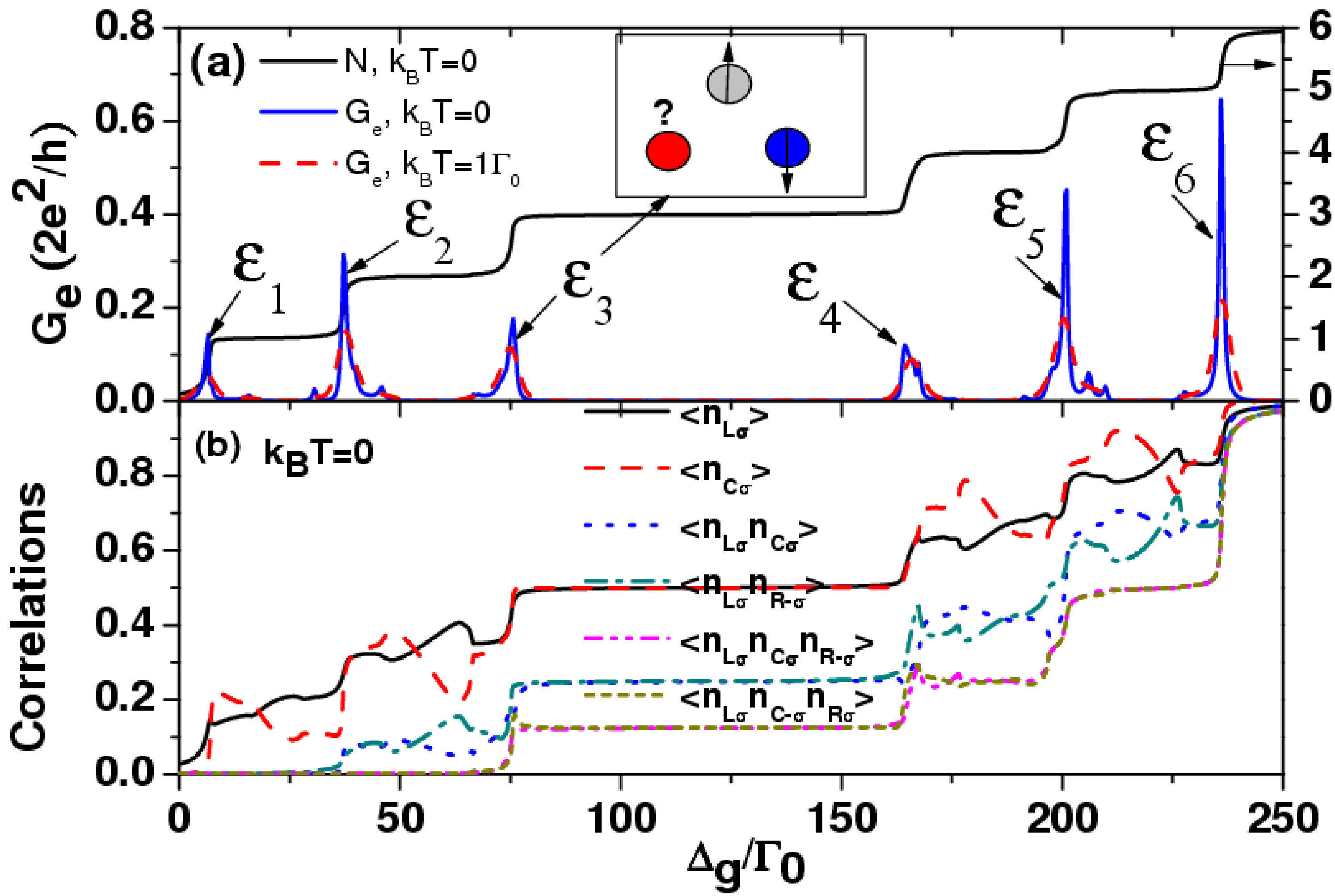
perature. The twelve peak positions of G_e are identified by $\epsilon_1 = E_0 - t_{LR}$, $\epsilon_2 = E_0 - t_{LR} + \frac{U_0+U_{LR}}{2} - \frac{1}{2}\sqrt{(U_0-U_{LR})^2+16t_{LR}^2}$, $\epsilon_3 = E_0+U_{LR}-t_{LR}$, $\epsilon_4 = E_0 + t_{LR}$, $\epsilon_5 = E_0 + t_{LR} + \frac{U_0+U_{LR}}{2} - \frac{1}{2}\sqrt{(U_0-U_{LR})^2+16t_{LR}^2}$, $\epsilon_6 = E_0 + U_{LR} + t_{LR}$, $\epsilon_7 = E_0 + U_0 + U_{LR} - t_{LR}$, $\epsilon_8 = E_0 - t_{LR} + \frac{U_0+3U_{LR}}{2} + \frac{1}{2}\sqrt{(U_0-U_{LR})^2+16t_{LR}^2}$, $\epsilon_9 = E_0 + U_0 + 2U_{LR} - t_{LR}$, $\epsilon_{10} = E_0 + U_0 + U_{LR} + t_{LR}$, $\epsilon_{11} = E_0 + t_{LR} + \frac{U_0+3U_{LR}}{2} + \frac{1}{2}\sqrt{(U_0-U_{LR})^2+16t_{LR}^2}$, and $\epsilon_{12} = E_0 + U_0 + 2U_{LR} + t_{LR}$. These poles do not involve any occupation numbers and correlation functions. This is a manifest result of integer charge picture.[14] The

[Re13]B R Bulka and T. Kostyrko, PRB, 70 205333 (2004)

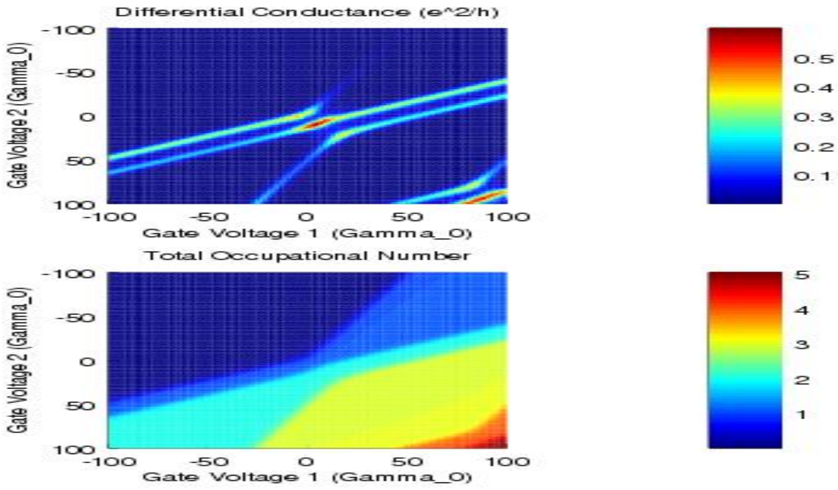
4-4:QI of TTQDs



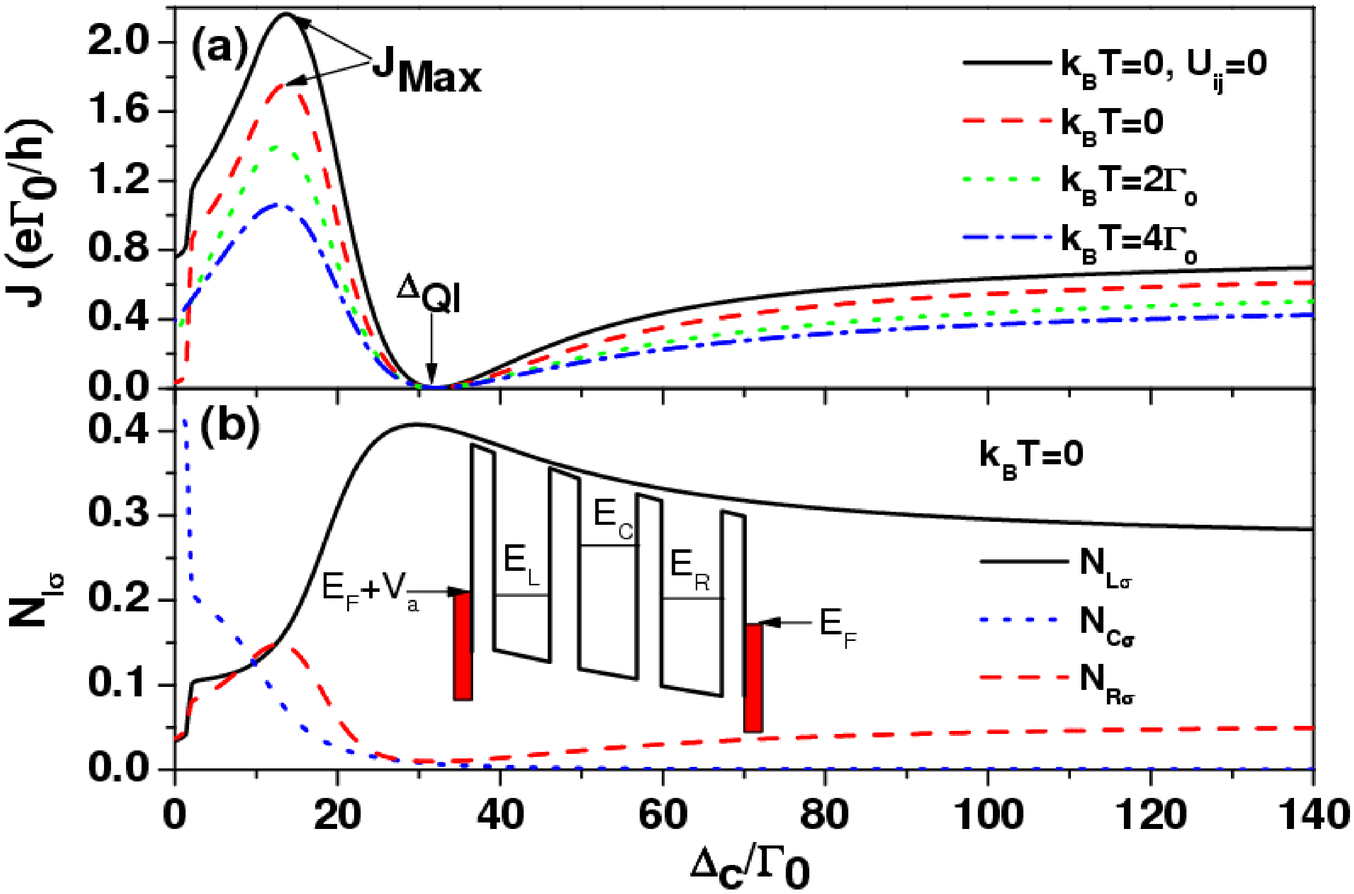
4-5:Spin frustration (TTQDs)



4-6:Charge stability diagram



4.7:QI effect on tunneling current



5:Conclusion

(1) Figure of merit, (ZT of QDs)

(2) Pauli spin blockade (DQDs)

(3) Thermal rectification (TQDs)

(4) Long distance coherent tunneling (TQDs)

(5)Quantum interference (TTQDs)

(6) Spin and charge frustrations (TTQDs)