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Thermoelectric properties of Kondo quantum dot in SU(N) Fermi liquid state

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Contents

Introduction

Mesoscopic system

Kondo effect and transport in QD

Thermal transport in QD 13 pages

Research related topic

Fermi liquid theory

Results

Thermal conductance formula
SU(2) and SU(4) cases

Conclusion and perspective

Introduction

Microscopic Quantum theory atom, molecule,…etc.	⟷	Macroscopic Classical mechanics …etc.

Intermediate μεσον

Mesoscopic 10nm~10μm

Quantum dot
Nano wire
…etc.

More precisely…

Larger than

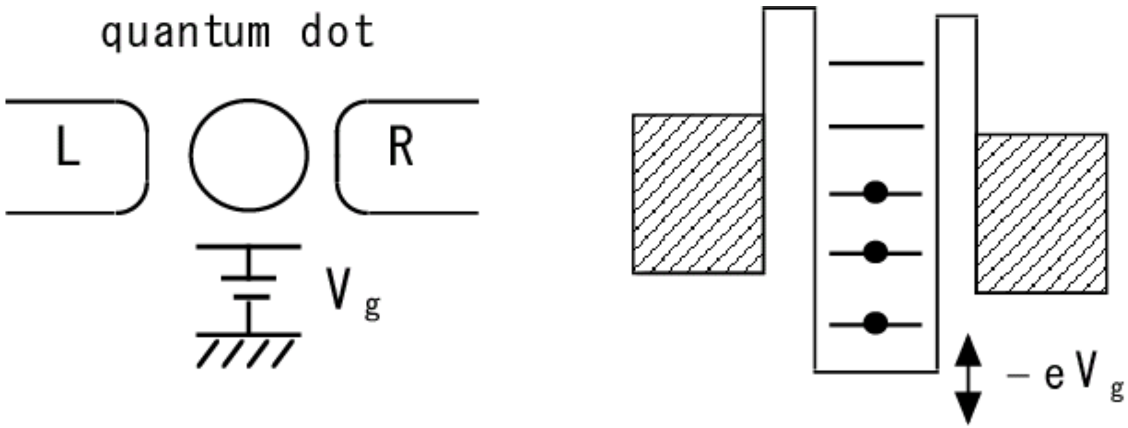
Lattice constant (cf. GaAs ~ 5.65 Å)

Smaller than

Phase decoherence length、Fermi wl ~100nm

One can control the quantum effect

Quantum dot + lead system



- Quantum dot: quasi zero dimension（nm scale）

  “confinement structure of electron”

- Connected with leads via tunnel coupling

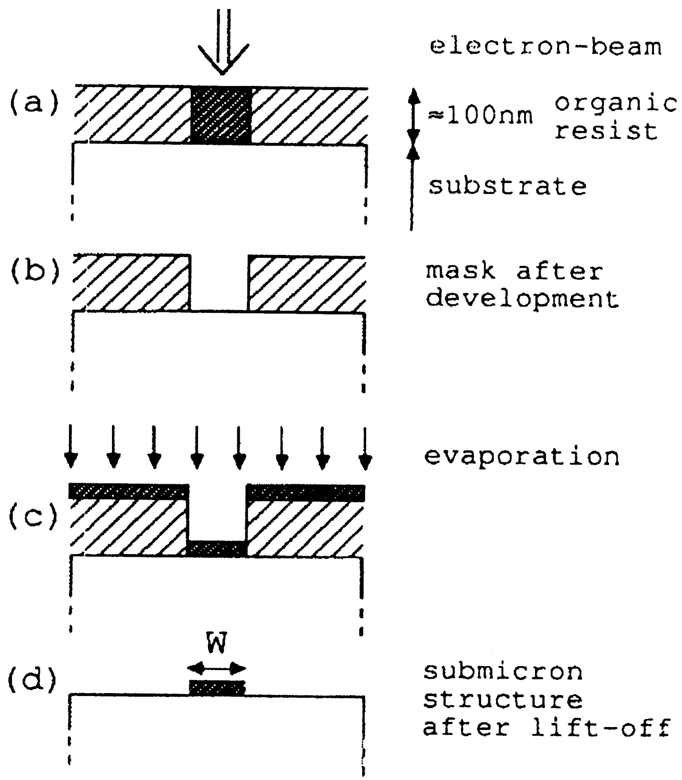
  “transport through discrete levels”

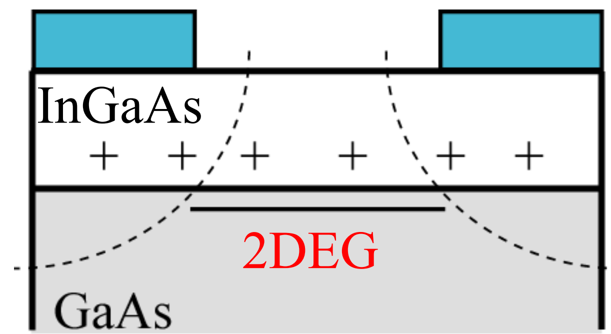
Quantum dot

(1) 2D electron gas in semiconductor

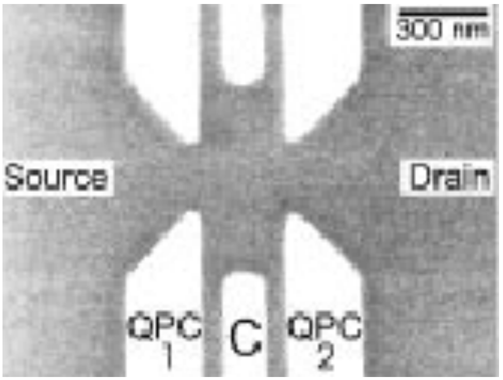
: Epitaxial Growth

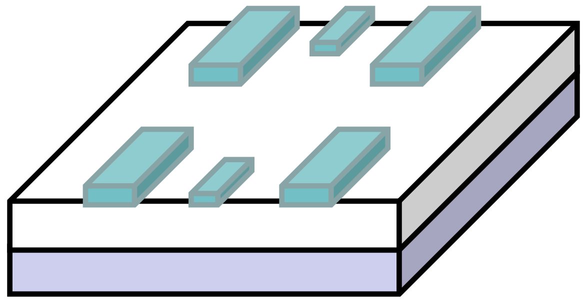
(2) Electron beam lithography : small electrode





Negative voltage
one can design the 2DEG





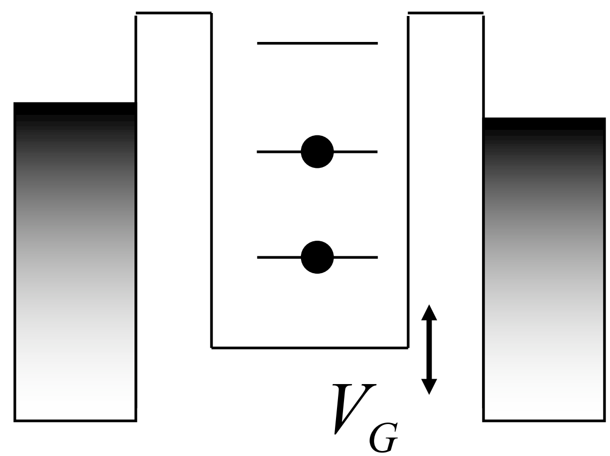
Gate voltage

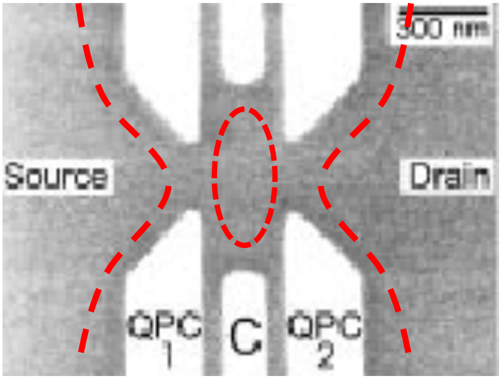
2DEG

Energy level: discretized

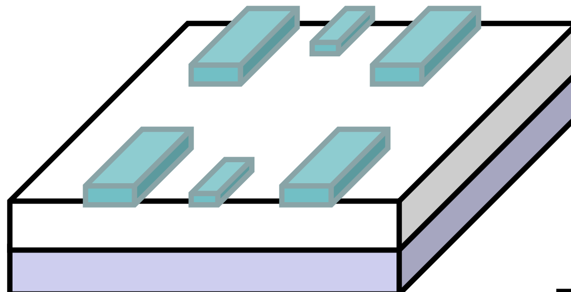
Gate voltage V_G

Static potential: tunable





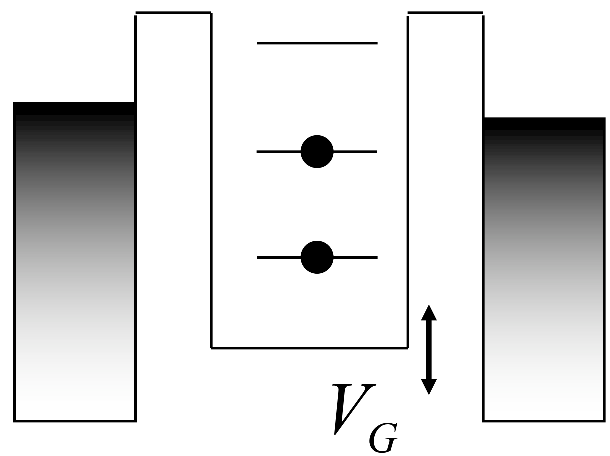
Gate voltage



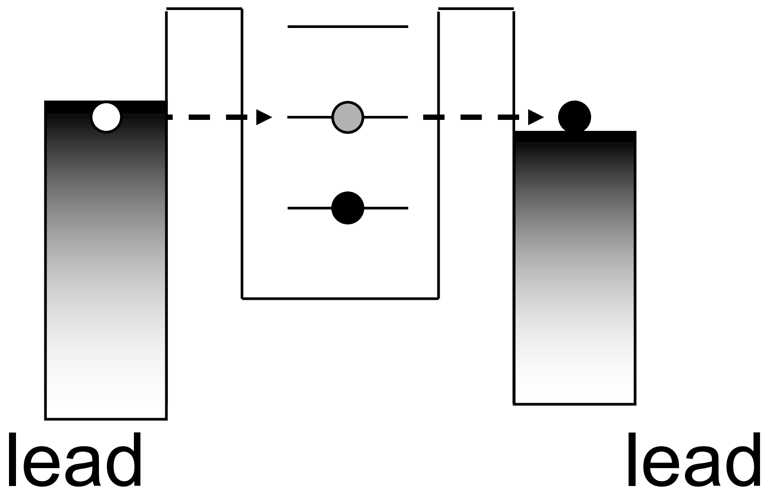
Energy level: discretized

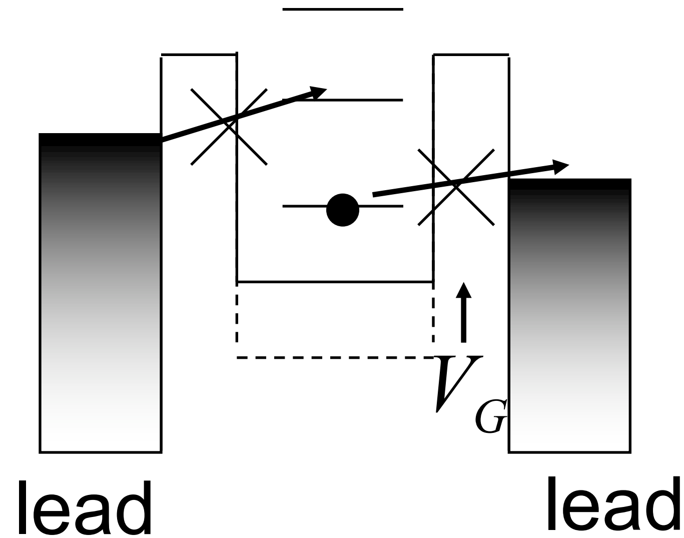
Gate voltage V_G

Static potential: tunable



Transport through quantum dot

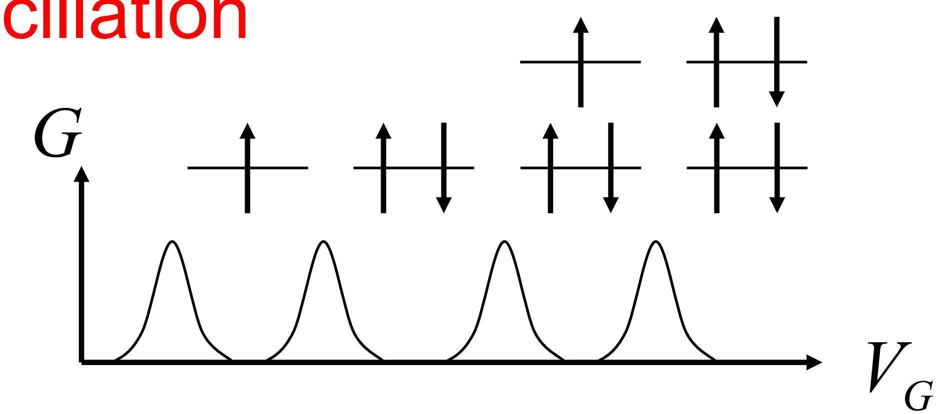




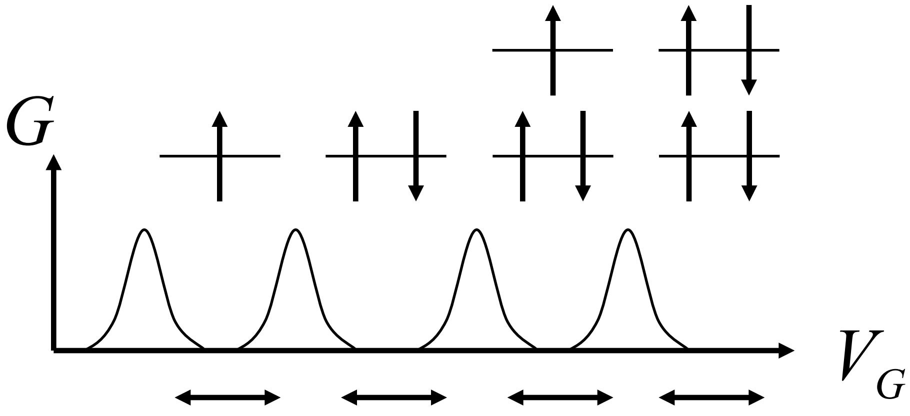
Tunneling: allowed

Tunneling: forbidden

Coulomb oscillation



Coulomb blockade

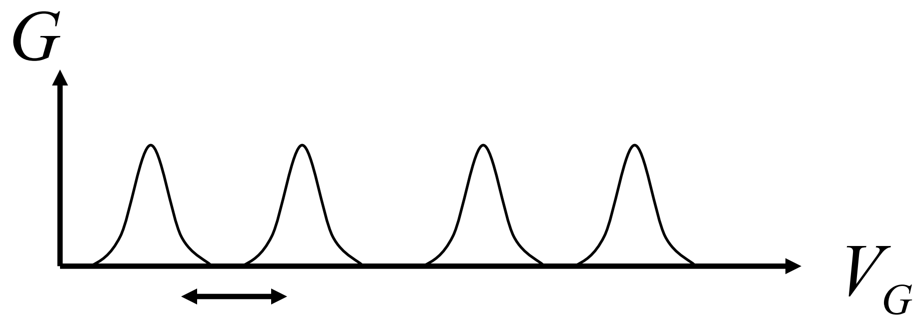


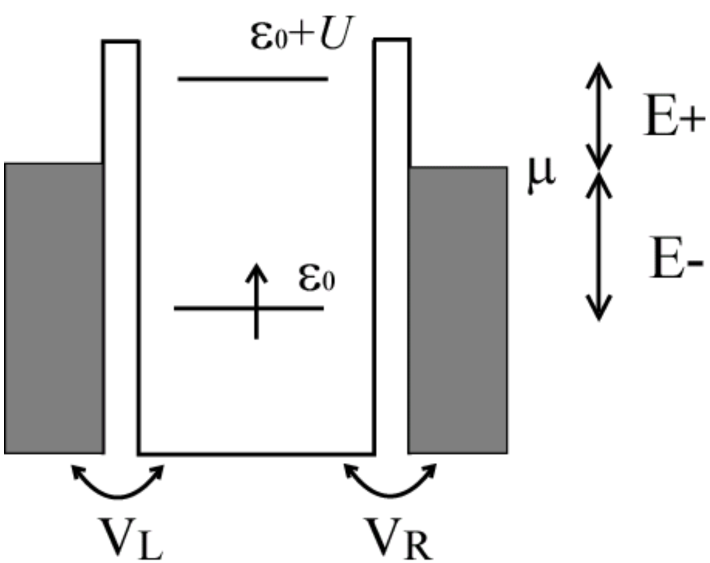
Number of electrons in quantum dot

Tunable one by one

Kondo effect in QD

Coulomb valley



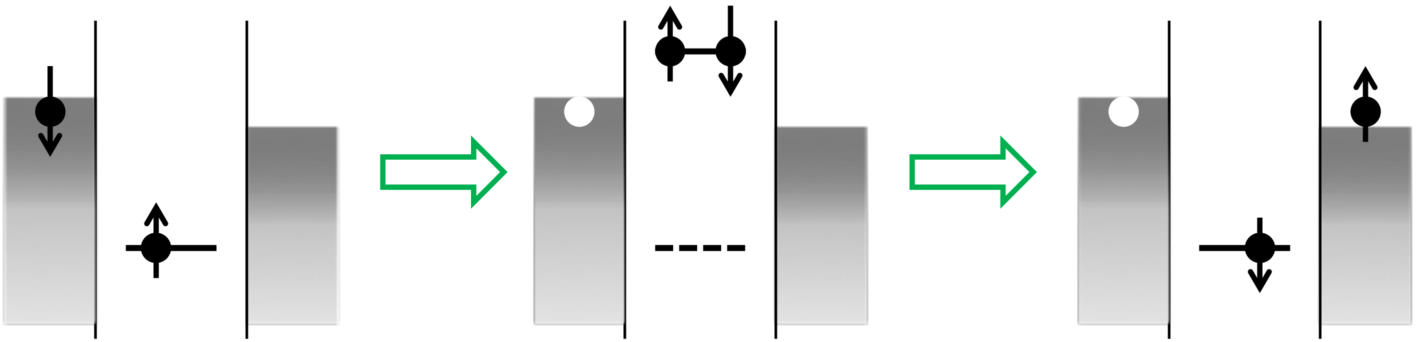


$$E^+, E^- \gg k_B T, \Gamma$$

$$\begin{cases} E^+ = \mu_2 - \mu = \varepsilon_0 + U - \mu \\ E^- = \mu - \mu_1 = \mu - \varepsilon_0 \end{cases}$$

$$\Gamma = \pi\nu\left(|V_L|^2 + |V_R|^2\right)$$

Second order tunneling process



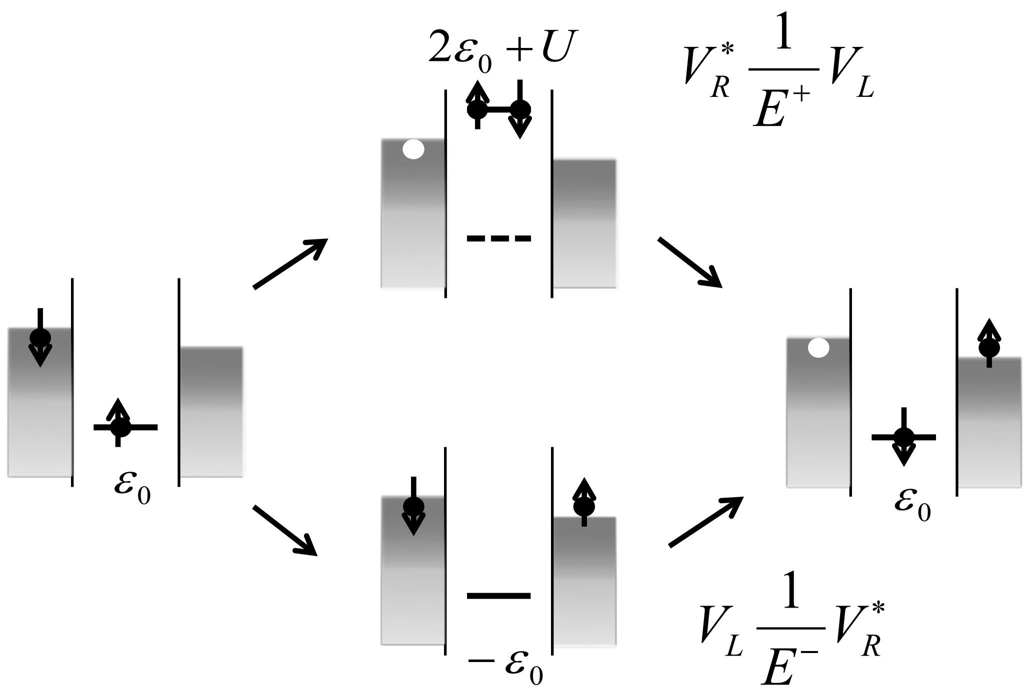
$$V_R^* \frac{1}{\varepsilon - H_0} V_L \approx -V_R^* \frac{1}{E^+} V_L$$

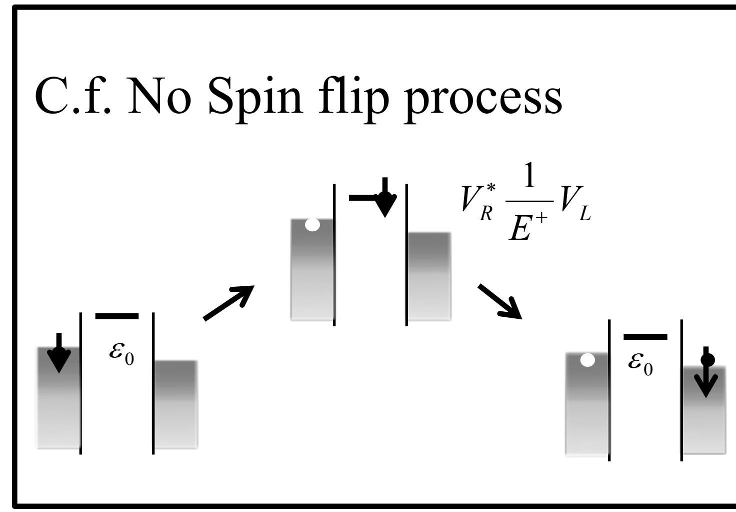
cotunneling

Dominant in Coulomb valley

Kondo effect

- Localized spin in QD S=1/2 : Spin flip process





Effective Hamiltonian $J \equiv \left(|V_L|^2 + |V_R|^2 \right) \left(\frac{1}{E^+} + \frac{1}{E^-} \right) > 0$

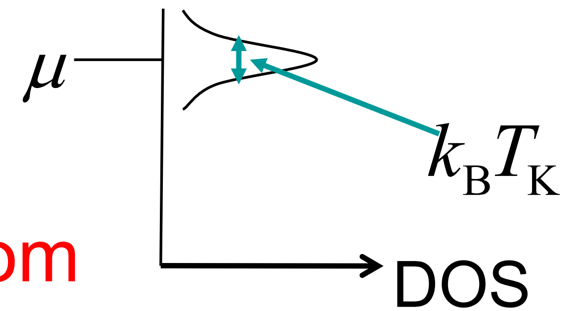
$$H = \sum_k \varepsilon_k a_{k\sigma}^\dagger a_{k\sigma} + 2J \sum_{k,k'} \mathbf{S} \cdot (\mathbf{s})_{k,k'}$$ Anti Ferromagnetic

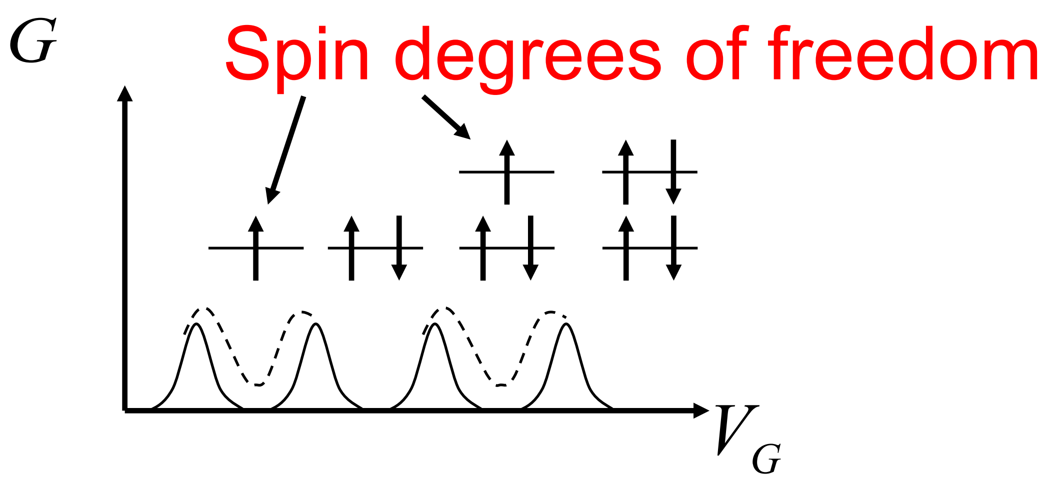
$$H = \sum_k \varepsilon_k a_k^\dagger a_k + 2J \sum_{k,k'} \mathbf{S} \cdot (\mathbf{s})_{k,k'}$$

Localized spin $\left(\frac{1}{2}\right)$
Spin in Fermi sea (leads)

→ Many body singlet state (spin screening)

Binding energy : Kondo temperature T_{K}





Odd valley: enhancement of conductance

Conductance

$$G = \frac{2e^2}{h}\alpha\int d\omega \frac{1}{2}\sum_s \left[-\pi\nu\,\mathrm{Im}T^s(\omega)\right]\left(-\frac{\partial f}{\partial\omega}\right)$$

$f(\omega)$: Fermi distribution function $\quad \alpha = \frac{4V_L^2V_R^2}{(V_L^2+V_R^2)^2} \quad 0<\alpha\le 1$

$T \ll T_\mathrm{K}$

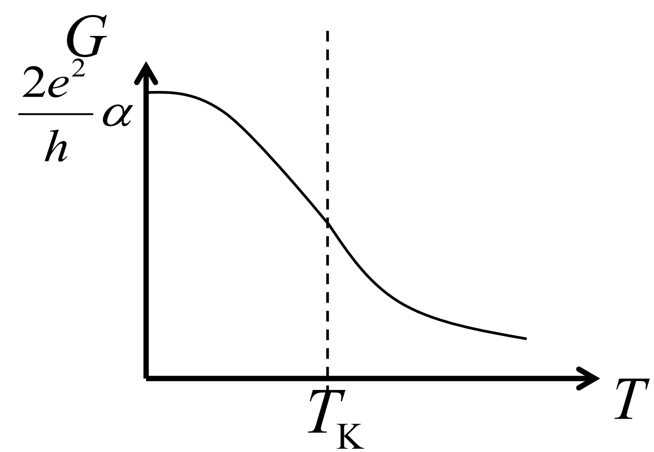
$$G = \frac{2e^2}{h}\alpha\left[1-\left(\frac{\pi T}{T_\mathrm{K}}\right)^2\right]$$

$T=0$

$$G = \frac{2e^2}{h}\alpha$$: resonant tunneling

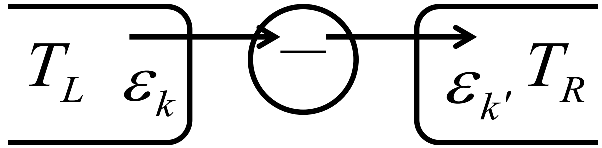
$T \gg T_\mathrm{K}$

$$G = \frac{2e^2}{h}\frac{3\pi^2}{16}\alpha\frac{1}{\left[\ln(T/T_\mathrm{K})\right]^2}$$



Thermal transport phenomena in QD

Landauer picture~ one particle picture



Thermal current

$$I_T = \sum_{k,k'} (\varepsilon_{k'} - \mu_R) v_{k'} T_{L,k\to R,k'} f_L(\varepsilon_k)[1 - f_R(\varepsilon_{k'})] - (\varepsilon_{k'} - \mu_L) v_{k'} T_{R,k\to L,k'} f_R(\varepsilon_k)[1 - f_L(\varepsilon_{k'})]$$

$v_{k'} = \partial \varepsilon_{k'} / \partial \hbar k'$:Group velocity

Linear response regime

$$T_L = T_R + \Delta T, \mu_L = \mu_R$$

$$G_T = \frac{I_T}{\Delta T} = \frac{2}{hT} \int d\varepsilon_{k'} (\varepsilon_{k'} - \mu)^2 \underline{|t_{k,k'}|}^2 [-f'(\varepsilon_k)]$$

Transmission probability
Calculable from T-matrix

Valid for non-interacting system

Interacting system ?

B. Dong and X L Lei, J. Phys.: Cond. Matt. **14** (2002).

Ng's ansatz

Interacting self energy $\Sigma^{<}(\varepsilon_{k'}), \Sigma^{>}(\varepsilon_{k'})$

Noninteracting Green functions $\Sigma_0^{<}(\varepsilon_{k'}), \Sigma_0^{>}(\varepsilon_{k'})$

Assumption

$$\Sigma^{<}(\varepsilon_{k'}) = A\Sigma_0^{<}(\varepsilon_{k'}), \Sigma^{>}(\varepsilon_{k'}) = A\Sigma_0^{>}(\varepsilon_{k'})$$

A :some function

$$\Rightarrow \quad G_T = \frac{2}{hT}\int d\varepsilon_{k'}(\varepsilon_{k'} - \mu)^2[-\Gamma \operatorname{Im} G^r(\varepsilon_{k'})][-f'(\varepsilon_{k'})]$$

$G^r(\varepsilon_{k'})$:retarded GF of QD

Purpose

- Derive the formula without using Ng's ansatz
- Detailed study for Strong coupling region

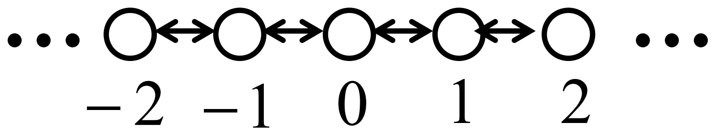
Fermi liquid theory

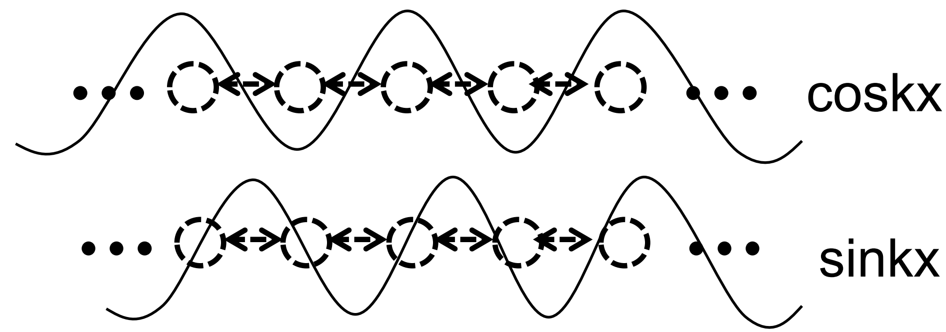
Schematic picture and some topics

5 pages

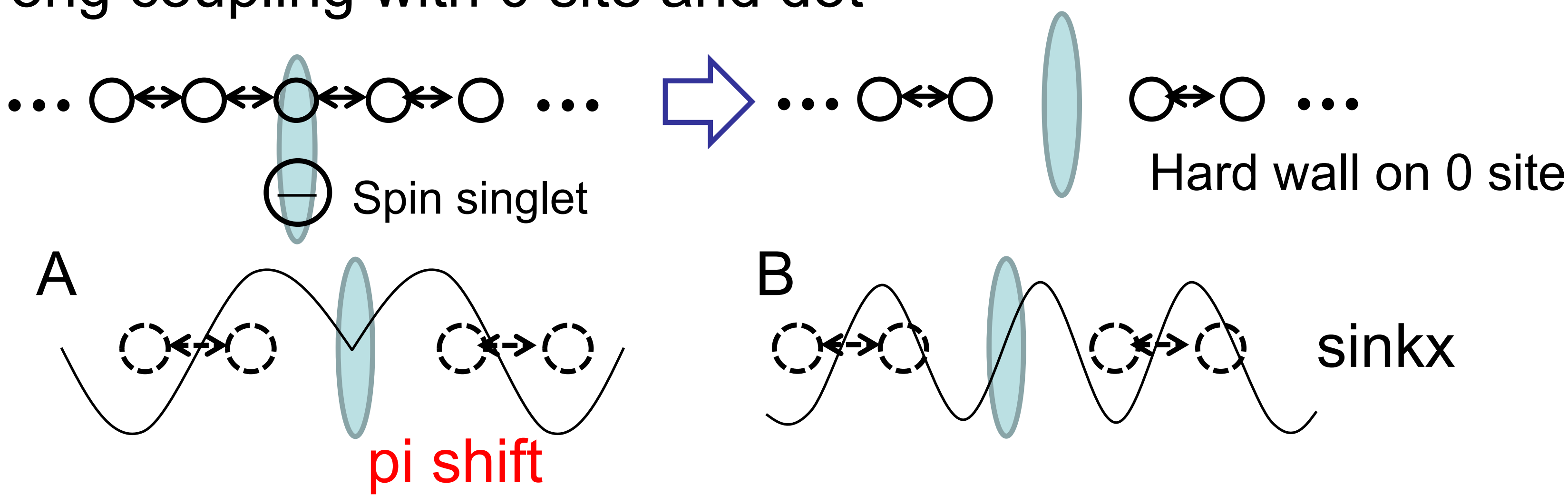
Fermi liquid theory (Schematics)

Free electrons in 1d lattice

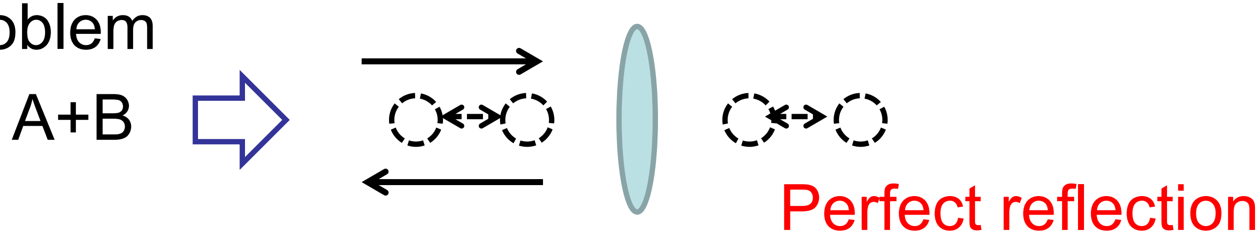




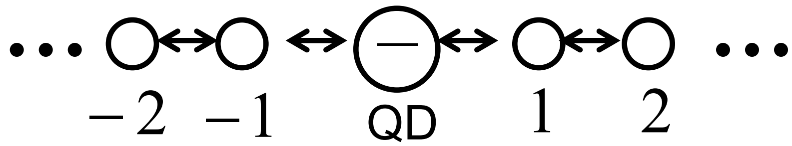
Strong coupling with 0 site and dot



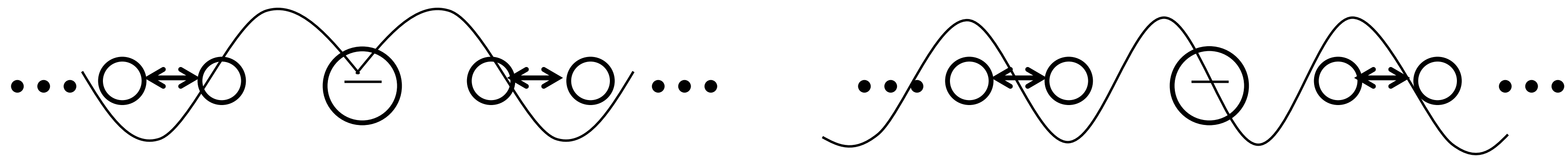
Scattering problem



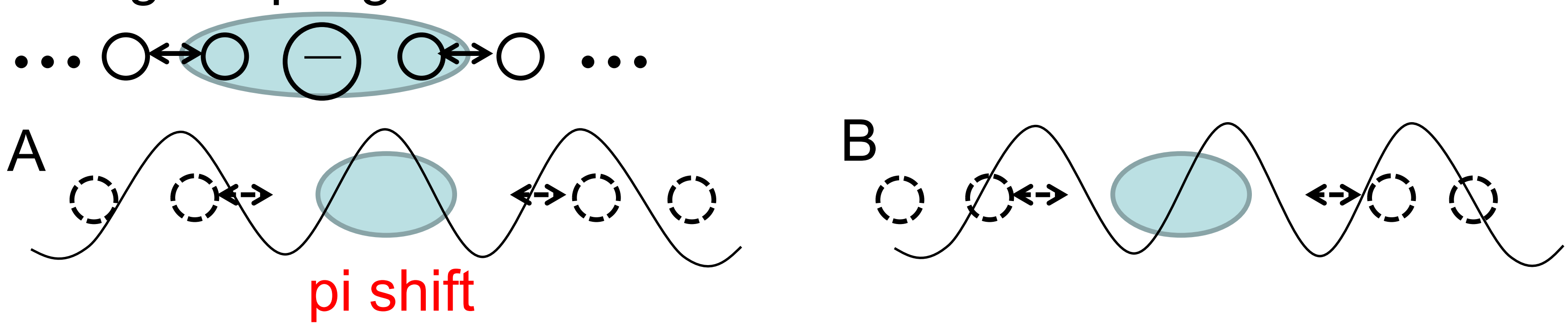
Quantum dot connected to two leads



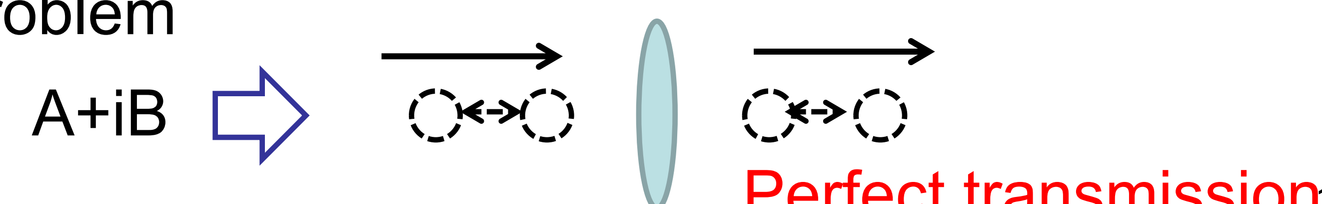
Coulomb blockade (no transmission)



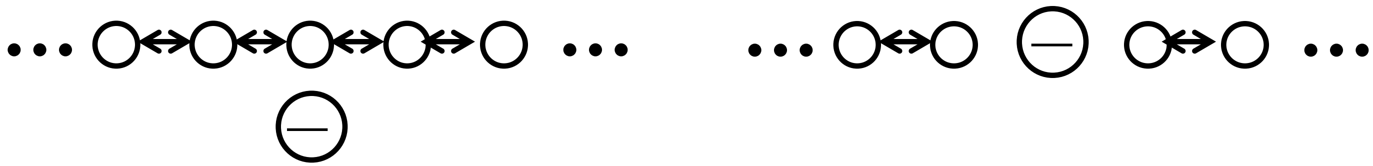
Strong coupling with leads and dot



Scattering problem



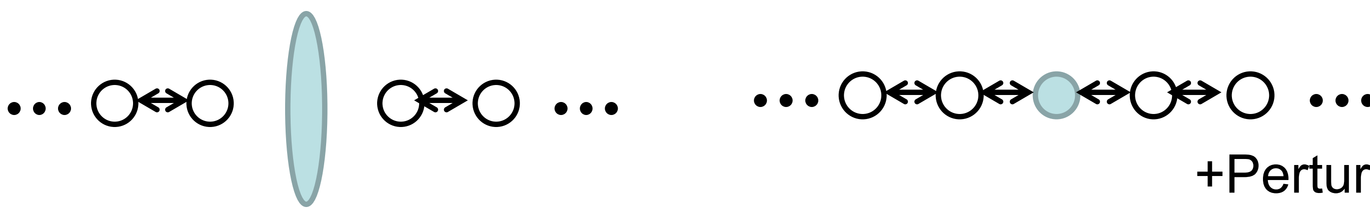
Weak coupling regime and strong coupling regime



Weak coupling

+Perturbation
Hopping term

Strong coupling



+Perturbation
With what ?

Fermi liquid theory ~ reverse transformation of renormalization

Strong coupling limit =fixed point of renormalization
Irreversible

Some input (and some times guess) is needed
- Symmetry (p-h, SU(2), etc) of the system
- Parameters need to be exported

Outline of the Fermi liquid expansion

C. Mora, PRB, **80**, 125304, (2009).

Expand the Phase shift

$$\delta_\sigma(\varepsilon, \delta n_{\sigma'}) = \delta_0 + \frac{\alpha_1}{T_\mathrm{K}}\varepsilon + \frac{\alpha_2}{T_\mathrm{K}^2}\varepsilon^2 \quad \text{(elastic scattering)}$$

$$-\sum_{\sigma'\neq\sigma}\frac{\phi_1}{T_\mathrm{K}}\int d\varepsilon'\delta n_{\sigma'}(\varepsilon') - \sum_{\sigma'\neq\sigma}\frac{\phi_1}{T_\mathrm{K}^2}\int d\varepsilon'(\varepsilon+\varepsilon')\delta n_{\sigma'}(\varepsilon') \quad \text{(4point vertex)}$$

$$-\sum_{\substack{\sigma''\neq\sigma \\ \sigma''<\sigma'}}\frac{\chi_2}{T_\mathrm{K}^2}\int d\varepsilon' d\varepsilon''\delta n_{\sigma'}(\varepsilon')\delta n_{\sigma''}(\varepsilon'') \quad \text{(6point vertex)}$$

Floating the Kondo resonance

Physics is the same except for energy shift

$$\delta_\sigma(\varepsilon+\delta\varepsilon, \delta n'_{\sigma'}) = \delta_\sigma(\varepsilon, \delta n_{\sigma'})$$

$$\Rightarrow \boxed{\alpha_1 = (N-1)\phi_1, \alpha_2 = \frac{N-1}{4}\phi_2, \phi_2 = (N-2)\chi_2} \quad \text{for SU(N)}$$

Fermi liquid theory

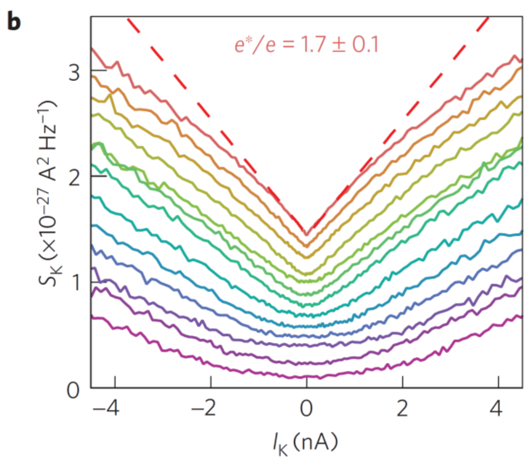
Once the Fermi liquid parameter is obtained…

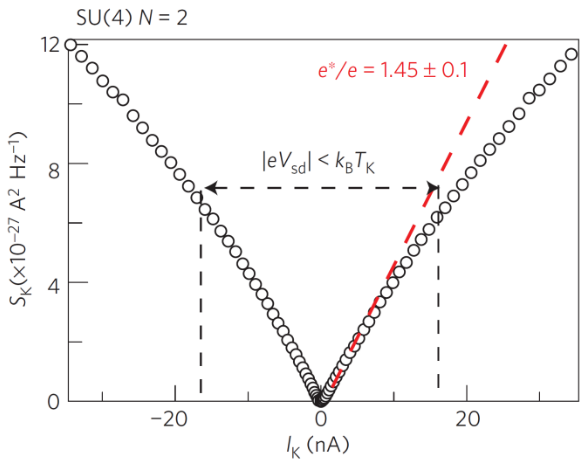
The powerful tool also in non equilibrium situation

c.f. Non-equilibrium Green's function,
exact up to O(eV, T, E)^3. A. Oguri, JPSJ, **74**, 110, (2005).

c.f. effective charge in Kondo effect detected by noise measurement

M. Ferrier, *et al*, Nat. Phys. **12**, 230–235 (2016).





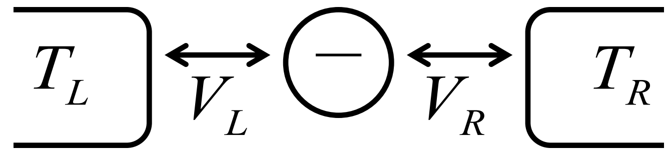
Results

7 pages

Outline of the derivation of conductances

Impurity Anderson model

$$H=\sum_{k,\sigma}(\varepsilon_k-\mu_\alpha)c^{+}_{\alpha,k,\sigma}c_{\alpha,k,\sigma}$$
$$+\varepsilon_d\sum_{\sigma}d^{+}_{\sigma}d_\sigma+U\sum_{\sigma<\sigma'}n_\sigma n_{\sigma'}$$
$$+\sum_{k,\sigma}V_\alpha c^{+}_{\alpha,k,\sigma}d_\sigma+h.c$$



Energy current = energy change in unit time

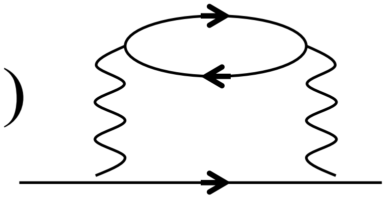
$$I^E_L=-\frac{d}{dt}\sum_{k,\sigma}(\varepsilon_k-\mu_L)c^{+}_{L,k,\sigma}c_{L,k,\sigma}$$

$$\Big\downarrow \text{ EOM technique}$$

$$I^E_L=-\frac{2\Gamma_L}{h}\int d\omega\sum_{\sigma}(\omega-\mu_L)[2f_L(\omega)\underbrace{\mathrm{Im}\,G^{r}_{d,\sigma}(\omega)}_{\text{retarded GF}}+\underbrace{\mathrm{Im}\,G^{<}_{d,\sigma}(\omega)}_{\text{lesser GF}}]$$

$$\Gamma_L=\underbrace{\pi\nu}_{\text{DOS}}V_L^2$$

Evaluation of $\Sigma^<(\varepsilon_{k'}), \Sigma^>(\varepsilon_{k'})$



$$\Sigma^<(\omega) = -ip\int d\varepsilon_1 d\varepsilon_2 \bar{f}(\varepsilon_1)\bar{f}(\varepsilon_2)[1-\bar{f}(\varepsilon_1+\varepsilon_2-\omega)]$$

$$p = 2\pi\nu^3 U^2,\ \bar{f}(\varepsilon) = \frac{\Gamma_L f_L(\varepsilon)+\Gamma_R f_R(\varepsilon)}{\Gamma_L+\Gamma_R}$$

$$T_L = T+\Delta T, T_R = T, \mu_L = \mu_R = 0$$

$$\Sigma^<(\omega) = -ipf(\omega)(\omega^2+\pi^2T^2)$$
$$-2ip\frac{\Gamma_L}{\Gamma_L+\Gamma_R}\frac{\partial}{\partial T}\left[\frac{f(\omega)}{2}(\omega^2+\pi^2T^2)\right]\Delta T + O(\Delta T^2)$$

$$\Sigma^>(\omega) = -\Sigma^<(-\omega)$$

Retarded self energy

$$\mathrm{Im}\Sigma^r(\omega) = \frac{\Sigma^<(\omega)-\Sigma^>(\omega)}{2i} = -\frac{p}{2}(\omega^2+\pi^2T^2) - p\frac{\Gamma_L}{\Gamma_L+\Gamma_R}\pi^2 T\Delta T$$

Result 1: Energy current conservation

$$\Delta I^E = I_L^E - I_R^E$$
$$= -\frac{4}{h}\int d\omega\omega\, |G_d^r(\omega)|^2 [2\bar{f}(\omega)\,\mathrm{Im}\Sigma^r(\omega) + \mathrm{Im}\Sigma^<(\omega)]$$
$$= O(\Delta T^2)$$

Conductance

One can also calculate

charge current with bias voltage

charge current with temperature gradient

energy current with bias voltage

$$\begin{pmatrix} G_{CC} & G_{CT} \\ G_{TC} & G_{TT} \end{pmatrix}\begin{pmatrix} \Delta V \\ \Delta T / T \end{pmatrix} = \begin{pmatrix} I^C \\ I^E \end{pmatrix}$$

Result 2: Conductance Formula

$$G_{CC} = \frac{2e^2}{h}\int d\omega[-\Gamma\,\mathrm{Im}\,G^r(\omega)][-f'(\omega)]$$

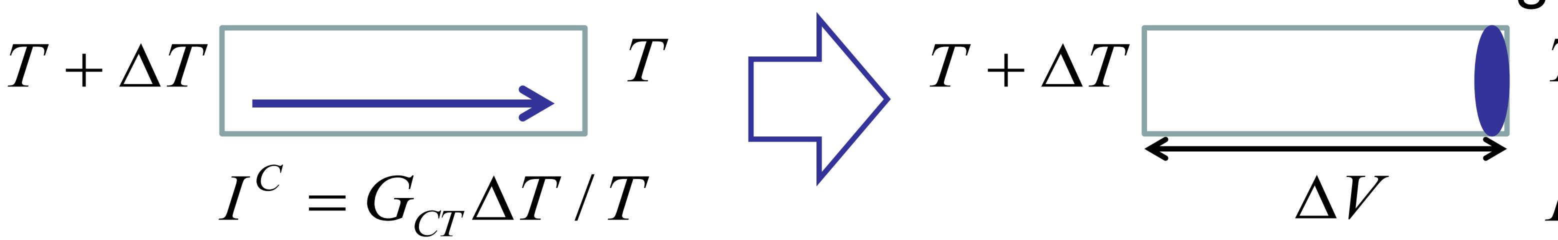
$$G_{TT} = \frac{2}{h}\int d\omega(\omega-\mu)^2[-\Gamma\,\mathrm{Im}\,G^r(\omega)][-f'(\omega)]$$

$$\underline{G_{CT} = G_{TC}} = \frac{2e}{h}\int d\omega(\omega-\mu)[-\Gamma\,\mathrm{Im}\,G^r(\omega)][-f'(\omega)]$$

Onsagar's reciprocity

Thermopower

charging



$I^C = G_{CT}\Delta T / T$

$I^C = 0$

$$\begin{pmatrix} G_{CC} & G_{CT} \\ G_{TC} & G_{TT} \end{pmatrix}\begin{pmatrix} \Delta V \\ \Delta T / T \end{pmatrix} = \begin{pmatrix} 0 \\ I^E \end{pmatrix}$$

$$\boxed{\Delta V = -G_{CT}/G_{CC} \times \Delta T / T}$$

$$\boxed{I^E = \kappa \Delta T / T \quad \kappa = G_{TT} - G_{CT}^2 / G_{CC}}$$

Result 3: Case of SU(2) Kondo (U=∞)

$$G_{CC} = \frac{2e^2}{h}\left[1-\left(\frac{T}{T_{\mathrm{K}}}\right)^2\right], \quad G_{TT} = \frac{2}{h}\frac{(\pi T)^2}{3}\left[1-\frac{13}{5}\left(\frac{T}{T_{\mathrm{K}}}\right)^2\right]$$

$$G_{CT} = G_{TC} = 0$$

$$\kappa = G_{TT} - G_{CT}^2 / G_{CC} = G_{TT}$$

Up to linear response, cross effect is absent

Particle-hole symmetry, time reversal symmetry, …?

+Small magnetic field B, T=0

$$\delta_\sigma = \delta_0 + \sigma g \mu_B B / T_{\mathrm{K}}$$

$$G_{CC} = \frac{2e^2}{h}\left[1-\left(\frac{g\mu_B B}{T_{\mathrm{K}}}\right)^2\right], \quad G_{TT} = \frac{2}{h}\frac{(\pi T)^2}{3}\left[1-\frac{13}{5}\left(\frac{g\mu_B B}{T_{\mathrm{K}}}\right)^2\right]$$

$G_{CT} = G_{TC} = 0$ T reversal symm. breaking $\nRightarrow$ cross effect

Result 4: Case of SU(4) Kondo (U=∞)

$$G_{CC} = \frac{2e^2}{h}, \quad G_{TT} = \frac{2}{h}\frac{(\pi T)^2}{3}\left[1 + \frac{16}{15}\left(\frac{T}{T_\mathrm{K}}\right)^2\right]$$

$$G_{CT} = G_{TC} = \frac{2e}{h}\frac{\pi T}{3}\left(\frac{\pi T}{T_\mathrm{K}}\right)$$

$$\kappa = G_{TT} - G_{CT}^2 / G_{CC} = \frac{2}{h}\frac{(\pi T)^2}{3}\left[1 + \frac{11}{15}\left(\frac{T}{T_\mathrm{K}}\right)^2\right]$$

Nonzero cross effect even in linear response regime

T=0 with magnetic field ⇒ cross effect is absent

SU(4) Kondo: Particle-hole symmetry is broken

Necessary for cross effect?

SU(2) Kondo + Particle-hole symmetry break?

In progress

Result 5: Case of SU(4) Kondo with Fermi liquid parameters

For general case,

$$\Gamma \operatorname{Im} G^r(\omega) \cong -\frac{1}{2} - \alpha_1 \frac{\omega}{T_{\mathrm{K}}} - \alpha_2 \frac{3\omega^2 - (\pi T)^2}{3T_{\mathrm{K}}^2}$$

c.f. SU(2) case

$$\Gamma \operatorname{Im} G^r(\omega) \cong -1 + \alpha_1 \frac{3\omega^2 + (\pi T)^2}{2T_{\mathrm{K}}^2}$$

$$G_{CC} = \frac{2e^2}{h}, \quad G_{TT} = \frac{2}{h}\frac{(\pi T)^2}{3}\left[1 + \frac{16}{15}\alpha_2\left(\frac{T}{T_{\mathrm{K}}}\right)^2\right]$$

$$G_{CT} = G_{TC} = \frac{2e}{h}\frac{\pi T}{3}\alpha_1\left(\frac{\pi T}{T_{\mathrm{K}}}\right)$$

SU(4) Kondo case: both α_1 α_2 appear

⇨ contains more information of micro process

Conclusion

- In the basis of Fermi liquid theory, the thermal conductance is exactly obtained in linear response regime.

- SU(2) and SU(4) case shows clear difference for the thermo-electric cross effect.

- Time reversal symmetry breaking cannot bring cross effect on SU(2) case.

- Thermal conductance and charge conductance contains the auxiliary information for SU(4) case.

Perspective

- Particle-hole symmetry breaking for SU(2)?
- Nonlinear response (Non equilibrium) regime?
- 2-Channel Kondo (Non Fermi liquid) case?

Expansion in energy is available