Kondo Physics, Out of Equilibrium Thermo-electricity

Karyn Le Hur

CPHT Ecole Polytechnique CNRS

Thanks to Collaborators
Thanks to Organizers

Karyn: PhD Thesis 05th October 1998
PhD Advisor: Bernard Coqblin

My First Article

The underscreened Kondo effect: a two S=1 impurity model

Karyn Le Hur and B. Coqblin

Laboratoire de Physique des Solides, Université Paris–Sud, Bât. 510, 91405 Orsay, France

1D S=1 Kondo Lattice Model with bosonization, KLH Phys. Rev. Lett., **83** (1999) 848
THANKS to B. Coqblin, H. J. Schulz, T. Giamarchi, T. Maurice Rice
C. Thomas, Acirete S. da Rosa Simões, J. R. Iglesias, C. Lacroix, N. B. Perkins, B. Coqblin
Phys. Rev. B **83**, 014415 (2011)

The Kondo problem is an active subject of intense research

Many materials, Topological Kondo insulators

Mesoscopic Structures Opening new probes of the Kondo Effect

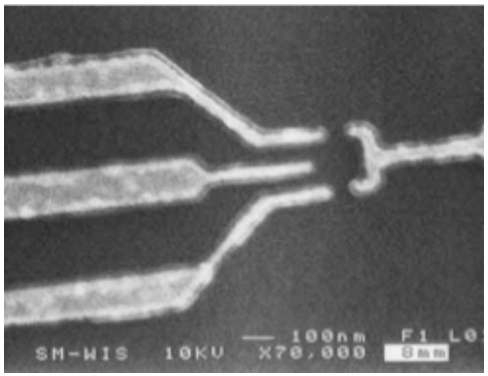
Recent Applications in ultra-cold Atoms and quantum optics

Thermo-electric applications

Transport in Nano-Matter:

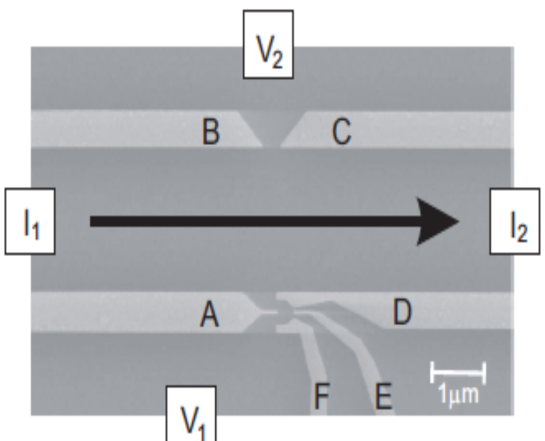
Transport: **current** and **noise** commonly accessible
Y. Blanter & M. Buettiker, Phys. Rep. 2000

D. Goldhaber-Gordon et al. 1998



Kondo model: Kondo, Anderson, Wilson, Nozieres, Blandin …
Schrieffer-Wolff; Coqblin – Schrieffer model, Friedel Phase
Integrability: N. Andrei; Tsvelik; Wiegmann; H. Saleur…
CFT: I. Affleck; A. Ludwig
Large-N approach: N. Read and Newns; P. Coleman
Applications to quantum dots: e.g. M. Pustilnik & L. Glazman, review

Noise in **Kondo** correlated regime: E. Sela et al. (2006)
O. Zarchin et al (2008); T. Delattre et al. (2009); Y. Yamauchi et al.
R. Deblock et al. (theory: P. Moca, P. Simon, G. Zarand)
C. Mora, P. Vitushinsky, X. Leyronas, A. Clerk & KLH
Also, recent works C.-H. Chung, KLH, M. Vojta, P. Woelfle



Thermopower:
L. Molenkamp et al (2005)

Schwinger-Keldysh 1961-64
Hershfield 1993

Thermoelectricity
Hybrid Systems

Generic Nano-System

Let us start with a **quantum impurity** problem $H = H_L + H_D + H_T$:

$$H_L = \sum_{\alpha k \sigma} \epsilon_{\alpha k} c^\dagger_{\alpha k \sigma} c_{\alpha k \sigma}$$

$$H_D = \sum_{\sigma} \epsilon_d d^\dagger_\sigma d_\sigma + H_{\text{int}}$$

$$H_T = \frac{1}{\sqrt{\Omega}} \sum_{\alpha k \sigma} t_{\alpha k} \left(c^\dagger_{\alpha k \sigma} d_\sigma + \text{h.c.} \right)$$

Quantum dot

Lead -1

Lead 1

The out-of-equilibrium situation is produced by **bias voltage**: $\Phi = \mu_1 - \mu_{-1}$

General question:

Out of equilibrium quantum problems difficult to solve?

S-matrix formulation :"Vacuum" at time $-\infty$ and $+\infty$

Interaction switched on and off adiabatically

Idea is that vacuum of the system does not evolve with
Time but just acquires a phase due to interaction events

$$iG(\mathbf{x},t;\mathbf{x}',t') = \frac{\langle \Phi_0 | T[S(\infty,-\infty)\hat{\psi}(\mathbf{x},t)\hat{\psi}^\dagger(\mathbf{x}',t')] | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty,-\infty) | \Phi_0 \rangle}$$

$$|\Phi(\infty)\rangle_I = S(\infty,-\infty)|\Phi(-\infty)\rangle_I$$

<u>Reality of nonequilibrium quantum problems:</u>

1. Vacuum not really known at all times
2. Interaction term is often important at all times
3. Interaction often not switched on and off adiabatically
4. Particle and Current production, dissipation, decoherence

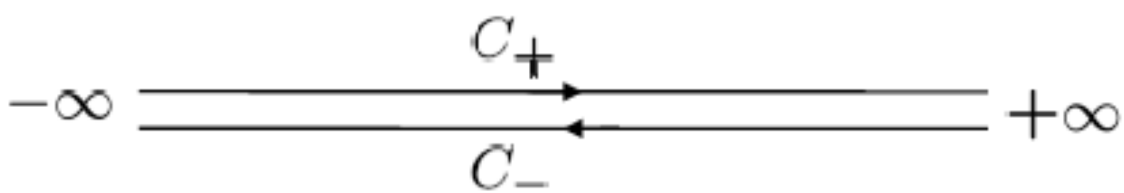
Schwinger (1961)
Keldysh (1964)

Example: Nonequilibrium Transport through a small cavity
Meir-Wingreen Formula (see later)

$$iG_{\Phi}(\mathrm{x},\tau;\mathrm{x}',\tau') = \langle \Phi(-\infty)|_I T_c[\mathcal{S}_c(-\infty,-\infty)\hat{\psi}(\mathrm{x},\tau)\hat{\psi}^{\dagger}(\mathrm{x}',\tau')]|\Phi(-\infty)\rangle_I$$

where the contour S-matrix is

$$\mathcal{S}_c(-\infty,-\infty) \equiv T_c \exp\left(-i \oint_C d\tau_1\, \hat{H}'(\tau_1)\right)$$



Schwinger-Keldysh contour

Other View:

Suppose we reach the steady state: stationary current

<u>IDEA BY S. HERSHFIELD (1993)</u>

Steady-state density matrix can be reformulated as usual Boltzmann form (papers by N. Andrei-Doyon; Schiller-Hershfield;…)

$$\boxed{\rho = \exp\left[-\beta(H - Y)\right]}$$

Y is the so-called BIAS OPERATOR

Quantum Mechanics view

$$Y = \frac{1}{\beta} \ln \rho + H$$

The Y operator can be written in terms of the **Lippmann-Schwinger operators**

$$H = \sum_{\alpha k} \epsilon_{\alpha k} \psi^{\dagger}_{\alpha k \sigma} \psi_{\alpha k \sigma}$$

Where: $$\psi^{\dagger}_{\alpha k \sigma} = c^{\dagger}_{\alpha k \sigma} + \frac{1}{\epsilon_{\alpha k} - \mathcal{L} + i\eta} \mathcal{L}_T c^{\dagger}_{\alpha k \sigma}$$

Liouvillians are defined as: $\mathcal{L}\mathcal{O} = [H, \mathcal{O}]$, $\mathcal{L}_T \mathcal{O} = [H_T, \mathcal{O}]$ and $\mathcal{L}_Y \mathcal{O} = [Y, \mathcal{O}]$

Hershfield showed that the Y operator has the general form

$$Y = \frac{\Phi}{2} \sum_{\alpha k \sigma} \alpha \psi^{\dagger}_{\alpha k \sigma} \psi_{\alpha k \sigma}.$$

We want to compute observables

P. Dutt, J. Koch, J. E. Han, KLH Annals of Physics **326**, 2963-99 (2011)

$$I = \frac{I_1 + I_{-1}}{2} = -\frac{e}{2}\left\langle \frac{d\left(N_1(t) - N_{-1}(t)\right)}{dt} \right\rangle$$

$$= i\frac{e}{2}\sum_{\alpha} \alpha \left\langle [N_\alpha(t), H] \right\rangle = i \sum_{\alpha k \sigma} \alpha \frac{e t_{\alpha k}}{2\sqrt{\Omega}} \left\langle \left(c^\dagger_{\alpha k \sigma} d_\sigma - d^\dagger_\sigma c_{\alpha k \sigma} \right) \right\rangle$$

$$= \mathrm{Im}\left[\sum_{\alpha k \sigma} \alpha \frac{e t_{\alpha k}}{\sqrt{\Omega}} \mathcal{G}_{c_{\alpha k \sigma} d^\dagger_\sigma}(\tau = 0) \right],$$

$$I = 2e \frac{\Gamma_1 \Gamma_{-1}}{\Gamma_1 + \Gamma_{-1}} \int d\epsilon_k A_d(\epsilon_k) \left[f\left(\epsilon_k + \frac{\Phi}{2}\right) - f\left(\epsilon_k - \frac{\Phi}{2}\right) \right]$$

Here,

$$A_d(\epsilon_k) = -\frac{1}{\pi} \sum_\sigma \mathrm{Im}\left[G^{\mathrm{ret}}_{d_\sigma d^\dagger_\sigma}(\epsilon_k) \right]$$

Formula also
obtained with Keldysh, Meir-Wingreen (1992)

$$\Gamma_\alpha = \pi t_\alpha^2 \nu$$

U=0 Quantum Mechanics

Resonant Level Model

$$\psi^{(0)\dagger}_{\alpha k\sigma} = c^{\dagger}_{\alpha k\sigma} + \frac{t}{\sqrt{\Omega}} g_d(\epsilon_k) d^{\dagger}_{\sigma} + \frac{t^2}{\Omega} \sum_{\alpha' k'} \frac{g_d(\epsilon_k)}{\epsilon_k - \epsilon_{k'} + i\eta} c^{\dagger}_{\alpha' k' \sigma}$$

$$g_d(\epsilon_k) = \frac{1}{\epsilon_k - \epsilon_d + i\Gamma} \qquad d^{\dagger}_{\sigma} = \frac{t}{\sqrt{\Omega}} \sum_{\alpha k} g^{*}_{d}(\epsilon_k) \psi^{(0)\dagger}_{\alpha k \sigma}$$

Key point, use Ψ−basis: $\mathcal{G}_{\psi^{(0)}_{\alpha' k' \sigma'}, \psi^{(0)\dagger}_{\alpha k \sigma}}(i\omega_n) = -\frac{e^{i\omega_n 0^+}}{-i\omega_n + \epsilon_k - \alpha\frac{\Phi}{2}} \delta_{\sigma\sigma'} \delta_{\alpha\alpha'} \delta_{kk'}.$

Linear relation between d and Ψ

$$I = \frac{e\Gamma^2}{\pi} \int_{-\infty}^{\infty} \frac{1}{(\epsilon - \epsilon_d)^2 + \Gamma^2} \left[f\left(\epsilon + \frac{\Phi}{2}\right) - f\left(\epsilon - \frac{\Phi}{2}\right) \right] d\epsilon$$

Double barrier problem at resonance (**no interaction**)

At T=0, Landauer-Buettiker formula: I varies linearly with bias in the linear regime

Large Bias, the current saturates (phase space argument)

Concrete Implementation:

P. Dutt, J. Koch, J. E. Han, KLH Annals of Physics **326**, 2963-99 (2011)

Anderson model, 1961:

$$H_{\text{int}} = \frac{U}{2}\hat{n}_d\left(\hat{n}_d - 1\right) = \frac{U}{2}\sum_{\sigma} d^{\dagger}_{\sigma} d^{\dagger}_{-\sigma} d_{-\sigma} d_{\sigma}$$

The Lippmann-Schwinger scattering states are simple for U=0 (no interaction)

NRG approach in the scattering state basis
F. B. Anders PRL 2008

In the presence of interactions, scattering states are complicated (not single-body like)

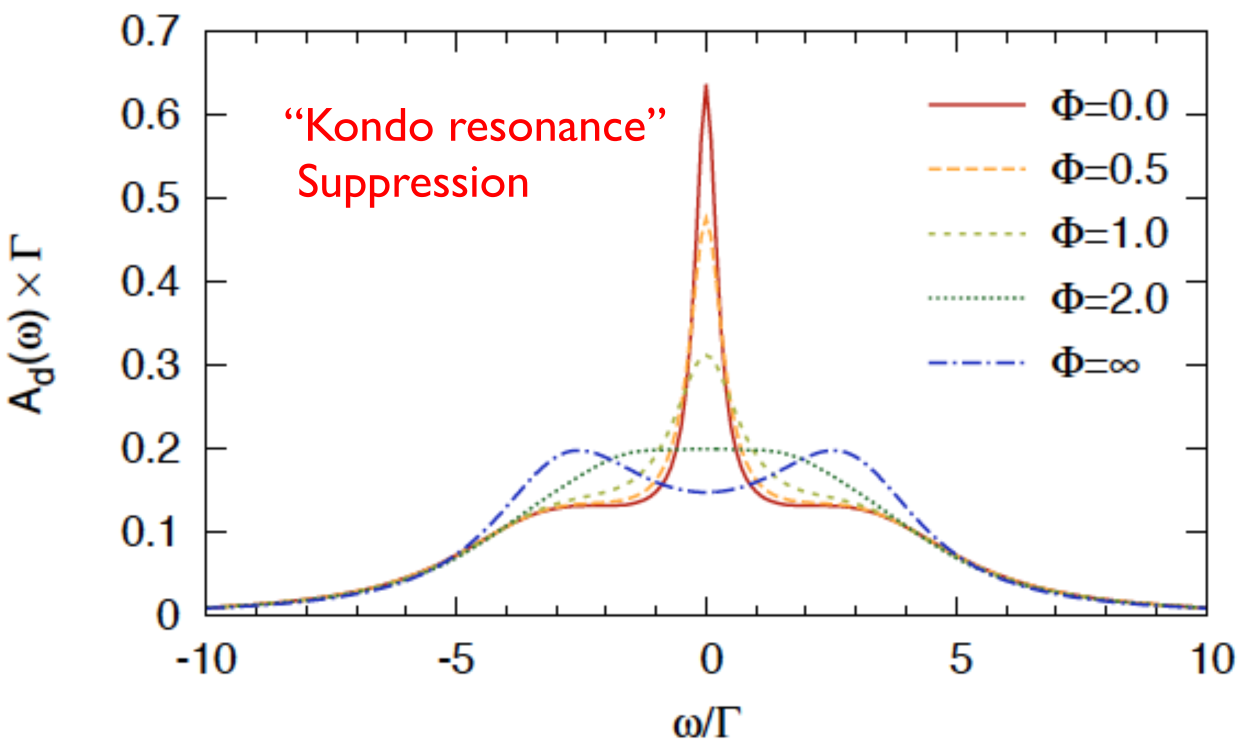
Next, we present results from a perturbation theory in the basis of scattering states

Numerical implementation:
collaboration with L. Messio and O. Parcollet

Possibility to implement this in the Coqblin-Schrieffer model

Results for all biases

Born approximation: self-energy computed to second order in U



Dephasing:

Kaminski, Nazarov & Glazman

Rosch, Kroha, Woelfle

Fig. 3. Spectral function (obtained using the Born approximation) for different values of the bias voltage for $U/(\pi\Gamma) = 2$, where we set $\Gamma = 1$. The limits $\Phi/\Gamma \to 0$ and $\Phi/\Gamma \to \infty$ agree with the results obtained via the Schwinger-Keldysh scheme [66,67].

Oguri

Main Results…

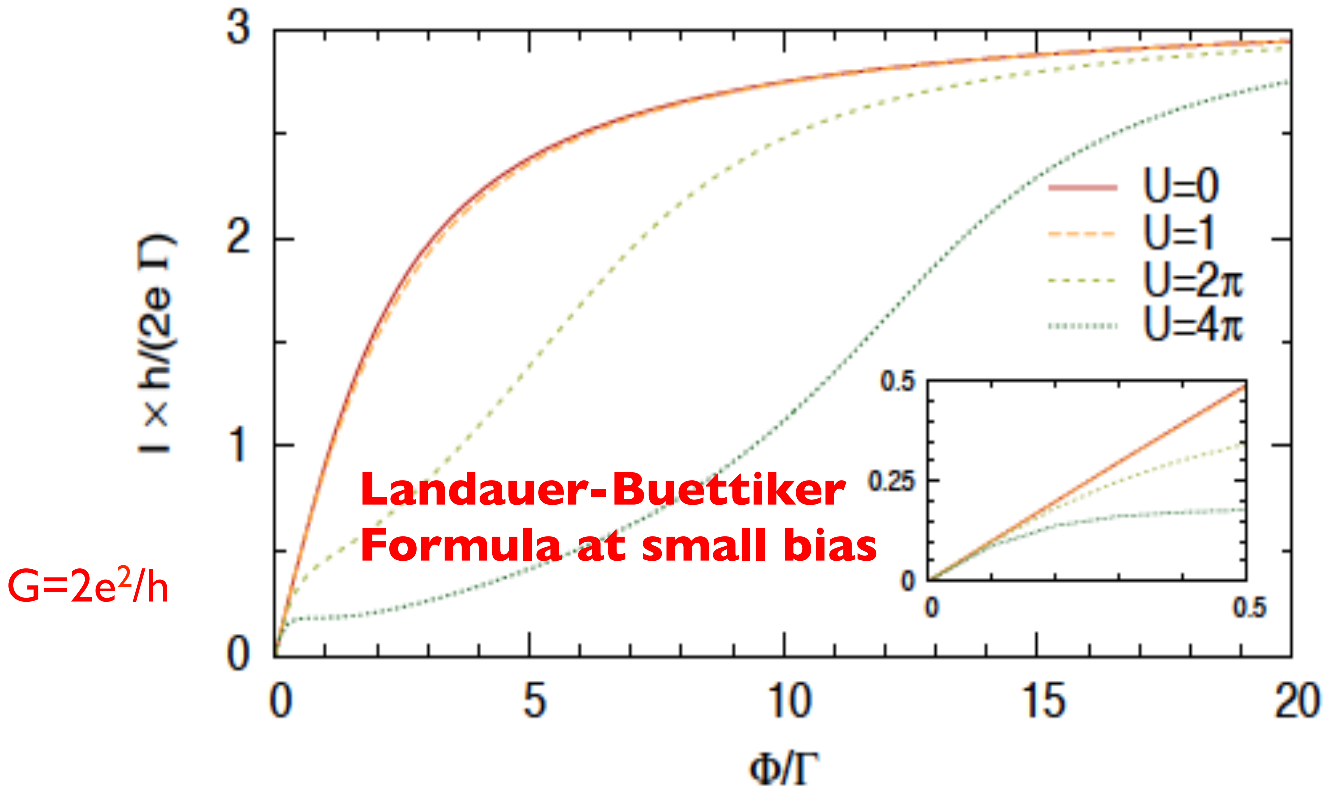


Fig. 6. The current-voltage curves for the Anderson model for $U/\Gamma = 0.0, 1.0, 2\pi$ and 4π, where $\Gamma = 1$. The inset shows the behavior of the curves for low bias. In the limit $\Phi \to 0$ the slope of the curves tend to 1, which corresponds to the value of the conductance quantum.

Zeeman splitting

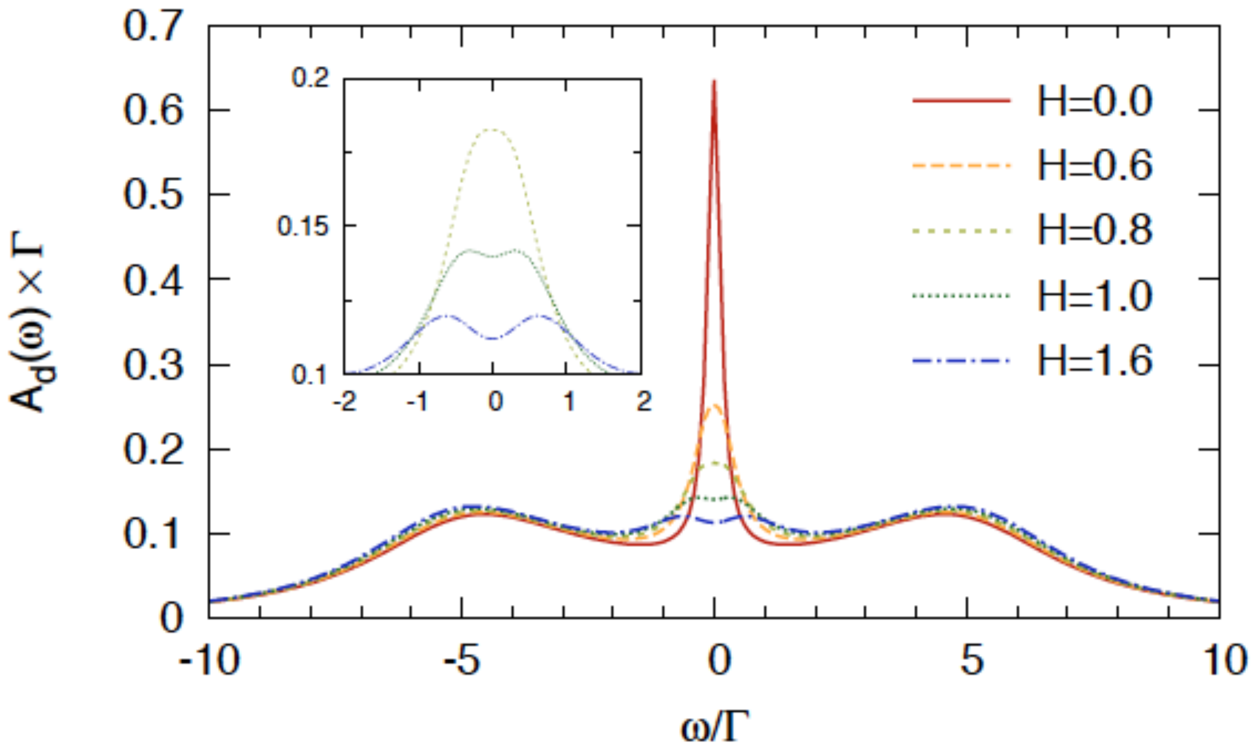


Fig. 5. Variation of the spectral function with an applied magnetic field (H), obtained using the second-order self-energy. Here $\Gamma = 1$, $\Phi = 0$, $U = 3\pi$ and H is given in the units defined by $g\mu_b$, where g is the g-factor and μ_b denotes the Bohr magneton. The inset shows the behavior of the Abriksov-Suhl resonance as a function of the magnetic field, for $H = 0.8$, 1.0 and 1.6.

Comparison with other methods & experiments

To second order in U, our results are valid for **all** bias voltages: they agree with the Schwinger-Keldysh results for **small** and **very large** biases (A. Oguri)

They are also in qualitative agreement with NRG in scattering state basis (F. Anders)

NOTE: Schwinger-Keldysh computation to fourth order observe a splitting of the Abrikosov-Suhl resonance, that is not obtained to second order (Fuji-Ueda, 2005)

Other methods do not see the splitting of the Kondo resonance,
Diagrammatic MC in Keldysh scheme: P. Werner, T. Oka and A. J. Millis, 2009-2010
M. Schiro & M. Fabrizio, 2008
T. Schmidt, Muehlbacher, Urban and Komnik 2011
Scattering states and QMC, with Matsubara voltage: J. Han (2010) & T. Pruschke (2012)

Experiments: for example, R. Leturcq et al. PRL 95, 126603 (2005)
Experimental groups: Harvard, Stanford, Duke, Orsay, CEA Saclay, Grenoble, ENS,, ETH

Thermal Transport Experiments

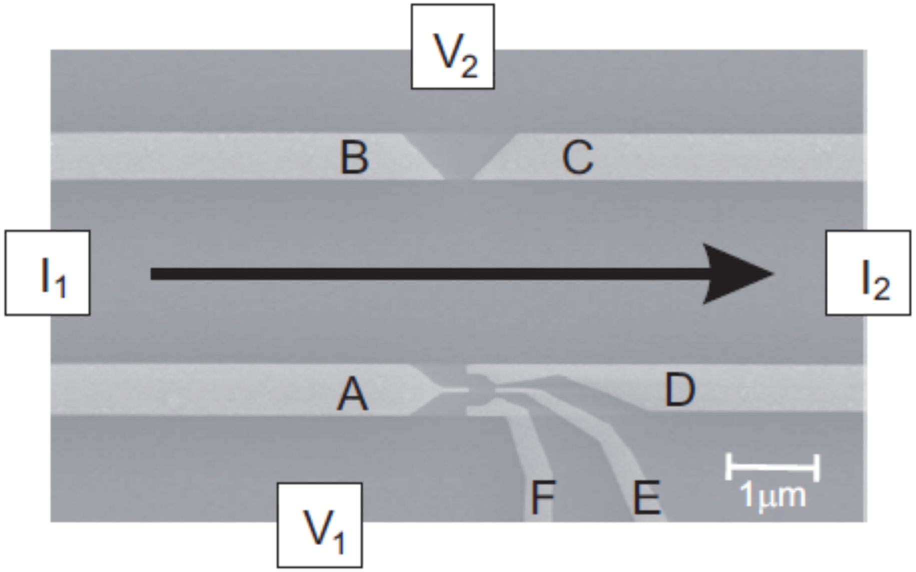
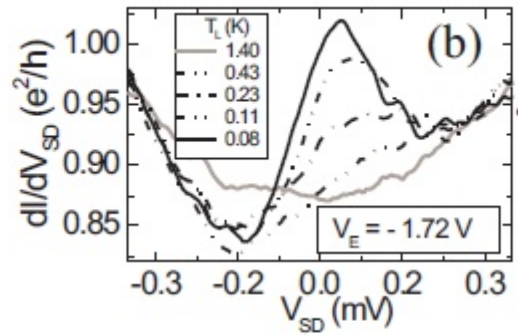


FIG. 1: SEM photograph of the quantum dot and the central part of the 20 μm long heating channel. The labels $V_{1,2}$ and $I_{1,2}$ indicate the 2DEG areas with ohmic contacts.



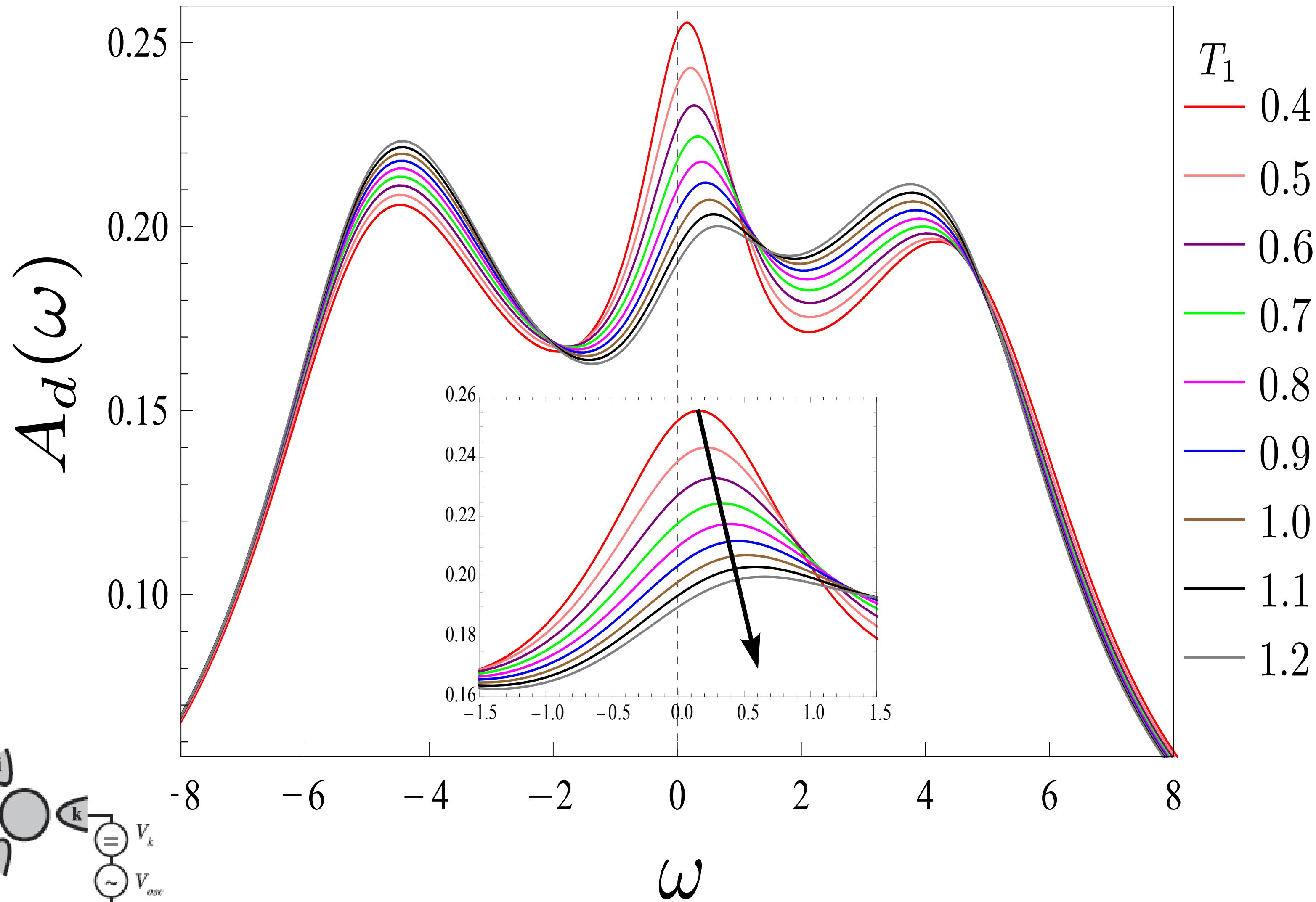
Breaking of particle-hole symmetry!
Combination of bias voltage and Temperature gradients

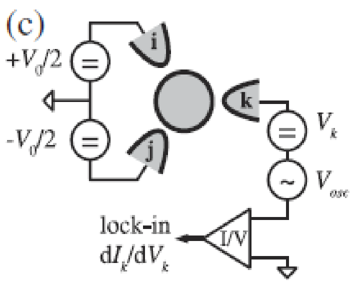
R.Scheibner, *et. al.*, Phys. Rev. Lett. **95**, 176602 (2005)

Nano-Engines: M. Buettiker, R. Lopez, D. Sanchez, Ph. Jacquod, many other references
Thermoelectric transport: V. Zlatic, T. Costi, A. Hewson, S. Kirchner, other works

Cold atoms: C. Grenier, C. Kollath and A. Georges (2012); J.-P. Brantut et al. 1306.5754

Thermoelectric Effects





P. Dutt and K. Le Hur, arXiv:1306.0840

Differential Conductance

$$\Delta = \epsilon_d + U/2$$

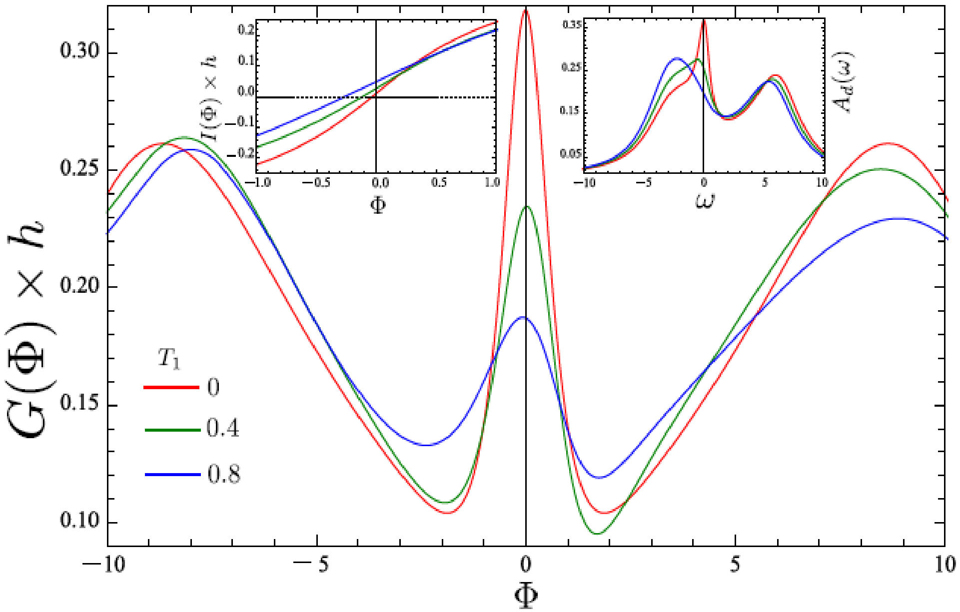


Figure 3.2.: Effect of ΔT on the differential conductance when $\Delta = 0.4$. We have used the units $\Gamma = 1$ and taken $U = 3\pi$. The inset on right shows the corresponding spectral function when $\Phi = 0$ and the current in the neighborhood of zero-bias is shown in the left inset.

P. Dutt and K. Le Hur, arXiv 1306.0840 (2013)

In principle, this formalism can also be applied to …

Hubbard model with electric fields or tilted lattices:
See for example Ph. Werner; C. Aron & C. Weber, G. Kotliar; Amaricci, Weber, Capone, Kotliar … see also work by Jong E. Han

DMFT: A. Georges, G. Kotliar, W. Krauth, M. Rozenberg RMP 1996
Non-equilibrium development: N. Tsuji et al. arXiv:1307.5946

This formalism can be easily applied in the case of "hybrid" systems

Example of Hybrid Systems
Anderson-Holstein model, where level coupled to "photon" mode
Experiments at LPA ENS, LPN Marcoussis, Princeton, ETH
M. Schiro & KLH, in preparation

Coupling a Microwave Resonator to Quantum Dot(s)+Leads

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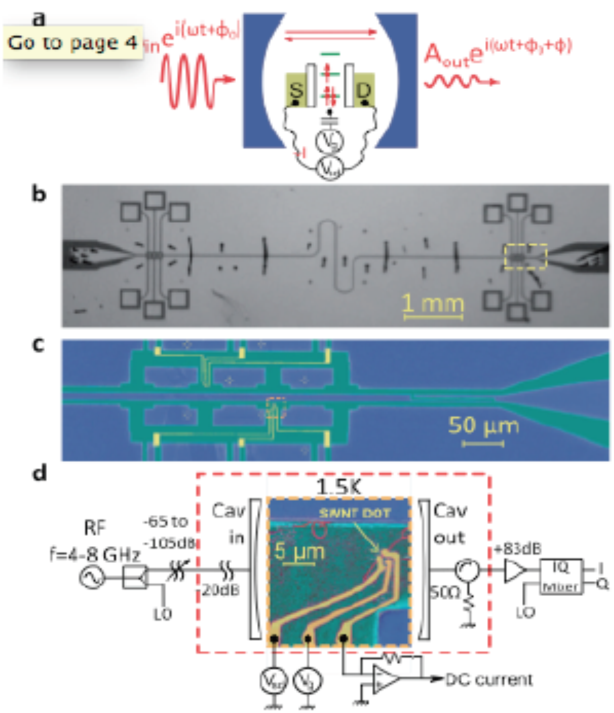
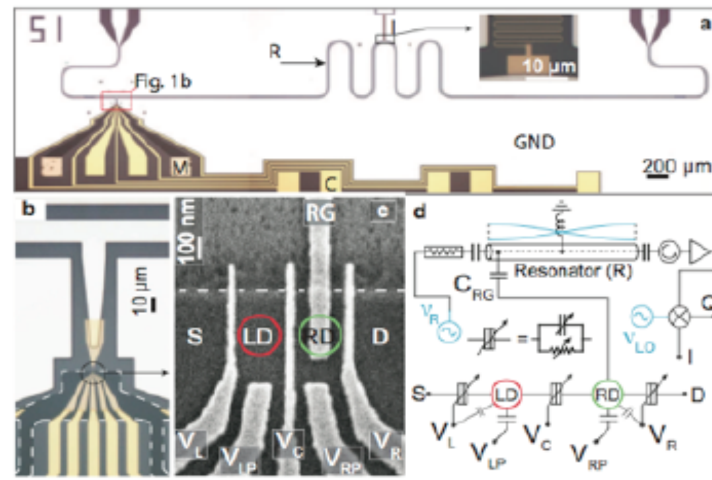




- M. Delbeq et al PRL **107** 256804 (2011) (ENS-Paris, T. Kontos Lab)
- T. Frey et al PRL **107** 256804 (2011) (ETH-Zurich, A. Wallraff Lab)

☑ <u>Similar</u> setup in Jason Petta experiment (Princeton)

« hybrid » experiments at LPN Marcoussis: A. Dousse et al. PRL 2008 & 2009

Phase Spectroscopy of a Resonator coupled to Dot+Leads

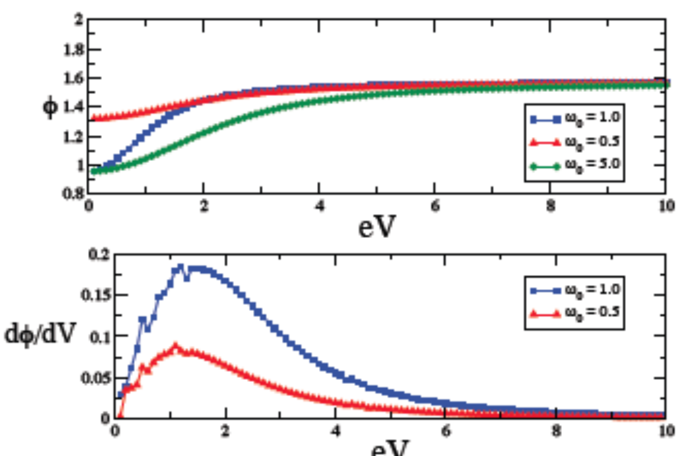
☑ Input-Output Relations

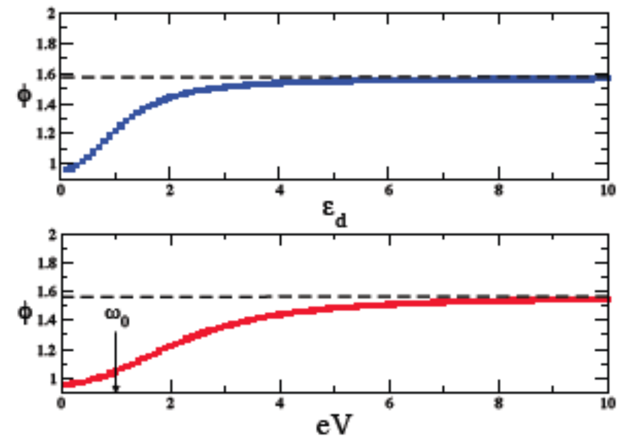
$$r(\omega) = \frac{\langle V_L^{out}(\omega)\rangle}{\langle V_L^{in}(\omega)\rangle} = 1 - 2i\, J_L(\omega)\, \chi_{xx}(\omega)$$

$$tan\,\varphi(\omega) = -\frac{2J_L(\omega)\,\chi^R_{xx}(\omega)}{1 - 2J_L(\omega)\,\chi^I_{xx}(\omega)}$$

Photon Propagator
(knows about electrons)

☑ U=0 (Holstein Model)





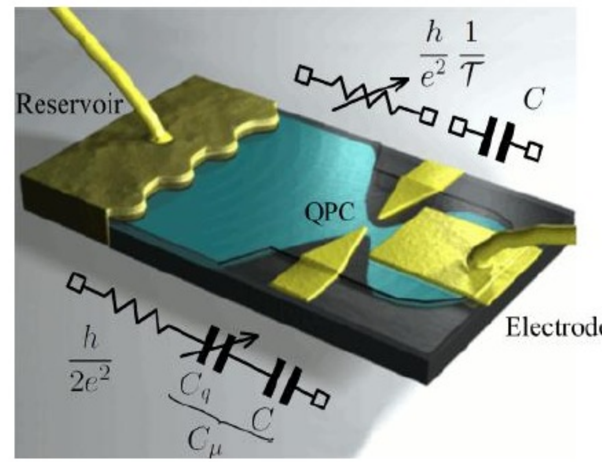
☑ Inelastic Features as the bias hits the photon frequency $eV \sim \omega_0$

Note 1: Charge Dynamics

$$\frac{Q(\omega)}{V_g(\omega)} = C_0(1 + i\omega C_0 R_q) + \mathcal{O}(\omega^2)$$

M. Buettiker, H. Thomas, and A. Pretre, Phys. Lett. A 180, 364 - 369,(1993)
J. Gabelli *et al.*, Science **313**, 499 (2006)
J. Gabelli, G. Feve, J.-M. Berroir, B. Placais, Rep. Progress 2012

$$R_q = \frac{h}{2e^2}$$



Interactions?

Mesoscopic crossover

C. Mora and K. Le Hur, Nature Phys. 6, 697 (2010)

Small Dot $R_q = \dfrac{h}{2e^2}$ $\Delta \gg \hbar\omega$

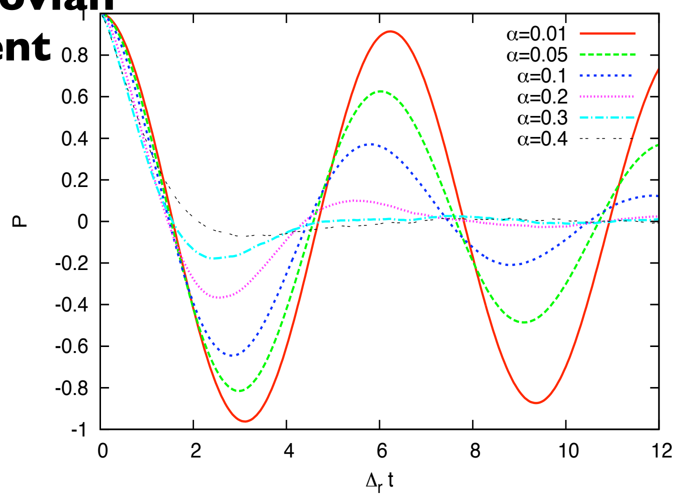
Metallic limit $R_q = \dfrac{h}{e^2}$ $\Delta \ll \hbar\omega$

Recent papers M. Filippone, KLH, C. Mora 2011, 2013; P. Dutt, T. Schmidt, C. Mora and KLH 2013
Y. Hamamoto, T. Jonckheere, T. Kato, T. Martin Phys. Rev. B **81**, (2010) 153305
Y. Etzioni, B. Horovitz and P. Le Doussal, Phys. Rev. Lett. **106**, 166803 (2011)

NOTE 2: P. Orth, A. Imambekov, K. Le Hur (stochastic) (2010, 2012)
Work at CPHT with Loic Henriet and Zoran Ristivojevic
P. Orth, D. Roosen, W. Hofstetter and K. Le Hur (t-dependent NRG, 2010)
R. Bulla, T. Costi, T. Pruschke, Rev. Mod. Phys. 80, 395 (2008)

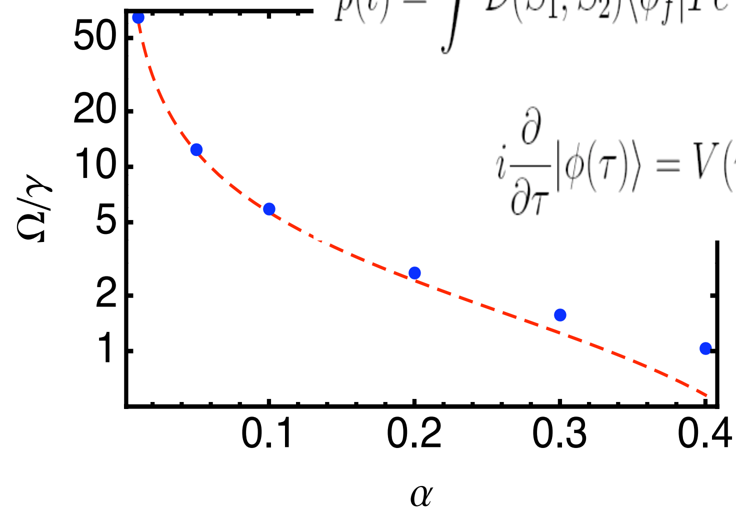
Non-Markovian environment

Rabi oscillations

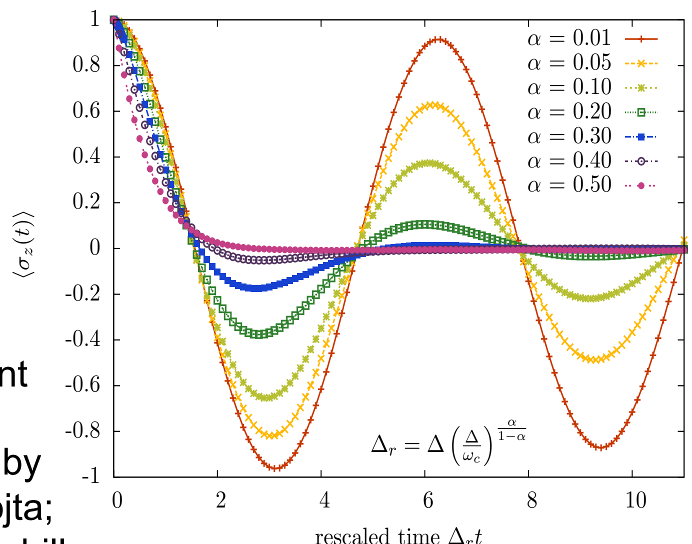


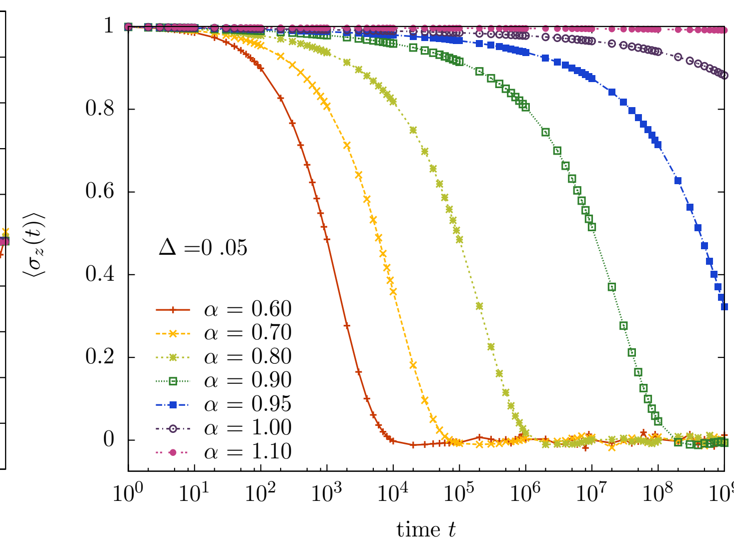
$$p(t) = \int \mathcal{D}(S_1, S_2)\langle \phi_f | T e^{-i\int_0^t dt' V(t')dt'} | \phi_i \rangle$$

$$i\frac{\partial}{\partial \tau}|\phi(\tau)\rangle = V(\tau)|\phi(\tau)\rangle$$



Time-dependent NRG
See also work by R. Bulla; M. Vojta; F. Anders; A. Schiller…





Way it works…

First, it is possible to expand the scattering state operators to the lth power in H_{int}

$$\mathcal{L}'\mathcal{O} = [H - H_{\text{int}}, \mathcal{O}] \text{ and } \mathcal{L}_I\mathcal{O} = [H_{\text{int}}, \mathcal{O}]$$

$$\psi^{\dagger}_{\alpha k\sigma} = \psi^{(0)\dagger}_{\alpha k\sigma} + \frac{t^2}{\Omega}\sum_{l=1}^{\infty}\left[\frac{1}{\epsilon_k - \mathcal{L}' + i\eta}\mathcal{L}_I\right]^l \sum_{\alpha' k'} \frac{g_d^*(\epsilon_{\alpha' k'})}{\epsilon_k - \epsilon_{k'} + i\eta}\psi^{(0)\dagger}_{\alpha' k'\sigma}.$$

This can be expressed symbolically as

$$\boxed{\psi^{\dagger}_{\alpha k\sigma} \equiv \sum_{l=0}^{\infty} \psi^{\dagger(l)}_{\alpha k\sigma},}$$

Then, expand density matrix to a given order in H_{int}

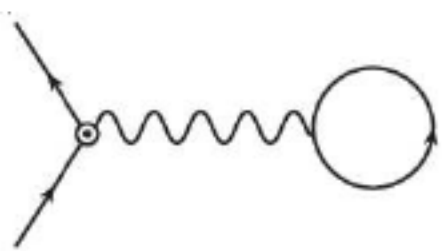
$$\boxed{\mathcal{H}^{(m)} = \left[\sum_{\alpha k\sigma}\left(\epsilon_k - \alpha\frac{\Phi}{2}\right)\sum_{p=0}^{m}\psi^{\dagger(p)}_{\alpha k\sigma}\psi^{(m-p)}_{\alpha k\sigma}\right]}$$

Current computation

$$\mathcal{H}^{(1)} = \sum_{\alpha k\sigma}\left(\epsilon_k - \frac{\alpha\Phi}{2}\right)\left[\psi^{\dagger(1)}_{\alpha k\sigma}\psi^{(0)}_{\alpha k\sigma} + \psi^{(0)\dagger}_{\alpha k\sigma}\psi^{(1)}_{\alpha k\sigma}\right]$$
$$= \sum_{121'2'\sigma}\left(12\left|\mathcal{V}\right|1'2'\right)\psi^{(0)\dagger}_{1\sigma}\psi^{(0)\dagger}_{2-\sigma}\psi^{(0)}_{2'-\sigma}\psi^{(0)}_{1'\sigma},$$

First order in U

Typical (Hartree) Diagram:



$$I^{(1)} = -\frac{et^2}{\Omega}\frac{1}{\beta}\,\mathrm{Im}\left[\sum_{11'\omega_n}\alpha g_{1'}\mathcal{G}^{(1)}_{\psi^{(0)}_{1'\sigma}\psi^{(0)\dagger}_{1\sigma}}(i\omega_n)\right]$$
$$= Un_d^{(0)}\left[\frac{e\Gamma^2}{\pi}\int d\epsilon_1\frac{(\epsilon_1-\epsilon_d)\left[f\left(\epsilon_1-\frac{\Phi}{2}\right)-f\left(\epsilon_1+\frac{\Phi}{2}\right)\right]}{\left[(\epsilon_1-\epsilon_d)^2+\Gamma^2\right]\left[(\epsilon_1-\epsilon_d)^2+\Gamma^2\right]}\right]$$

In agreement with mean-field theory results (developed to first order in U)!

First order result just shifts the position of the particle-hole symmetric point

Mean-Field argument

Shift of the level position:

$$H_D^{\mathrm{MF}} = \sum_\sigma (\epsilon_d + U\langle \hat{n}_{-\sigma}\rangle)\, d_\sigma^\dagger d_\sigma$$

$$I = \frac{e\Gamma^2}{2\pi} \sum_\sigma \int_{-\infty}^{\infty} \frac{1}{(\epsilon - \epsilon_d - U\langle \hat{n}_{-\sigma}\rangle)^2 + \Gamma^2} \left[f\left(\epsilon + \frac{\Phi}{2}\right) - f\left(\epsilon - \frac{\Phi}{2}\right)\right] d\epsilon$$

$$\langle \hat{n}_\sigma \rangle = \frac{\Gamma}{2\pi} \int_{-\infty}^{\infty} \frac{1}{(\epsilon - \epsilon_d - U\langle \hat{n}_{-\sigma}\rangle)^2 + \Gamma^2} \left[f\left(\epsilon + \frac{\Phi}{2}\right) + f\left(\epsilon - \frac{\Phi}{2}\right)\right] d\epsilon.$$

One observes that the condition for particle-hole symmetry, *i.e.*, $\langle \hat{n}_\sigma \rangle = 1/2$ is realized for $\epsilon_d = -U/2$, as confirmed by first order in perturbation theory.

Dynamics around p-h symmetric point

Self-energy computed to second order in U for all bias voltages
Expanding our results to second order in the bias voltage agrees with **Fermi liquid regime (Nozieres 1974) - T. A. Costi, A. Hewson, V. Zlatic**

$$A_d^{(2)}(\omega) = \frac{2}{\pi\Gamma}\Bigg[1 - \left\{1 + \left(\frac{13}{2} - \frac{\pi^2}{2}\right)\left(\frac{U}{\pi\Gamma}\right)^2\right\}\left(\frac{\omega}{\Gamma}\right)^2 - \frac{1}{2}\left(\frac{U}{\pi\Gamma}\right)^2\left(\frac{\pi T}{\Gamma}\right)^2 - \frac{3}{8}\left(\frac{U}{\pi\Gamma}\right)^2\left(\frac{\Phi}{\Gamma}\right)^2 + \ldots\Bigg],$$

and similarly

$$G^{(2)} = G_0\Bigg[1 - \left\{\frac{1}{3} + \frac{16-\pi^2}{6}\left(\frac{U}{\pi\Gamma}\right)^2\right\}\left(\frac{\pi T}{\Gamma}\right)^2 - \left\{\frac{1}{4} + \frac{22-\pi^2}{8}\left(\frac{U}{\pi\Gamma}\right)^2\right\}\left(\frac{\Phi}{\Gamma}\right)^2 \ldots\Bigg].$$

This result agrees with known results
for Anderson model at/close to equilibrium