Vyacheslavs Kashcheyevs
Amnon Aharony
Ora Entin-Wohlman

אוניברסיטת תל-אביב
TEL AVIV UNIVERSITY

Applicability of the **equations-of-motions** technique for **quantum dots**

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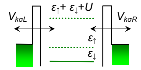
Objective: Tractable analytic approximation for electron Green function applicable to both strong and weak coupling regimes of a small quantum dot.

Strategy: Self-consistent truncation of exact hierarchy of equations of motions for double time Green functions.

Testbed: Generalized single impurity Anderson model:

$$\mathcal{H} = \sum_{\sigma=\uparrow,\downarrow} \epsilon_\sigma d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow + \sum_{\substack{\alpha=L,R\\ k\sigma}} \left(\epsilon_{k\alpha\sigma} c_{k\alpha\sigma}^\dagger c_{k\alpha\sigma} + V_{k\alpha\sigma} c_{k\alpha\sigma}^\dagger d_\sigma + V_{k\alpha\sigma}^* d_\sigma^\dagger c_{k\alpha\sigma}\right)$$



Summary

Empty orbital ("even valley")

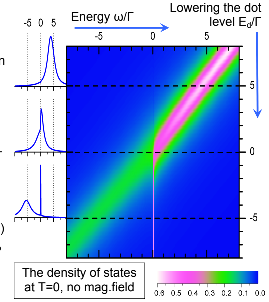
- Better than 5% agreement with known exact results (Bethe ansatz)
- Continuous Lorentzian DOS

Mixed valence ("CB peak")

- Exponential increase in susceptibility
- Continuous asymmetric DOS at low T

Kondo regime ("odd valley")

- All qualitative features of the Kondo effect (singlet ground state, universal scaling, narrow peak in the DOS, etc.)
- Friedel sum rule broken by up to 30%
- Problems at the point of exact particle-hole symmetry



Exact hierarchy of equations of motion

- Equilibrium Green function (GF) of two fermionic operators:

$$\langle\langle A;B\rangle\rangle_z = -i\int_0^{+\infty} \langle A(t)\,B + B\,A(t)\rangle\, e^{izt} dt \qquad \text{(retarded, Im } z>0)$$

- Interested in the GF on the quantum dot, $G_\sigma(z) \equiv \langle\langle d_\sigma; d_\sigma^\dagger\rangle\rangle_z$.
- Heisenberg time evolution generates a hierarchy of equations [1–4]:

$$\boxed{[z-\epsilon_\sigma]\langle\langle d_\sigma; d_\sigma^\dagger\rangle\rangle = 1 + U\langle\langle n_{\bar\sigma} d_\sigma; d_\sigma^\dagger\rangle\rangle + \sum_{k\alpha} V_{k\alpha\sigma}^* \langle\langle c_{k\alpha\sigma}; d_\sigma^\dagger\rangle\rangle}$$

$$[z-\epsilon_{k\alpha\sigma}]\langle\langle c_{k\alpha\sigma}; d_\sigma^\dagger\rangle\rangle = V_{k\alpha\sigma}\langle\langle d_\sigma; d_\sigma^\dagger\rangle\rangle$$

$$[z-\epsilon_\sigma-U]\langle\langle n_{\bar\sigma} d_\sigma; d_\sigma^\dagger\rangle\rangle = \langle n_{\bar\sigma}\rangle + \\ + \sum_{k\alpha}\Big[-V_{k\alpha\bar\sigma}\langle\langle c_{k\alpha\bar\sigma}^\dagger d_{\bar\sigma} d_\sigma; d_\sigma^\dagger\rangle\rangle + V_{k\alpha\sigma}^*\langle\langle c_{k\alpha\sigma} n_{\bar\sigma}; d_\sigma^\dagger\rangle\rangle + V_{k\alpha\bar\sigma}^*\langle\langle d_{\bar\sigma}^\dagger c_{k\alpha\bar\sigma} d_\sigma; d_\sigma^\dagger\rangle\rangle\Big]$$

$$\boxed{\begin{aligned}[z-\epsilon_{k\alpha\sigma}]\langle\langle c_{k\alpha\sigma} n_{\bar\sigma}; d_\sigma^\dagger\rangle\rangle &= V_{k\alpha\sigma}\langle\langle n_{\bar\sigma} d_\sigma; d_\sigma^\dagger\rangle\rangle + \\ &+ \sum_{k'\alpha'}\Big[V_{k'\alpha'\bar\sigma}^*\langle\langle c_{k\alpha\sigma} d_{\bar\sigma}^\dagger c_{k'\alpha'\bar\sigma}; d_\sigma^\dagger\rangle\rangle - V_{k'\alpha'\bar\sigma}\langle\langle c_{k'\alpha'\bar\sigma}^\dagger d_{\bar\sigma} c_{k\alpha\sigma}; d_\sigma^\dagger\rangle\rangle\Big]\end{aligned}}$$

$$\boxed{\begin{aligned}[z-\epsilon_\sigma+\epsilon_{\bar\sigma}-\epsilon_{k\alpha\bar\sigma}]\langle\langle d_{\bar\sigma}^\dagger c_{k\alpha\bar\sigma} d_\sigma; d_\sigma^\dagger\rangle\rangle &= \langle d_{\bar\sigma}^\dagger c_{k\alpha\bar\sigma}\rangle + V_{k\alpha\bar\sigma}\langle\langle n_{\bar\sigma} d_\sigma; d_\sigma^\dagger\rangle\rangle + \\ &+ \sum_{k'\alpha'}\Big[-V_{k'\alpha'\bar\sigma}\langle\langle c_{k'\alpha'\bar\sigma}^\dagger c_{k\alpha\bar\sigma} d_\sigma; d_\sigma^\dagger\rangle\rangle + V_{k'\alpha'\sigma}^*\langle\langle d_{\bar\sigma}^\dagger c_{k\alpha\bar\sigma} c_{k'\alpha'\sigma}; d_\sigma^\dagger\rangle\rangle\Big]\end{aligned}}$$

$$\boxed{\begin{aligned}[z-\epsilon_\sigma-\epsilon_{\bar\sigma}-U+\epsilon_{k\alpha\bar\sigma}]\langle\langle c_{k\alpha\bar\sigma}^\dagger d_{\bar\sigma} d_\sigma; d_\sigma^\dagger\rangle\rangle &= \langle c_{k\alpha\bar\sigma}^\dagger d_{\bar\sigma}\rangle - V_{k\alpha\bar\sigma}^*\langle\langle n_{\bar\sigma} d_\sigma; d_\sigma^\dagger\rangle\rangle + \\ &+ \sum_{k'\alpha'}\Big[V_{k'\alpha'\sigma}^*\langle\langle c_{k\alpha\bar\sigma}^\dagger d_{\bar\sigma} c_{k'\alpha'\sigma}; d_\sigma^\dagger\rangle\rangle - V_{k'\alpha'\bar\sigma}^*\langle\langle c_{k\alpha\bar\sigma}^\dagger d_\sigma c_{k'\alpha'\bar\sigma}; d_\sigma^\dagger\rangle\rangle\Big]\end{aligned}}$$

Decoupling closes the chain

$$\underbrace{\langle\langle c_{k\alpha\bar\sigma}^\dagger d_{\bar\sigma} c_{k'\alpha'\sigma}; d_\sigma^\dagger\rangle\rangle_z}_{\text{No more than one dot operator, } d_\sigma} \Rightarrow \langle c_{k\alpha\bar\sigma}^\dagger d_{\bar\sigma}\rangle\langle\langle c_{k'\alpha'\sigma}; d_\sigma^\dagger\rangle\rangle_z - \overbrace{\langle c_{k\alpha\bar\sigma}^\dagger c_{k'\alpha'\sigma}\rangle\langle\langle d_{\bar\sigma}; d_\sigma^\dagger\rangle\rangle_z}^{0 \text{ (spin conservation)}}$$

Choosing this path is crucial!

Uncorrelated values [2]

$$\langle c_{k\alpha\sigma}^\dagger c_{k'\alpha'\sigma}\rangle \simeq \delta_{kk'}\delta_{\alpha\alpha'} f(\epsilon_{k\alpha\sigma}) \\ \langle c_{k\alpha\sigma}^\dagger d_\sigma\rangle \simeq 0$$

\+ Immediate solution

− Near failure for Kondo

Fluctuation-dissipation theorem [3,4]

$$\langle A^\dagger B\rangle = \frac{i}{2\pi}\int_C f(z)\langle\langle A^\dagger; B\rangle\rangle_z\, dz$$

\+ Self-consistency ⇒ better results

− Need to solve coupled equations

The main self-consistent equations

$$\begin{cases} G_\sigma(z) = \dfrac{u(z) - \langle n_{d\bar\sigma}\rangle - P_{\bar\sigma}(z_1) - P_{\bar\sigma}(z_2)}{u(z)\,[z-\epsilon_\sigma-\sigma h-\Sigma_\sigma(z)] + [P_{\bar\sigma}(z_1)+P_{\bar\sigma}(z_2)]\,\Sigma_\sigma(z) - Q_{\bar\sigma}(z_1) + Q_{\bar\sigma}(z_2)} \\ P_\sigma(z) = \dfrac{i}{2\pi}\oint_C f(z')\Big[G_\sigma(z')\dfrac{\Sigma_\sigma(z)-\Sigma_\sigma(z')}{z'-z}\Big]dz' \\ Q_\sigma(z) = \dfrac{i}{2\pi}\oint_C f(z')\Big[\{1+\Sigma_\sigma(z')G_\sigma(z')\}\,\dfrac{\Sigma_\sigma(z)-\Sigma_\sigma(z')}{z'-z}\Big]dz' \end{cases}$$

$$z_1 \equiv z - \epsilon_\sigma + \epsilon_{\bar\sigma} \\ z_2 \equiv -z + \epsilon_\sigma + \epsilon_{\bar\sigma} + U \\ u(z) \equiv U^{-1}\big[U - z + \epsilon_\sigma + \\ + \Sigma_\sigma(z) + \Sigma_{\bar\sigma}(z_1) - \Sigma_{\bar\sigma}(z_2)\big]$$

Input parameters

- Quantum dot levels $\epsilon_\uparrow, \epsilon_\downarrow$
- Coulomb on-site repulsion U
- Self-energy for the $U = 0$ problem:

$\Sigma_\sigma(z)$ encodes everything about the external network

$$\Sigma_\sigma(z) \equiv \sum_{k\alpha}\frac{|V_{k\alpha\sigma}|^2}{z-\epsilon_{k\alpha\sigma}} = z - \epsilon_\sigma - [G_\sigma(z)]^{-1}_{U=0}$$

Exactly solvable case I

- At the particle-hole symmetric point of Anderson Hamiltonian…

$$\boxed{2\epsilon_\sigma + U = 0 \text{ and } \Sigma_\sigma(z) = \Sigma_\sigma^*(-z)}$$

- …equations lead to *temperature-independent* Green function

$$[G_\sigma(z)]^{-1} = z - \Sigma_\sigma(z) - \frac{U^2}{4\,[z-\Sigma_\sigma(z)-2\Sigma_{\bar\sigma}(z)]}$$

- Breaks a Fermi liquid relation (S-matrix unitarity at T=0)

$$\text{Im}\,[G_\sigma(0)]^{-1} \neq -\text{Im}\,[\Sigma_\sigma(0)]^{-1}$$

- **Good news:** any deviation from exact symmetry restores temperature dependence and saves the Fermi liquid relation

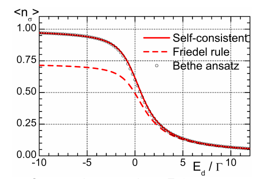
Exactly solvable case II

$\boxed{U\to\infty \text{ and } \Sigma_\sigma(z) = \text{const}}$ Generalization to the method of Bloomfield and Hamann [5]

- Non-linear coupled equations are re-written in terms of sectionally holomorphic functions → A combination of unknown functions is proven to be fully holomorphic, thus polynomial → Two independent **linear Riemann-Hilbert problems**
- Asymptotic and self-consistency conditions → Two independent **linear Riemann-Hilbert problems**
- Asymptotic and self-consistency conditions → Transcendent equations for **three real self-consistent parameters** (including $\langle n_\sigma\rangle$)
- Two independent **linear Riemann-Hilbert problems** → **Explicit solution** containing a Cauchy-type integral and self-consistent parameters
- Transcendent equations for **three real self-consistent parameters** (including $\langle n_\sigma\rangle$) → **Explicit solution** containing a Cauchy-type integral and self-consistent parameters

Results

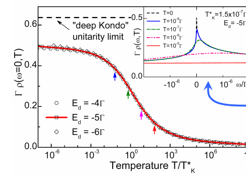
$$\epsilon_\uparrow = \epsilon_\downarrow \equiv \epsilon_0;\ U\to\infty \\ \Sigma_\uparrow = \Sigma_\downarrow = -i\Gamma$$



Quantum dot occupation at T=0.

At zero temperature

- Correct scaling with $E_d = \epsilon_0 + (\Gamma/\pi)\ln(D/\Gamma)$
- Self-consistent $\langle n_\sigma\rangle$ agree within 3% with Bethe ansatz
- $\langle n_\sigma\rangle$ from the Friedel sum rule is underestimated in the Kondo regime

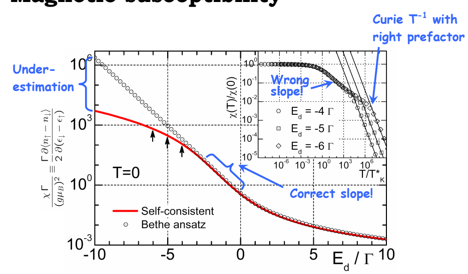


The density of states at the Fermi level.

At finite temperature

- Temperature dependencies scale with T/T_K^*, where $T_K^* = \Gamma e^{\pi E_d/\Gamma} = D e^{-\pi|\epsilon_0|/\Gamma}$
- The Kondo peak melts away for $T > T_K^*$.
- Correct high-T asymptotics
- Note: exact $T_K/\Gamma = \sqrt{T_K^*/\Gamma}$

Magnetic susceptibility



Conclusions

- Equations-of-motions can describe physical properties over a wide parameter range.
- High order truncation and self-consistency are essential in the Kondo regime.
- Limiting cases provide comprehensive analytical tests, while general equations need to be solved numerically.

References

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