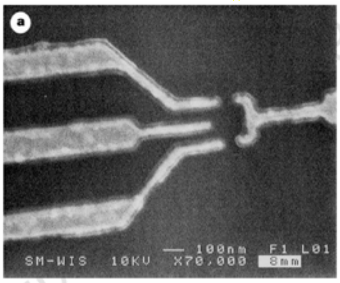
(i)

The 4th Windsor Summer School on Condensed Matter Theory
Quantum Transport and Dynamics in Nanostructures
Great Park, Windsor, UK, August 6 - 18, 2007

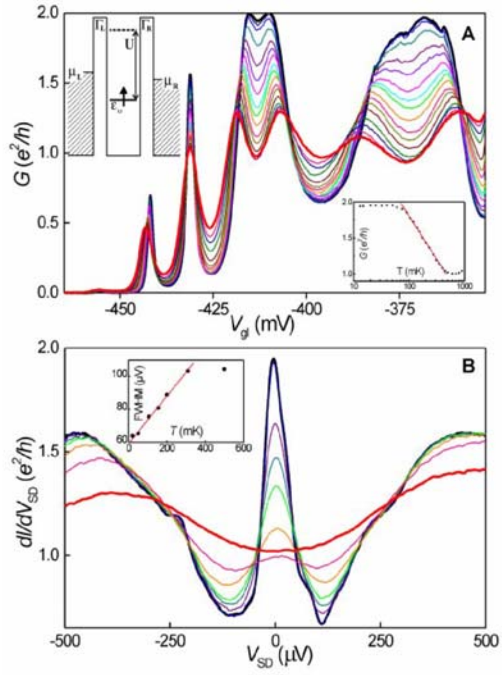
Kondo Effect in Metals and Quantum Dots

Jan von Delft



Goldhaber-Gordon et al., Nature **391**, 156 (1998)

Cronenwett et al., Science **281**, 540 (1998)
Simmel et al., PRL **83**, 804 (1999)
van der Wiel et al., Sience 289, 2105 (2000)



van der Wiel et al., Sience 289, 2105 (2000)

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Lecture 1: Kondo effect in metals: Kondo model
- T-matrix in perturbation theory, log(T/D) divergencies
- Anderson's "poor man's scaling", Kondo temperature
- Strong coupling regime, Fermi liquid theory, Friedel sum rule
- Kondo resonance

Lecture 2: Kondo effect in quantum dots: Anderson model
- Experimental Results
- Mapping of Anderson to Kondo model by Schrieffer-Wolff transformation
- Anderson model with two leads

Lecture 3: Flow equation Renormalization Group
- General idea: diagonalize Hamiltonian by unitary transformation
- Application to Kondo model in equilibrium
- out of equilibrium

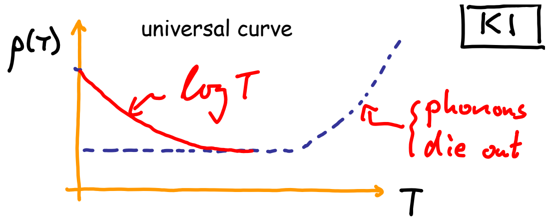
Lecture 4: Numerical Renormalization Group
- General idea: map model to linear chain and diagonalize numerically
- Wilson's iterative RG scheme
- Matrix product states
- Relation to DMRG
- Finite temperature

Lecture 1: Kondo model

[Kondo, Phys Rev 1964]

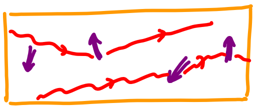
K1

anomalous resistivity minimum in dilute magnetic alloys
(localized spins scatter conduction electrons)



Kondo Model:

$H_{Kondo} = H_{band} + H_{scat}$



$$H_{band} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \qquad (1)$$

conduction electron spin

$$H_{scat} = J \sum_{kk'\sigma\sigma'} \big(\overbrace{c^\dagger_{k\sigma} \tfrac{1}{2}\vec{\sigma}_{\sigma\sigma'} c_{k'\sigma'}}^{=:\vec{s}} \cdot \vec{S} \big) \qquad (2)$$

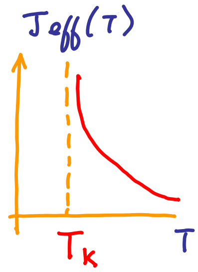
magnetic impurity

Spin-flip scattering:

final state: $k\uparrow$ $\Downarrow$ $\qquad$ initial state: $\Uparrow$ $k'\downarrow$

turns out to be enhanced at low temperatures:

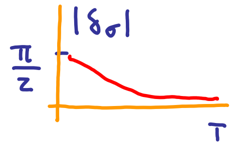
$$T \lesssim T_K = D e^{-\frac{1}{\nu J}} \qquad (3)$$



T = 0: Fermi liquid theory

ground state = spin singlet $= (\Downarrow\uparrow) = k\uparrow \otimes k'\uparrow$

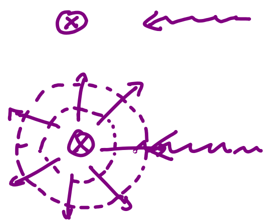
$$\frac{e^{i(kr - \delta_\sigma)}}{r} \leftarrow \frac{e^{-ikr}}{r}$$



Scattering states and T-matrix

K2

$$H = H_0 + H_1 \qquad (1)$$



Free state: $\quad H_0 |k\sigma\rangle = \varepsilon_k |k\sigma\rangle \qquad (2)$

Scattering state: $\quad H |\tilde{k\sigma}\rangle = \varepsilon_k |\tilde{k\sigma}\rangle \qquad (3)$

Ansatz:

$$|\tilde{k\sigma}\rangle = |k\sigma\rangle + \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 |\tilde{k\sigma}\rangle \qquad (4)$$

Check:

$$(\varepsilon_k - H_0 + \underbrace{\cancel{i\eta}}_{=0}) |\tilde{k\sigma}\rangle = (\underbrace{\cancel{\varepsilon_k - H_0}}_{=0\ (2)} + \underbrace{\cancel{i\eta}}_{=0}) |k\sigma\rangle + H_1 |\tilde{k\sigma}\rangle \qquad (5)$$

$$(\varepsilon_k - H_0 - H_1) |\tilde{k\sigma}\rangle \overset{(3)}{=} 0$$

Iterate (4):

$$|\tilde{k\sigma}\rangle = \left[1 + \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 + \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 + \dots \right]$$

$$= \left[1 + \frac{1}{\varepsilon_k - H_0 + i\eta} \mathcal{T} \right] |k\sigma\rangle \qquad (6)$$

T-matrix:

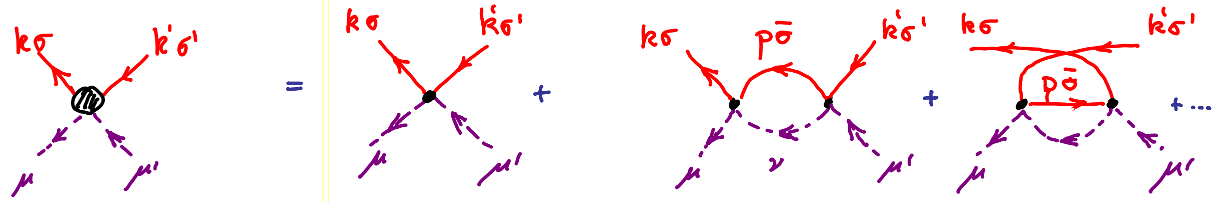
$$\mathcal{T} = H_1 + H_1 \frac{1}{\varepsilon_k - H_0 + i\eta} H_1 + H_1 \frac{1}{(\ )} H_1 \frac{1}{(\ )} H_1 + \dots \qquad (7)$$

Matrix elements of T

$$\langle k\sigma| \otimes \langle \mu| \; T \; |k'\sigma'\rangle \otimes |\mu'\rangle$$

K3

pert. exp: $$T^{\mu\mu'}_{k\sigma,k'\sigma'} = T^{(1)} + \underbrace{T^{(2)} \qquad\qquad\qquad}\; + \dots \qquad (1)$$



(2)

$$T^{(1)\,\mu\mu'}_{k\sigma,k'\sigma'} = \frac{1}{2} J \, \vec{\sigma}_{\sigma\sigma'} \cdot \vec{S}_{\mu\mu'} \qquad (3)$$

$$T^{(2)\,\mu\mu'}_{k\sigma,k'\sigma'} = J^2 \sum_{\substack{p\bar\sigma\\ \nu}} \frac{(\frac{1}{2}\vec{\sigma}_{\sigma\bar\sigma}\cdot\vec{S}_{\mu\nu})\cdot(\frac{1}{2}\vec{\sigma}_{\bar\sigma\sigma'}\cdot\vec{S}_{\nu\mu'})}{\varepsilon_k - \varepsilon_p \quad + i\eta} \, [1 - f(\varepsilon_p)] \qquad (4a)$$

relative minus: $1 - f(\varepsilon_p)$

final state is $c^\dagger_k \overbrace{c_p \, c^\dagger_p} c_{k'} |k'\sigma\rangle$

versus $\underbrace{c^\dagger_p c_{k'} c^\dagger_k c_p}_{f(\varepsilon_p)} |k'\sigma\rangle$

$c^\dagger_k$, $c_{k'}$ act in opposite order

$$\ominus \; J^2 \sum_{\substack{p\bar\sigma\\ \nu}} \frac{(\frac{1}{2}\vec{\sigma}_{\bar\sigma\sigma'}\cdot\vec{S}_{\mu\nu})\cdot(\frac{1}{2}\vec{\sigma}_{\sigma\bar\sigma}\cdot\vec{S}_{\nu\mu'})}{\varepsilon_k - (\varepsilon_{k'} - \varepsilon_p + \varepsilon_k) \;+ i\eta} \, f(\varepsilon_p) \qquad (4b)$$

K4

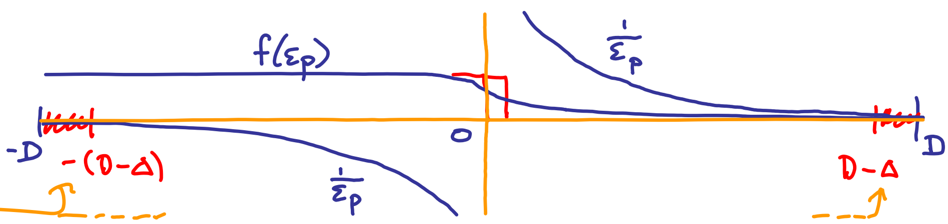
$$T^{(2)} \overset{(3.4b)}{=} J^2 \sum_{\substack{aa'=\\ xyz}} (S^a S^{a'})_{\mu\mu'} \left[\nu \int_{-D}^{D} d\varepsilon_p \, \frac{1}{4} \left\{ (\sigma^a \sigma^{a'})_{\sigma\sigma'} \frac{f(\varepsilon_p) - 1}{\varepsilon_p - \varepsilon_k - i\eta} - (\sigma^{a'} \sigma^{a})_{\sigma\sigma'} \frac{f(\varepsilon_p)}{\varepsilon_p - \varepsilon_{k'} + i\eta} \right\} \right] \qquad (1)$$

Consider $\varepsilon_k \simeq \varepsilon_{k'} \simeq \varepsilon_F$:

$$\frac{1}{4}[\sigma^a, \sigma^{a'}]_{\sigma\sigma'} \, \nu \int_{-D}^{D} d\varepsilon_p \frac{f(\varepsilon_p)}{\varepsilon_p} \propto \int_{-D}^{T} d\varepsilon_p \frac{1}{\varepsilon_p} = \ln T/D \xrightarrow{T \to 0} \infty \qquad (2)$$

↳ performing entire integral yields log. divergence

Anderson "poor man's scaling" idea: split off contribution from strips near band edges:



$$T^{(2)}_{(D)} = T^{(2)}_{(D-\Delta)} + \delta T^{(2)} \qquad (3)$$

$$\delta T^{(2)} = \underbrace{J^2 \sum_{aa'} (S^a S^{a'})_{\mu\mu'} \overbrace{\frac{1}{4}[\sigma^a, \sigma^{a'}]_{\sigma\sigma'}}^{\frac{1}{2} i \varepsilon_{aa'b} \sigma^b}} \, \nu \left[\int_{D-\Delta}^{D} d\varepsilon_p + \int_{-D}^{-(D-\Delta)} d\varepsilon_p \right] \frac{f(\varepsilon_p)}{\varepsilon_p} \qquad (4)$$

check algebra yourself! $\boxed{\Sigma}$

$$= J^2 \left(-\frac{1}{2} \vec{S}_{\mu\mu'} \cdot \vec{\sigma}_{\sigma\sigma'}\right) \nu\Delta \begin{cases} \frac{0}{D} + \frac{1}{-D} & \text{for } T \ll D \quad (5a) \\ \frac{1/2}{D} + \frac{1/2}{-D} \simeq 0 & \text{for } D \ll T \quad (5b) \end{cases}$$

K5

Integrated-out strips yield term of same form as bare vertex:

$T^{(1)} \overset{(3.3)}{=} \frac{1}{2} J \, \vec{\sigma}\cdot\vec{S}$

$$\delta T^{(2)}(J) \overset{(4.5a)}{=} \underbrace{J^2 \frac{\nu\Delta}{D}}_{\delta J} \frac{1}{2}\vec{\sigma}\cdot\vec{S} = T^{(1)}(\delta J) \qquad (1)$$

Scaling of T-matrix under band-width reduction:

$$T(D,J) \overset{(3.2)}{=} T^{(1)}(J) + T^{(2)}(D,J) + O(J^3) \qquad (2)$$

$$\overset{(4.4)}{=} T^{(1)}(J) + T^{(2)}(D-\Delta, J) + \overset{T^{(1)}(\delta J)}{\overset{\overset{(1)}{\parallel}}{\delta T^{(2)}(J)}} \qquad (3)$$

$$\overset{(1)}{=} T^{(1)}(J+\delta J) + T^{(2)}(D+\delta D, J+\delta J) + O(\cancel{J^3}) \qquad (4)$$

$$= T(D', J') \qquad (5)$$

So, reducing bandwidth $D \to D' = D + \delta D$, $\delta D = -\Delta$ (6)

generates increase in coupling constant: $J \to J' = J + \delta J$, $\underbrace{\delta J \nu}_{\delta g} \overset{(1)}{=} -\underbrace{J^2 \nu^2}_{g^2} \frac{\delta D}{D}$ (7)

Scaling eq. for dimensionless coupling: $g(D) := \nu J$ $\qquad \boxed{\frac{dg}{d(\ln D)} = -g^2}$ (8)

K6

Flow to strong coupling; Kondo temperature

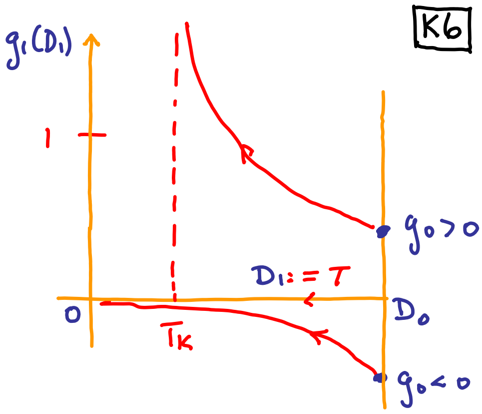
Scaling equation:

$$-\int_{g_0}^{g_1} \frac{dg}{g^2} \overset{(5.8)}{=} \int_{D_0}^{D_1} d(\ln D) \qquad (1)$$

$$\frac{1}{g_1} - \frac{1}{g_0} = \ln D_1/D_0 \qquad (2)$$

$$g_1(D_1) = \frac{1}{\frac{1}{g_0} - \underbrace{\ln(D_0/D_1)}_{>0}} \qquad (3)$$

, grows as $D_1 \to 0$



Reduce bandwidth until $D_1 = T$ [because by (4.5b), renormalization of coupling stops for $D_1 \ll T$; lecture 3 will illustrate this in more detail !]

and use as effective coupling constant at temperature T:

$$g_{eff}(T) = g_1(D_1 = T) \overset{(3)}{=} \frac{1}{\frac{1}{g_0} - \ln(D/T)} = \frac{1}{\ln(T/T_K)} \qquad (4)$$

for $T > T_K$

For $g_0 > 0$, scaling approach eventually breaks down: eff. coupling diverges at a scale T_K:

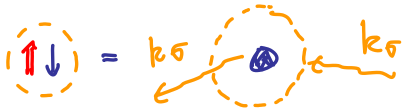
$$\ln D/T_K := \frac{1}{g_0} \Rightarrow \boxed{T_K = D e^{-\frac{1}{g_0}}} \qquad (5)$$

Strong coupling fixed point: Fermi liquid theory

P. Nozières, J. Low Temp. Phys. 17, 31 (1974)

K7

* Scaling approach breaks down for $T \le T_K$ Nevertheless, it allows qualitative conclusion:
* For T→0, "KM flows to strong-coupling fixed point", dominated by $J\,\vec{\sigma}\cdot\vec{S}$ (1)
* Local spin binds "one" electron from band into a singlet: (conduction band "screens" local spin to form a singlet)



* Other electrons form Fermi liquid, for which singlet acts a (static) potential scatterer, causing only phase shifts: $\frac{e^{i(kr-\delta_\sigma)}}{r} \leftarrow \frac{e^{-ikr}}{r}$ (2)

standard relation between S and T

S- [or T-] matrix: $e^{2i\delta_\sigma(\varepsilon_k)} = S_\sigma(\varepsilon_k) \quad [=: 1 - i2\pi\nu\, T_\sigma(\varepsilon_k)]$ (3)

Choose: $|\delta_\sigma| \le \pi/2$

KM is invariant under particle-hole symmetry: $c_{k\sigma} \to \sigma\, c^\dagger_{-k-\sigma}$ (4)

Thus, particle scatteres same way as hole

This relates phase shifts for spin up and down: $e^{i2\delta_\sigma(\varepsilon_k)} \overset{(3)}{=} S_\sigma(\varepsilon_k) \overset{(4)}{=} S^\dagger_{-\sigma}(-\varepsilon_{-k}) = e^{-i2\delta_\sigma(-\varepsilon_{-k})}$ (5)

At Fermi level: $\varepsilon_k = 0$ $\quad \boxed{\delta_\uparrow(0) = -\delta_\downarrow(0)} = ?$ (6)

Friedel sum rule:

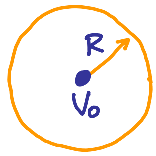
Friedel, Can. J. Phys. 34, 1190 (1956)

$\boxed{\frac{1}{\pi}\delta_\sigma(0) = \Delta n_\sigma}$ = charge displaced by local potential scatterer (1)

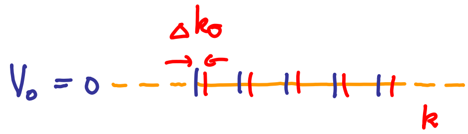
K8

Derivation:

Use radial box, radius R, radial wavefunctions $j_\ell(kr)$: $0 = j_{\ell=0}\left(kR - \delta_\sigma(\varepsilon_k)\right) = \frac{\sin(kR - \delta_\sigma(\varepsilon_k))}{kR}$ (2)



to quantize momenta of radial waves: $k_n = \frac{\pi n}{R} + \underbrace{\frac{\delta_\sigma(\varepsilon_k)}{R}}_{\Delta k_\sigma}$ (3)



Radial momentum sums: $\xi_k = \frac{k^2}{2m} = \varepsilon_F + \varepsilon_k$

$$\sum_k \simeq R\int\frac{dk}{\pi} = \int d\varepsilon_k\, \underbrace{\frac{R}{\pi}\frac{\partial}{\partial\varepsilon_k}(k + \Delta k_\sigma)}_{\nu(\varepsilon_k) + \Delta\nu_\sigma(\varepsilon_k)} \quad (4)$$

Potential scatterer $\delta_\sigma(\varepsilon_k)$, $\quad \Delta k_\sigma \overset{(3)}{=} \frac{\delta_\sigma(\varepsilon_k)}{R}$, $\quad \Delta\nu_\sigma(\varepsilon_k) \overset{(4)}{=} \frac{1}{\pi}\frac{\partial\delta_\sigma(\varepsilon_k)}{\partial\varepsilon_k}$ (5)

Change in charge of cond. electrons around impurity ("screening charge"):

$$\Delta n_\sigma \overset{(T=0)}{=} \int_{-D}^{0} d\varepsilon_k\, \Delta\nu_\sigma(\varepsilon_k) \overset{(5)}{=} \frac{1}{\pi}\left[\delta_\sigma(0) - \delta_\sigma(-D)\right] = (1)\checkmark \quad (6)$$

$= 0$ if $|D| \gg V_0$

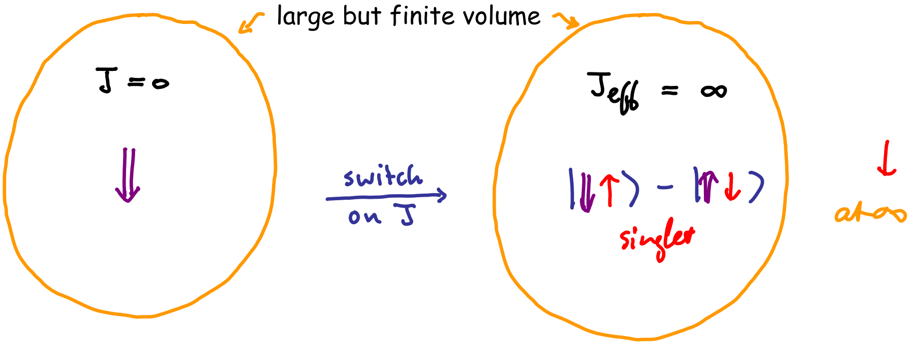
for Kondo problem, scattering near band edge is weak, $= 0$ see (6.3)

Screening of local spin to form singlet:

Pustilnik, Glazman, "Nanophysics: Coherence and Transport," eds. H. Bouchiat et al., pp. 427-478 (Elsevier, 2005).

K9

Consider how charge inside a large but finite volume changes when J is switched on:



total spin inside volume: $S_{z,tot} = -\frac{1}{2}$ $\qquad$ $S_{z,tot} = 0$ $\qquad$ (1)

conduction band is initially unpolarized: $n_\uparrow - n_\downarrow = 0$

change in cond. band charge inside volume to achieve screening: $\Delta n_\uparrow - \Delta n_\downarrow = 1$ $\qquad$ (2)

$\downarrow (8.6)$

$$\frac{1}{\pi}\left[\underbrace{\delta_\uparrow(0) - \delta_\downarrow(0)}_{= \delta_\uparrow(0) \ (7.6)}\right] = 1 \qquad (3)$$

Phase shifts at Fermi energy:

$$\boxed{\delta_\uparrow(0) \overset{(7.6)}{=} -\delta_\downarrow(0) \overset{(3)}{=} \frac{\pi}{2}}$$

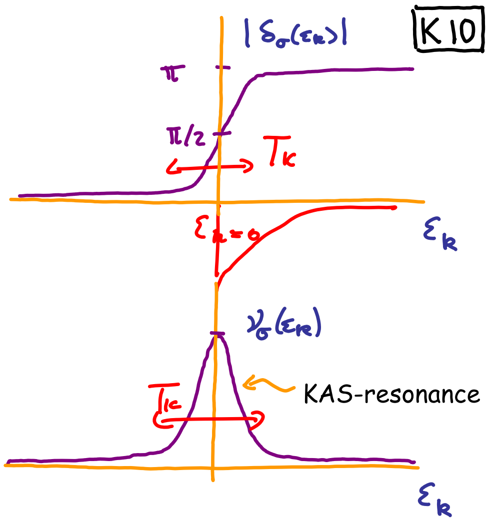
maximal possible value $\qquad$ (4)

Kondo-Abrikosov-Suhl resonance in density of states

K10

* $g_{eff}(D')$ becomes large only for $D' \leq T_K$

* phase shifts change on scale of T_K



* similarly for DOS: $\Delta\nu_\sigma(\varepsilon) \overset{(8.5)}{=} \frac{1}{\pi}\frac{\partial \delta_\sigma(\varepsilon_k)}{\partial \varepsilon_k}$

This resonance also arises in:

- T-matrix
- electron scattering rate (causing resistivity anomaly)
- in dynamical correlation function of composite operator F:

Costi, Phys. Rev. Lett. 85, 1504 (2000)

$$F_\sigma := \sum_{k\sigma'} \vec{S} \cdot \vec{\sigma}_{\sigma\sigma'} c_{k\sigma'} \qquad (1)$$

$$-\frac{\mathrm{Im}\, T_{\sigma\sigma}(\omega)}{\pi} = A_{\sigma\sigma}(\omega) := \mathrm{Im} \int_0^\infty \frac{dt}{\pi} e^{-i\omega t} (-i) \langle \{ F_\sigma(t), F_\sigma^\dagger(0) \} \rangle \qquad (2)$$