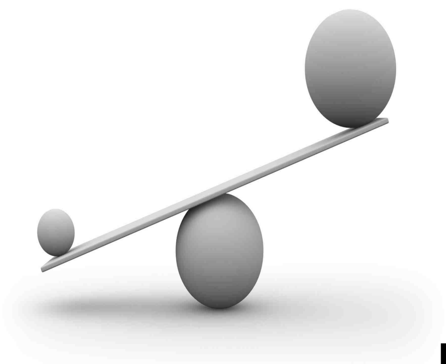
# Effective Equilibrium Description Of Non-Equilibrium Transport

Les Houches, August 2012

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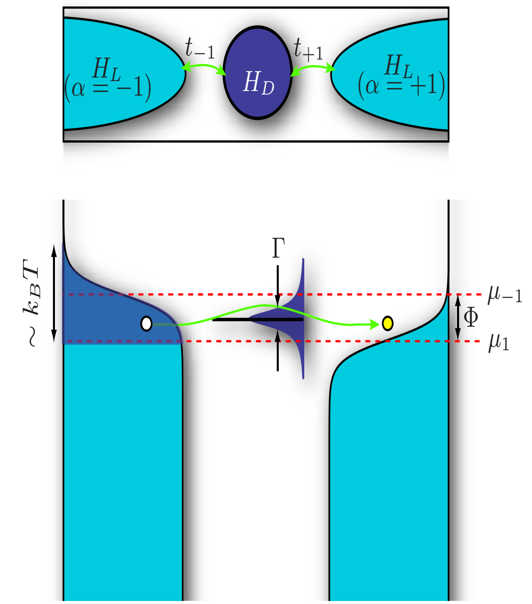
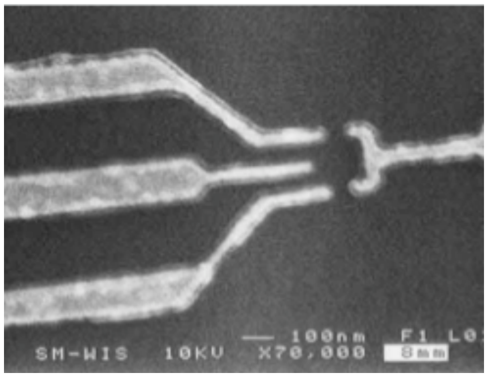
Prasenjit Dutt, Yale (**PhD thesis**)
Jens Koch, Northwestern University
Jong Han, Buffalo University



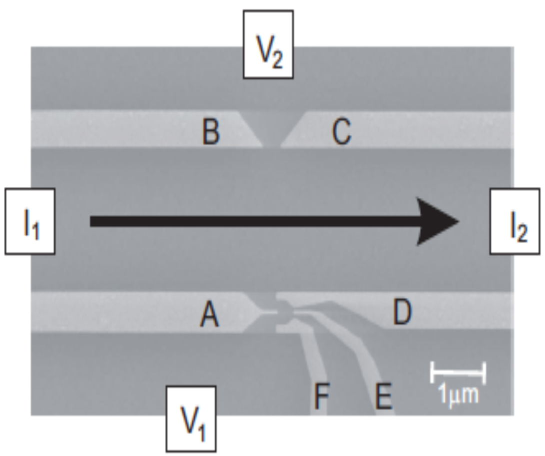
Review: Annals of Physics **326**, 2963-99 (2011)

# Transport in Nano-Matter: QPCs, dots and quantum wires

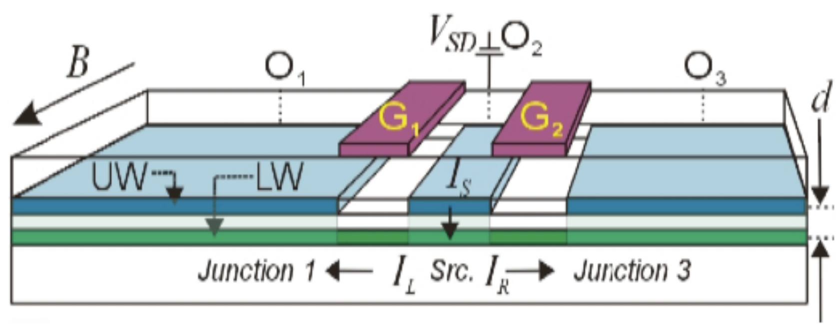



Quantum impurity models: **courses** H. Saleur, N. Andrei
Transport: **current** and **noise** commonly accessible

Noise in strong correlation regime: T. Delattre et al. (2009)
Y. Yamauchi et al. (2011); News and Views: R. Egger
Theory: C. Mora, P. Vitushinsky, X. Leyronas, A. Clerk & KLH




**Thermopower:**
L. Molenkamp et al (2005)

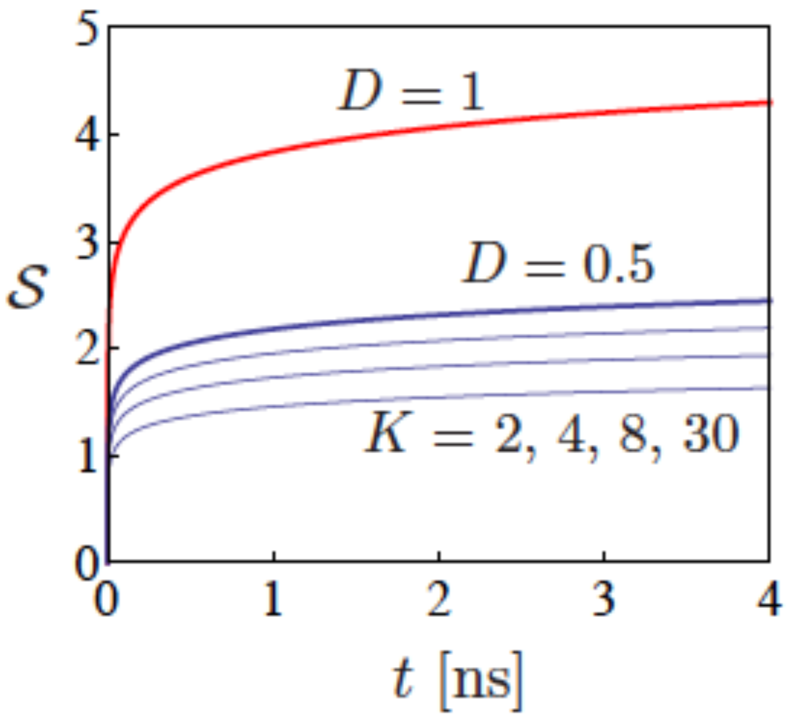



Low-D Luttinger liquids and Beyond: A. Yacoby (Harvard)

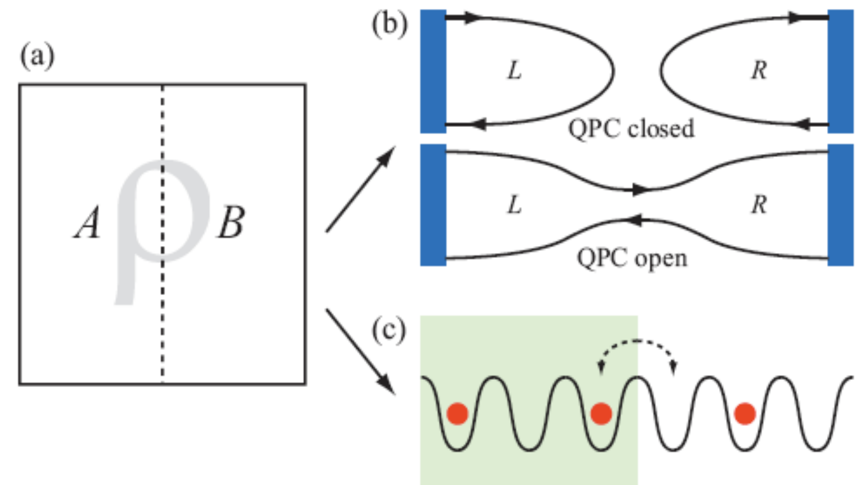
# Noise & Entanglement Entropy

QPC to perform a quantum quench:

Klich-Levitov, Gaussian case D=1: 2009
H. F. Song, S. Rachel, C. Flindt, N. Laflorencie
I. Klich & KLH, 2012 (general case)




D = transparency of the barrier




D=1: Results from CFT (Klich-Levitov): entropy grows logarithmically with time
D=0.5: Higher cumulants matter, but the entropy maintains its logarithmic growth
**noise: Lower bound on the full entanglement entropy**

See C. Glattli's course

# General question:

**Out of equilibrium quantum problems difficult to solve?**

S-matrix formulation :"Vacuum" at time -∞ and +∞

**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

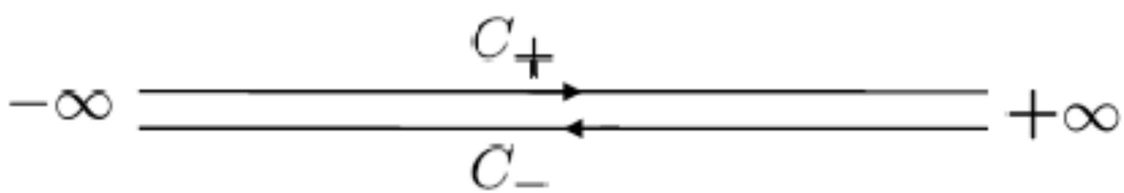
# Schwinger (1961)
# Keldysh (1964)

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

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

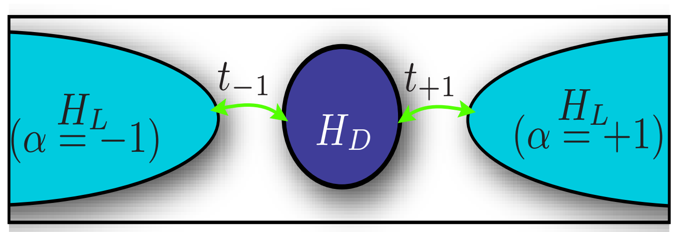
where the contour $S$-matrix is

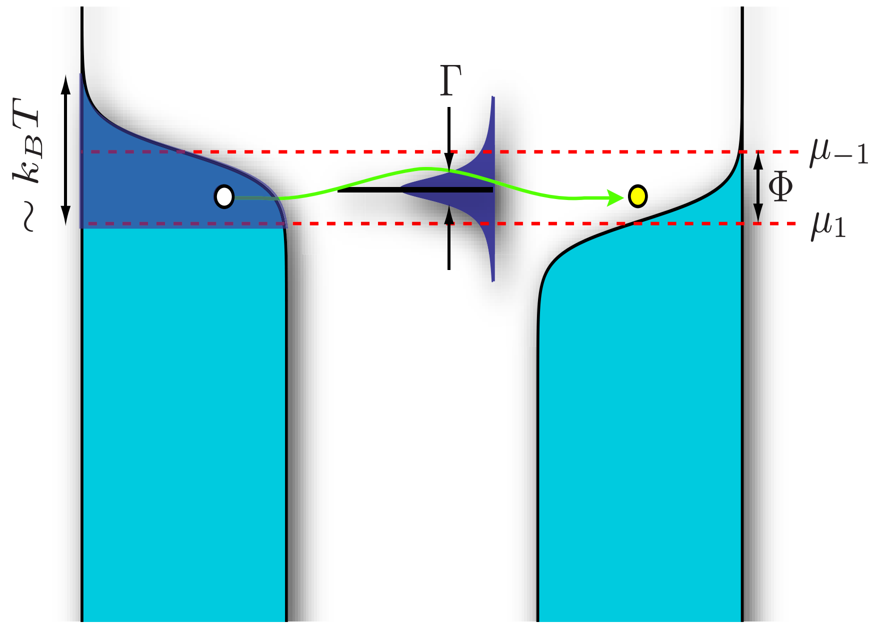
$$\mathcal{S}_c(-\infty,-\infty) \equiv T_c \exp\left(-i \oint_C d\tau_1\, \hat{H}'(\tau_1)\right)$$




**Schwinger-Keldysh contour**

# Typical Setup out of equilibrium:




## OUTLINE, Course:

Define notion of Steady State

Introduce Hershfield equilibium view
Show Equivalence with Schwinger-Keldysh
for current computation

Application:
Resonant level model
Anderson model

Comparisons with other methods
and experiments

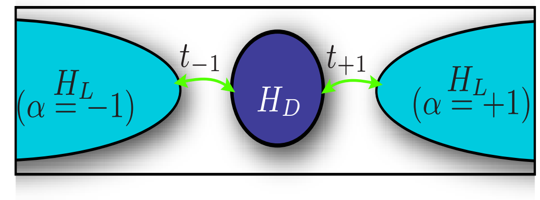
# Generic Nano-System

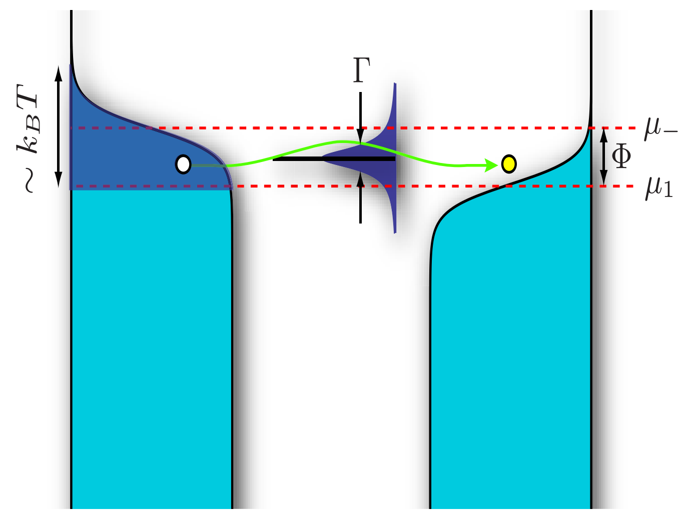
Let us start with a **quantum impurity** problem $H = H_L + H_D + H_T$:

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

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

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




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

# Notion of Steady State

Typically, steady state is reached after short times in the leads (relaxation mechanisms)

To avoid microscopic relaxation mechanisms, one can also resort to **open system Doyon and Andrei (2006)** and **Mehta-Andrei**

**Initially:** time $t_0$, electron leads and dot are totally decoupled $H_0=(H_L+H_D)$

Tunneling term **switched on adiabatically** at negative time t,

$$H = H_0 + H_T e^{\eta t}\theta(t - t_0)$$

Observables can be evaluated **at time t=0**, where $H_T$ has reached its full strength

$$\boxed{v_F/L \ll |t_0|^{-1} \ll \eta}$$

Infinite Leads ($L \rightarrow +\infty$): Hot particle escapes to infinity (and is not reflected back)

# Switching on tunneling

Exact Protocol not important, but the process needs to be adiabatic:
Irreversibility of the turning on process ($H_T$ needs to be treated **exactly**)

On the other hand, the way of switching on interactions does not matter and can be done in a non-adiabatic manner
**Interactions can be then treated perturbatively**

**IDEA BY S. HERSHFIELD (1993)**

**Steady-state density matrix can be reformulated as usual Boltzmann form** (see also papers by A. Oguri; J. Han; Doyon-Andrei)

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

Y is the so-called BIAS OPERATOR

# What is the Y-bias operator?

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

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

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

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

# How to show this?

For a pedestrian derivation of Hershfield's proof (1993), without relaxation mechanisms,
See Appendix A and B of : Annals of Physics **326**, 2963-99 (2011)

**Goals:**
Show that the density matrix of the system in the interaction representation at time t=0
is equivalent to the Hershfield's density matrix for all orders in $H_T$

Show that it is also true for any observable

There is a non-trivial step in the proof: One must use the open system limit (**Doyon-Andrei**)
and the **factorization** of correlation functions at long times (see Eq. B11)

**Question:** Is this "factorization" always rigorous ?
For electron leads, described by a Fermi liquid theory, at T=0, correlation functions decay
as power laws and not exponential decays

# Another proof for current (for any T)

Based on **imaginary time** formulation (similar to finite-T field theory)

In imaginary-time, we define the propagation of an operator by

$$\mathcal{O}(\tau) = e^{\tau(H-Y)}\mathcal{O}e^{-\tau(H-Y)} = e^{\tau(\mathcal{L}-\mathcal{L}_Y)}\mathcal{O}.$$

The nonequilibrium thermal Green's function is defined on $0 < \tau < \beta$ as

$$\mathcal{G}_{\mathcal{O}_1\mathcal{O}_2}(\tau) = -\langle T\left[\mathcal{O}_1(\tau)\mathcal{O}_2(0)\right]\rangle = -\langle \mathcal{O}_1(\tau)\mathcal{O}_2(0)\rangle.$$

The subsequent Fourier transform in imaginary-time results in

$$\mathcal{G}_{\mathcal{O}_1\mathcal{O}_2}(i\omega_n) = \left\langle \left\{ \mathcal{O}_1, \frac{e^{i\omega_n 0^+}}{i\omega_n - \mathcal{L} + \mathcal{L}_Y}\mathcal{O}_2 \right\} \right\rangle,$$

where $\omega_n = (2n+1)\pi/\beta$ ($n \in \mathbb{Z}$) denotes the fermionic Matsubara frequencies.

# Real-time formulation

Switching to real-time, the Heisenberg representation of an operator $\mathcal{O}$ is given by $\mathcal{O}(t) = e^{iHt}\mathcal{O}e^{-iHt}$. The nonequilibrium real-time retarded Green's function can then be expressed as

$$\begin{aligned} G^{\mathrm{ret}}_{\mathcal{O}_1\mathcal{O}_2}(t) &= -i\theta(t)\langle\{\mathcal{O}_1(t), \mathcal{O}_2(0)\}\rangle \\ &= -i\theta(t)\frac{\mathrm{tr}\left[e^{-\beta(H-Y)}\{\mathcal{O}_1(t), \mathcal{O}_2(0)\}\right]}{\mathrm{tr}\left[e^{-\beta(H-Y)}\right]}. \end{aligned}$$

By using the spectral representation and then Fourier transforming, we obtain

$$G^{\mathrm{ret}}_{\mathcal{O}_1\mathcal{O}_2}(\omega) = \left\langle\left\{\mathcal{O}_1, \frac{1}{\omega - \mathcal{L} + i\eta}\mathcal{O}_2\right\}\right\rangle.$$

$\mathcal{G}_{\mathcal{O}_1\mathcal{O}_2}(i\omega_n)$ and $G^{\mathrm{ret}}_{\mathcal{O}_1\mathcal{O}_2}(\omega)$ are not related by analytical continuation

# Exact Formulation

CURRENT:

$$
\begin{aligned}
I &= \frac{I_1 + I_{-1}}{2} = -\frac{e}{2}\left\langle \frac{d\left(N_1(t) - N_{-1}(t)\right)}{dt} \right\rangle \\
&= i\frac{e}{2}\sum_{\alpha} \alpha \left\langle [N_\alpha(t), H] \right\rangle = i\sum_{\alpha k\sigma} \alpha \frac{e t_{\alpha k}}{2\sqrt{\Omega}} \left\langle \left( c^\dagger_{\alpha k\sigma} d_\sigma - d^\dagger_\sigma c_{\alpha k\sigma} \right) \right\rangle \\
&= \mathrm{Im}\left[ \sum_{\alpha k\sigma} \alpha \frac{e t_{\alpha k}}{\sqrt{\Omega}} \mathcal{G}_{c_{\alpha k\sigma} d^\dagger_\sigma}(\tau = 0) \right],
\end{aligned}
$$

We have used the fact that we are in steady state: current invariant under translation
For a diagrammatic analysis, it is convenient to **Fourier transform** this formula:

$$
I = \mathrm{Im}\left[ \sum_{\alpha k\sigma\omega_n} \alpha \frac{e t_{\alpha k}}{\sqrt{\Omega}} \frac{1}{\beta} \mathcal{G}_{c_{\alpha k\sigma} d^\dagger_\sigma}(i\omega_n) \right]
$$

# Equivalence with Meir-Wingreen

$$\frac{1}{\beta}\sum_{\omega_n}\mathcal{G}_{c_{\alpha k\sigma}d^\dagger_\sigma}(i\omega_n)=\frac{1}{\beta}\sum_{\omega_n}\left\langle\left\{c_{\alpha k\sigma},\frac{e^{i\omega_n 0^+}}{i\omega_n-\mathcal{L}+\mathcal{L}_Y}d^\dagger_\sigma\right\}\right\rangle$$

Then, we use the definition of Eq. (*) defined ealier and assume that we don't apply a magnetic field, and that the tunneling matrix elements are constant

$$\frac{1}{\beta}\sum_{\omega_n}\mathcal{G}_{c_{\alpha k\sigma}d^\dagger_\sigma}(i\omega_n)=\frac{1}{\beta}\sum_{\omega_n}\left[\left\langle\left\{\psi_{\alpha k\sigma},\frac{e^{i\omega_n 0^+}}{i\omega_n-\mathcal{L}+\mathcal{L}_Y}d^\dagger_\sigma\right\}\right\rangle\right.$$
$$\left.-\left\langle\left\{\frac{1}{\epsilon_k+\mathcal{L}-i\eta}d_\sigma,\frac{e^{i\omega_n 0^+}}{i\omega_n-\mathcal{L}+\mathcal{L}_Y}d^\dagger_\sigma\right\}\right\rangle\right].$$

One can show that the second term does not need to be evaluated

Essentially, the current at the left and right junction must be equivalent
In steady state which implies that I = $\left(t_1^2 I_{-1} + t_{-1}^2 I_1\right) / \left(t_1^2 + t_{-1}^2\right)$
Using this second formulation this second term vanishes

Then, a calculation allows to show that:

$$\frac{1}{\beta}\sum_{\omega_n}\left\langle\left\{\psi_{\alpha k\sigma}, \frac{e^{i\omega_n 0^+}}{i\omega_n - \mathcal{L} + \mathcal{L}_Y} d_\sigma^\dagger\right\}\right\rangle = \frac{t_\alpha}{\sqrt{\Omega}} f\left(\epsilon_k - \alpha\frac{\Phi}{2}\right) G^{\mathrm{ret}}_{d_\sigma d_\sigma^\dagger}(\epsilon_k)$$

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

Here,

Spectral function in general depends on bias voltage

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

Similar formula
Obtained with Keldysh

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

We have also shown that we recover the Meir-Wingreen (Keldysh) form:
**Meir-Wingreen, 1992-1993**

$$I = i\frac{e}{2\pi}\sum_{\alpha\sigma}\alpha\Gamma_\alpha\int_{-\infty}^{\infty} d\epsilon_k\left\{f\left(\epsilon_k-\alpha\frac{\Phi}{2}\right)\left[G^{\text{adv}}_{d_\sigma d_\sigma^\dagger}(\epsilon_k)-G^{\text{ret}}_{d_\sigma d_\sigma^\dagger}(\epsilon_k)\right]+G^{<}_{d_\sigma d_\sigma^\dagger}(\epsilon_k)\right\}$$

This (exact) formula works in the presence of interactions on the level

$$2i\pi\mathcal{G}_{d_\sigma d_\sigma^\dagger}(\tau=0) = 2i\pi\left\langle d_\sigma^\dagger d_\sigma\right\rangle = 2\pi G^{<}_{d_\sigma d_\sigma^\dagger}(t=0) = \int_{-\infty}^{\infty} d\epsilon_k G^{<}_{d_\sigma d_\sigma^\dagger}(\epsilon_k)$$

$$\begin{aligned}
n_d &= \sum_\sigma \langle d_\sigma^\dagger d_\sigma\rangle = \frac{1}{\beta}\sum_{\sigma,\omega_n}\mathcal{G}_{d_\sigma d_\sigma^\dagger}(i\omega_n)\\
&= \frac{1}{2}\int d\epsilon_k A_d(\epsilon_k)\left[f\left(\epsilon_k-\frac{\Phi}{2}\right)+f\left(\epsilon_k+\frac{\Phi}{2}\right)\right]\\
&= \int d\epsilon_k A_d(\epsilon_k) f^{\text{eff}}(\epsilon_k,\Phi),\\
f^{\text{eff}}(\epsilon_k,\Phi) &= \frac{1}{2}\left[f\left(\epsilon_k-\frac{\Phi}{2}\right)+f\left(\epsilon_k+\frac{\Phi}{2}\right)\right]
\end{aligned}$$

Useful formula
for level occupancy

# In principle, these exact relations can also be applied to …

DMFT spirit: Hubbard model with electric fields or tilted lattices
See for example, C. Aron & G. Kotliar,
Hershfield's approach: as impurity solver

This formalism can be easily applied in the case of "hybrid" systems:
Anderson-Holstein model, where level coupled to "photon" mode

Possibility to extract exact relations for Friedel-Langreth sum rule

Application to a gradient of Temperature

# (Trivial) Application: resonant level

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

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

$$g_d(\epsilon_k) = \frac{1}{\epsilon_k - \epsilon_d + i\Gamma}$$ (this relation can be easily inverted)

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

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

At T=0, Landauer formula: we recover that I varies linearly with bias in the linear regime (see next slide, curve at U=0, no interaction)

# At U=0, tractable case

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

$$g_d(\epsilon_k) = \frac{1}{\epsilon_k - \epsilon_d + i\Gamma}$$

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

**<u>Note:</u> Don’t use the original (c,d) basis since**

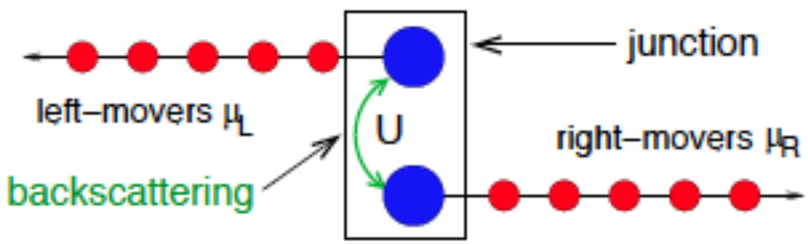
$$Y = \sum_{\alpha k\sigma} \frac{\alpha\Phi}{2} \Big[ c^\dagger_{\alpha k\sigma} c_{\alpha k\sigma} + \frac{t}{\sqrt{\Omega}} \left( g_d(\epsilon_k) d^\dagger_\sigma c_{\alpha k\sigma} + \mathbf{h.c.} \right) + \frac{t^2}{\Omega} \sum_{\alpha' k'} \left( \frac{g_d(\epsilon_k)}{\epsilon_k - \epsilon_{k'} + i\eta} c^\dagger_{\alpha' k' \sigma} c_{\alpha k\sigma} + \mathbf{h.c.} \right) \Big]$$

# Concrete Implementation:

**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)



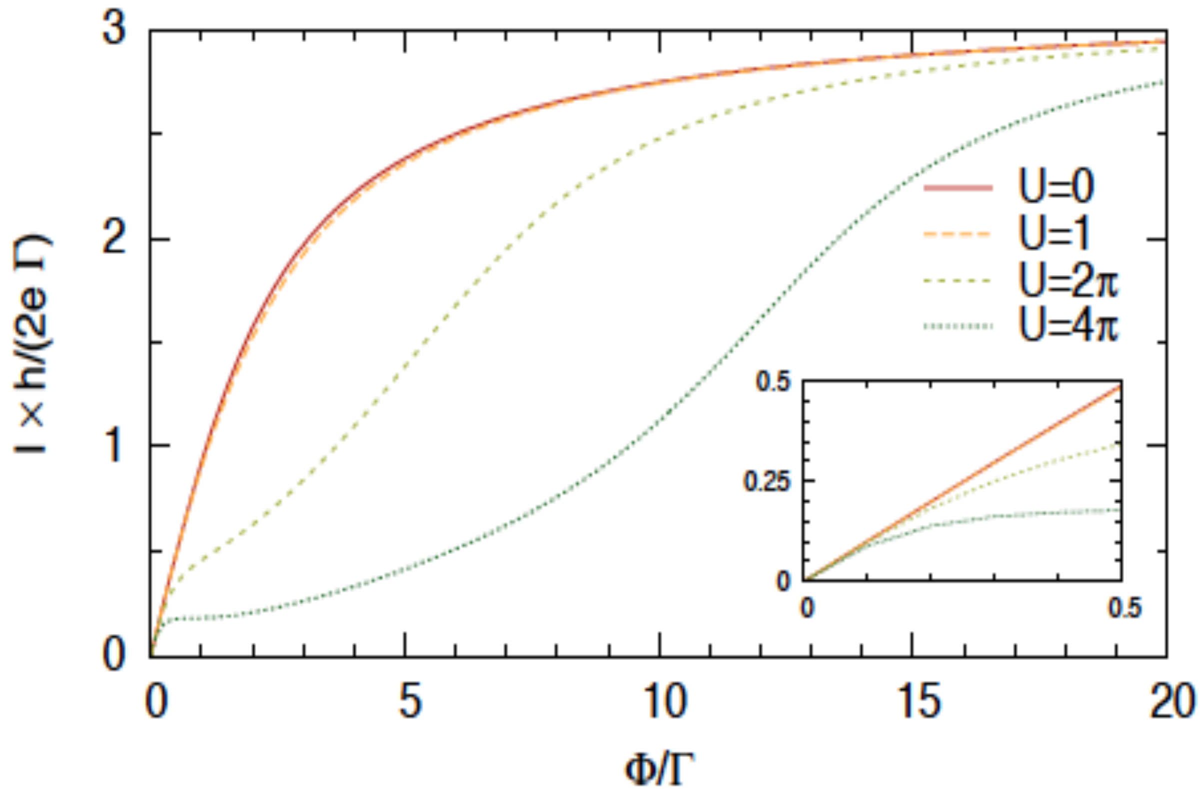

In the presence of interactions, scattering states are complicated (not single-body like)

NRG approach in the scattering state basis
**F. Anders et al.**

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

Idea: Hershfield density matrix simple $\rho_0$ for U=0
Switch on U and let $\rho$ evolve to steady state

# Main goal: explain…




**Landauer view at small bias**

Fig. 6. The current-voltage curves for the Anderson model for $U/\Gamma = 0.0, 1.0, 2\pi$ and $4\pi$, 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.

# Mean-Field argument

Shift of the level position:

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

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

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

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.

# First order level:

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

Then, we can use: $$d_{\sigma}^{\dagger} = \frac{t}{\sqrt{\Omega}}\sum_{\alpha k} g_d^*(\epsilon_k)\psi_{\alpha k\sigma}^{(0)\dagger}$$

$$H_{\rm int} = \frac{U}{2}\left(\frac{t^2}{\Omega}\right)^2 \sum_{1,2,3,4,\sigma} g_1^* g_2^* g_3 g_4 \psi_{1\sigma}^{(0)\dagger}\psi_{2-\sigma}^{(0)\dagger}\psi_{3-\sigma}^{(0)}\psi_{4\sigma}^{(0)}$$

This already affects the form of the scattering states to first order

$$\psi_{\alpha k\sigma}^{\dagger(1)} = U g_d(\epsilon_k)\left(\frac{t^2}{\Omega}\right)^2 \sum_{123} \frac{g_1^* g_2^* g_3}{\epsilon_k - \epsilon_1 - \epsilon_2 + \epsilon_3 + i\eta}\psi_{1\sigma}^{(0)\dagger}\psi_{2-\sigma}^{(0)\dagger}\psi_{3-\sigma}^{(0)}$$

# 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 $H_{int}$

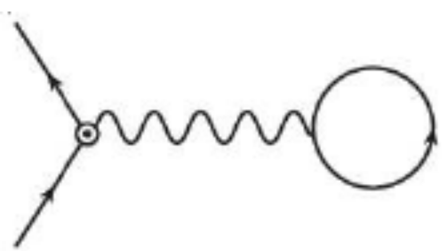
$$\boxed{\mathcal{H}^{(m)} = \left[\sum_{\alpha k\sigma}\left(\epsilon_k - \alpha\frac{\Phi}{2}\right)\sum_{p=0}^{m}\psi^{\dagger(p)}_{\alpha k\sigma}\psi^{(m-p)}_{\alpha k\sigma}\right]}$$

# 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:



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

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

# 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**

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

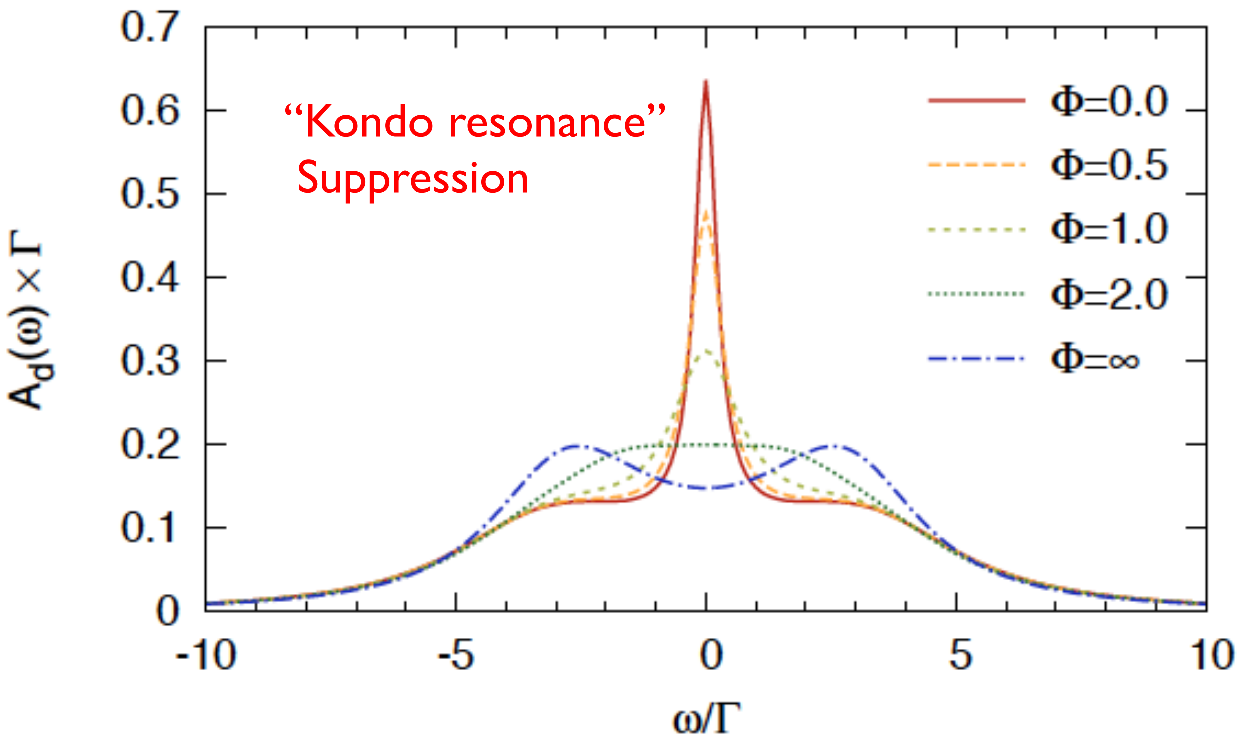
and similarly

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

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

# 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**

# Zeeman splitting

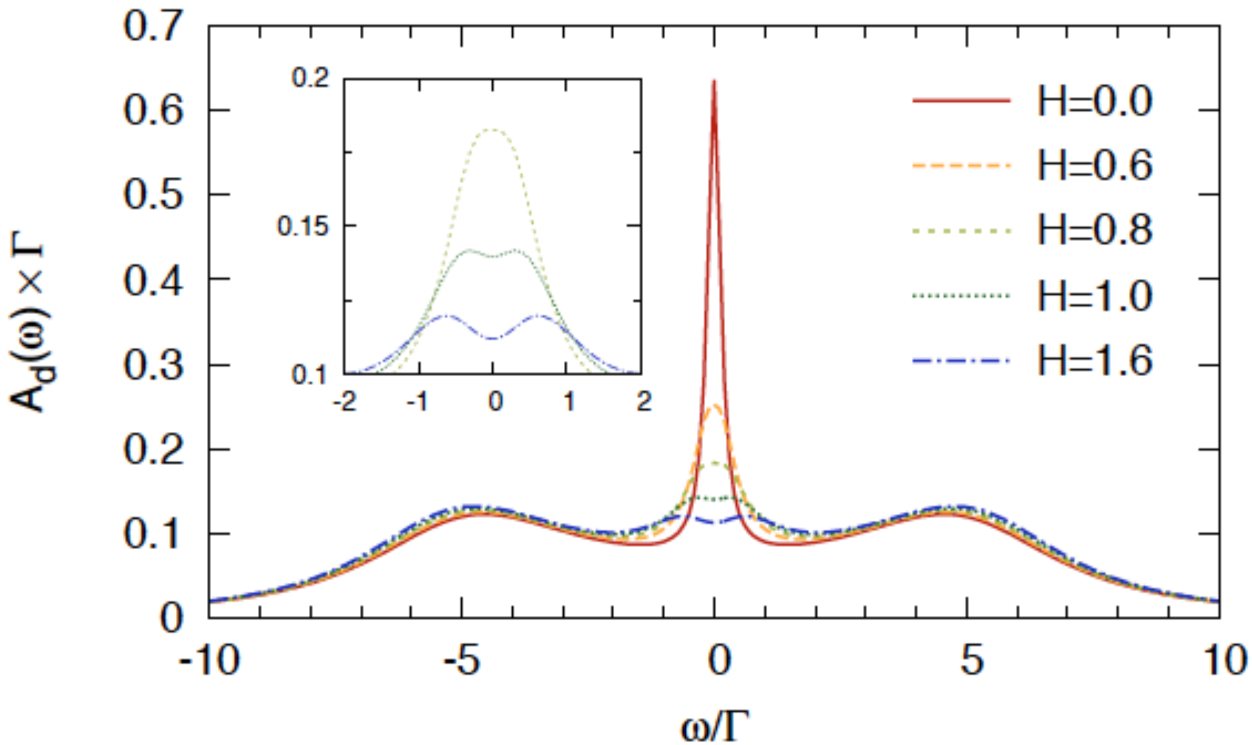



Fig. 5. Variation of the spectral function with an applied magnetic field ($H$), obtained using the second-order self-energy. Here $\Gamma = 1$, $\Phi = 0$, $U = 3\pi$ and $H$ is given in the units defined by $g\mu_b$, where $g$ is the g-factor and $\mu_b$ denotes the Bohr magneton. The inset shows the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