Solution of the Anderson impurity model via the functional renormalization group

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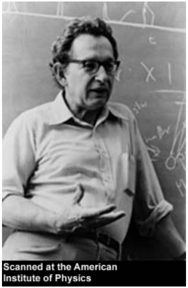
Simon Streib, Aldo Isidori, and Peter Kopietz, Phys. Rev. B 87, 201107(R), 2013

Anderson Impurity Model

- localized impurity in contact with a conduction bath (Anderson, 1961)



$$\begin{aligned}\hat{H} \;&=\; \sum_{k\sigma} (\epsilon_k - \sigma H)\, \hat{c}^\dagger_{k\sigma} \hat{c}_{k\sigma} + \sum_{\sigma} (E_d - \sigma H)\, \hat{d}^\dagger_{\sigma} \hat{d}_{\sigma} \\ &\quad + U \hat{d}^\dagger_{\uparrow} \hat{d}_{\uparrow} \hat{d}^\dagger_{\downarrow} \hat{d}_{\downarrow} + \sum_{k\sigma} \left(V_k^* \hat{d}^\dagger_{\sigma} \hat{c}_{k\sigma} + V_k \hat{c}^\dagger_{k\sigma} \hat{d}_{\sigma} \right)\end{aligned}$$

- ϵ_k: dispersion of the conduction electrons
- E_d: atomic energy of the localized impurity state
- V_k: hybridization energy
- U: on-site interaction of the impurity electrons
- H: Zeemann energy due to an external magnetic field

Impurity action

- integrate over conduction electrons $\rightarrow$ impurity action

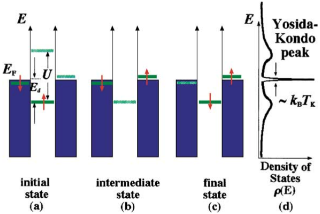
$$S_{\text{imp}} = -\int_\omega \sum_\sigma G_{0,\sigma}^{-1}(i\omega)\bar{d}_{\omega\sigma} d_{\omega\sigma} + U \int_0^{1/T} d\tau \, n_\uparrow n_\downarrow$$

- bare Green's function (here only particle-hole symmetric case)

$$G_{0,\sigma}(i\omega) = \frac{1}{i\omega + U/2 + \sigma H + i\Delta \operatorname{sgn}\omega}$$

- $\Delta = \pi |V|^2 \rho(0)$ hybridization energy

- experimental realization in quantum dots:



Exact and approximate results on the AIM

- spin- and charge susceptibilities from Bethe-Ansatz (Wiegmann, Andrei, Kawakami, Okiji, 1980-81)

$$\begin{aligned}\pi\Delta\chi_s &= \sqrt{\frac{2}{\pi u}} e^{\pi^2 u/8} \int_0^\infty dx e^{-x^2/(2u)} \frac{\cos(\pi x/2)}{1-x^2}, \\ \pi\Delta\chi_c &= \sqrt{\frac{2}{\pi u}} e^{-\pi^2 u/8} \int_0^\infty dx e^{-x^2/(2u)} \frac{\cosh(\pi x/2)}{1+x^2}.\end{aligned}$$

- in strong coupling regime ($u \equiv U/(\pi\Delta) \gtrsim 2$) there is only one energy scale (Kondo temperature)

$$T_K = \Delta\sqrt{\frac{\pi u}{2}} e^{-\frac{\pi^2 u}{8}+\frac{1}{2u}} \quad , \quad \chi_s \sim 1/(2T_K) \quad , \quad Z \sim 2/(\pi\Delta\chi_s)$$

- all previous FRG studies have so far failed to reproduce correct exponential Kondo scale in χ_s and Z.

Partial bosonization of the interaction

- Partial bosonization of the interaction ($U = U_\parallel + U_\perp$):

$$U n_\uparrow(\tau) n_\downarrow(\tau) = U_\parallel n_\uparrow(\tau) n_\downarrow(\tau) - U_\perp \bar{s}(\tau) s(\tau)$$

$$s(\tau) = \bar{d}_\downarrow(\tau) d_\uparrow(\tau), \text{ and } \bar{s}(\tau) = \bar{d}_\uparrow(\tau) d_\downarrow(\tau)$$

- Hubbard-Stratonovich transformation:

$$\int \mathcal{D}\left[\bar{\chi}, \chi\right] e^{\int_{\bar{\omega}} \left(-U_\perp^{-1} \bar{\chi}_{\bar{\omega}} \chi_{\bar{\omega}} - \bar{s}_{\bar{\omega}} \chi_{\bar{\omega}} - s_{\bar{\omega}} \bar{\chi}_{\bar{\omega}} \right)} = e^{U_\perp \int_{\bar{\omega}} \bar{s}_{\bar{\omega}} s_{\bar{\omega}}},$$

- Partially bosonized action:

$$\begin{aligned} S_0[\bar{d}, d, \bar{\chi}, \chi] &= -\int_\omega \sum_\sigma G_{0,\sigma}^{-1}(i\omega) \bar{d}_{\omega\sigma} d_{\omega\sigma} + \int_{\bar{\omega}} U_\perp^{-1} \bar{\chi}_{\bar{\omega}} \chi_{\bar{\omega}}, \\ S_1[\bar{d}, d, \bar{\chi}, \chi] &= \int_{\bar{\omega}} \left(\bar{s}_{\bar{\omega}} \chi_{\bar{\omega}} + s_{\bar{\omega}} \bar{\chi}_{\bar{\omega}} \right) + U_\parallel \int_0^{1/T} \mathrm{d}\tau \, n_\uparrow(\tau) n_\downarrow(\tau). \end{aligned}$$

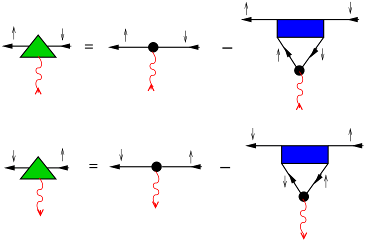
Skeleton equations

- bosonic self-energy in terms of three-legged vertex:

$$\Pi_{\perp}\left(i\bar{\omega}\right) = -\int_{\omega} \Gamma^{\bar{d}_{\uparrow} d_{\downarrow} \chi}\left(\omega, \omega - \bar{\omega}; \bar{\omega}\right) G_{\uparrow}\left(i\omega\right) G_{\downarrow}\left(i\omega - i\bar{\omega}\right)$$

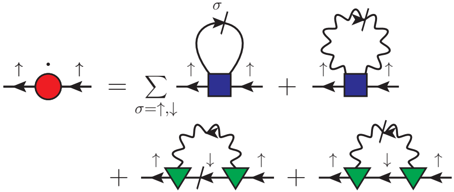
- three and four legged vertices are not independent:

$$\begin{aligned} \Gamma^{\bar{d}_{\uparrow} d_{\downarrow} \chi}\left(\omega + \bar{\omega}, \omega; \bar{\omega}\right) \quad &= \quad 1 - \int_{\omega'} G_{\uparrow}\left(i\omega' + i\bar{\omega}\right) G_{\downarrow}\left(i\omega'\right) \\ &\quad \times \tilde{\Gamma}^{\bar{d}_{\uparrow} \bar{d}_{\downarrow} d_{\downarrow} d_{\uparrow}}\left(\omega + \bar{\omega}, \omega'; \omega, \omega' + \bar{\omega}\right) \end{aligned}$$



FRG with magnetic field cutoff

- use the external magnetic field H as an FRG flow paramater: $\Lambda = H$ [Edwards and Hewson, J. Phys.: Cond. Mat. 23, 045601 (2011)]
- additional bosonic regulator: $U_{\perp}^{-1} = U^{-1} + R_H$ with $R_0 = 0$ and $R_{\infty} = \infty$
- fermion propagator: $G_{\sigma}^{-1}(i\omega) = G_{0,\sigma}^{-1}(i\omega) - \Sigma_{\sigma}(i\omega)$
- boson propagator: $F_{\perp}^{-1}(i\bar{\omega}) = U_{\perp}^{-1}(H) - \Pi_{\perp}(i\bar{\omega})$
- single scale propagators: $\dot{G}_{\sigma}\,(i\omega) = -\sigma G_{\sigma}^{2}\,(i\omega),\ \dot{F}_{\perp}\,(i\bar{\omega}) = -\frac{\partial R_H}{\partial H} F_{\perp}^{2}\,(i\bar{\omega})$
- FRG flow equation: $\dfrac{\partial \Sigma_{\uparrow}(i\omega)}{\partial H} =$



Low-energy expansion

- neglect the frequency-dependence of the vertices:

$$\Gamma_4^{\bar{d}_\sigma \bar{d}_{\sigma'} d_{\sigma'} d_\sigma}(\omega_1, \ldots, \omega_4) \approx \Gamma_4^{\bar{d}_\sigma \bar{d}_{\sigma'} d_{\sigma'} d_\sigma}(0)$$

$$\Gamma_4^{\bar{d}_\sigma d_\sigma \bar{\chi}\chi}(\omega_1, \ldots, \bar{\omega}_4) \approx \Gamma_4^{\bar{d}_\sigma d_\sigma \bar{\chi}\chi}(0)$$

$$\Gamma_3^{\bar{d}_\uparrow d_\downarrow \chi}(\omega_1, \omega_2, \bar{\omega}_3) \approx \Gamma_3^{\bar{d}_\uparrow d_\downarrow \chi}(0) \equiv \gamma$$

- expand the fermionic self-energy:

$$\Sigma_\sigma(i\omega) = U/2 - \sigma M + (1 - Z^{-1}) i\omega + \mathcal{O}(\omega^2)$$

  - flowing parameters M and Z
  - for $H \to \infty$, $\quad M \to U/2$ and $Z \to 1$ (Hartree-Fock)

- how to close the FRG hierarchy?
  - bosonic self-energy $\Pi_\perp(i\bar{\omega})$ $\to$ skeleton equation [Bartosch *et al.* (2009)]
  - flow equations for the vertices $\to$ Ward identities

Ward identities

- Koyama-Tachiki Ward identities [Prog. Theor. Phys. Supp. **80**, 108 (1984)]

$$\Gamma^{\bar{d}_\sigma d_{-\sigma} \chi_\sigma}(0,0;0) \equiv \gamma = \frac{H+M}{H+U_\perp s}, \quad \chi_\perp = \frac{\Pi_\perp(i0)}{1-U_\perp \Pi_\perp(i0)} = \frac{s}{H},$$

where magnetic moment $s = \frac{\langle n_\uparrow - n_\downarrow \rangle}{2}$ satisfies Friedel sum rule:

$$s = \frac{1}{\pi} \arctan\left(\frac{H+M}{\Delta}\right)$$

- Yamada-Yosida Ward identities [Yamada-Yosida, Prog. Theor. Phys. (1975); Kopietz *et al.*, J. Phys. A: Math. Theor. **43**, 385004 (2010)]

$$Z^{-1} = \frac{\tilde{\chi}_c + \tilde{\chi}_\parallel}{2} \quad , \quad \rho \Gamma_\perp^{(4)} = -\frac{\tilde{\chi}_c - \tilde{\chi}_\parallel}{2}$$

where $\tilde{\chi}_c = \chi_c/\rho$, $\tilde{\chi}_\parallel = \chi_\parallel/\rho$ and $\Gamma_\perp^{(4)} = \Gamma^{\bar{d}_\sigma \bar{d}_{\sigma'} d_{\sigma'} d_\sigma}(0,0;0,0)$ is the full four-point vertex (without bosonization)

Restoring rotational invariance in FRG flow

- flow equation for Z: $\frac{\partial \ln Z}{\partial \ln H} = ZH \lim_{\omega \to 0} \frac{\partial}{\partial(i\omega)} \frac{\partial \Sigma_\sigma(i\omega)}{\partial H}$
- flow equation for M: $\frac{\partial M}{\partial H} = -\sigma \frac{\partial}{\partial H} \Sigma_\sigma(i0)$
- problem: (truncated) FRG flow equation for M does not restore the rotational invariance for $H \to 0$:

$$\lim_{H \to 0} M \neq 0!$$

- solution: use Yamada-Yosida Ward identities to derive an alternative flow equation which restores rotational invariance for $H \to 0$:

$$\frac{\partial M}{\partial H} = \rho \Gamma_\perp^{(4)} + \frac{1}{Z} - 1 \approx \frac{1}{1+b^2} \frac{b}{\arctan b} \left[\frac{b}{h} - \frac{1}{Z} \right] + \frac{1}{Z} - 1$$

where $b = (H + M)/\Delta$ and $h = H/\Delta$.

- $\Rightarrow \lim_{H \to 0} M = 0$ without fine-tuning.

Initial conditions and bosonic regulator

- start FRG flow for $H \to \infty \Rightarrow$ first order perturbation theory becomes exact; small parameter: U/H:

$$\Sigma_\sigma^{(1)}(i\omega) = \frac{U}{2} - \sigma\frac{U}{2} \Rightarrow Z_0 = 1,\ M_0 = \frac{U}{2},\ \text{for } H \to \infty$$

- bosonization depends on the bosonic regulator: $U_\perp^{-1} = U^{-1} + R_H$
  use two-slope function: $r = \pi\Delta^2 R_H = \begin{cases} \alpha H & \text{for } H \lesssim \Delta \\ \beta H & \text{for } H \gtrsim \Delta \end{cases}$,

- ansatz: $\alpha(u) = \frac{\alpha_0}{\alpha_2+u^2}$, $\beta(u) = \frac{\beta_1 u}{\beta_2+u^2}$, with $u = \frac{U}{\pi\Delta}$
  need four constraints to fix four parameters $\alpha_0, \alpha_2, \beta_1, \beta_2$.

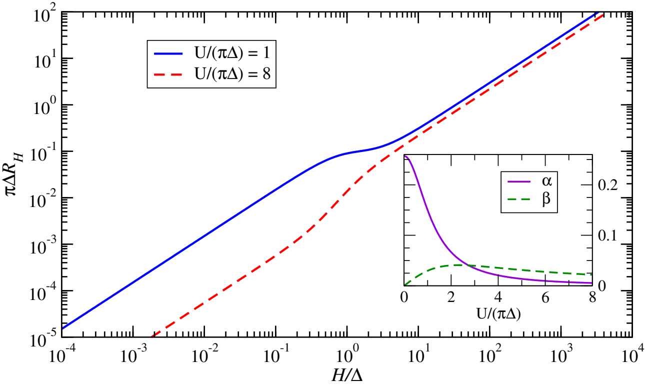
- two constraints: weak coupling limit for $\tilde{\chi}_s$ and Z (e.g., at $u = 0.1$)

- two more constraints: strong coupling limit of Wilson ratio $R_W = 2$ for two strong coupling values (e.g., $u = 4$, $u = 8$).

$$R_W = \tilde{\chi}_s Z = 2\tilde{\chi}_s/(\tilde{\chi}_s + \tilde{\chi}_c) \to 2,\ u \gtrsim 2$$

Our bosonic regulator

- two-slope function: $\pi\Delta^2 R_H = (\alpha - \beta)\frac{h}{1+h^2} + \beta h$



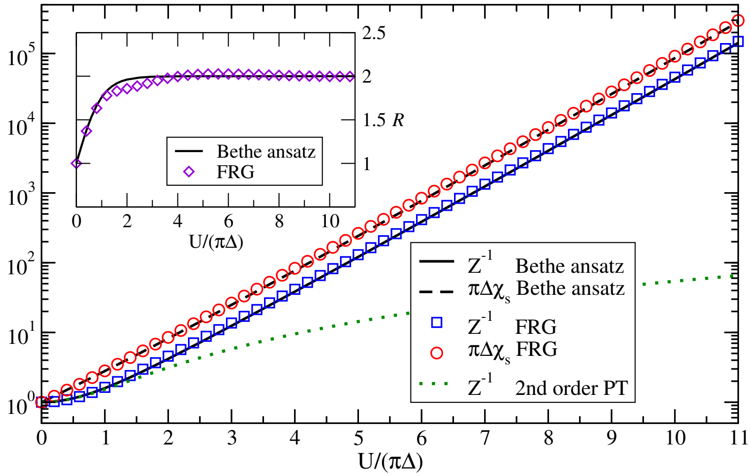
$$\alpha(u) = \frac{\alpha_0}{\alpha_2 + u^2}$$

$$\beta(u) = \frac{\beta_1 u}{\beta_2 + u^2}$$

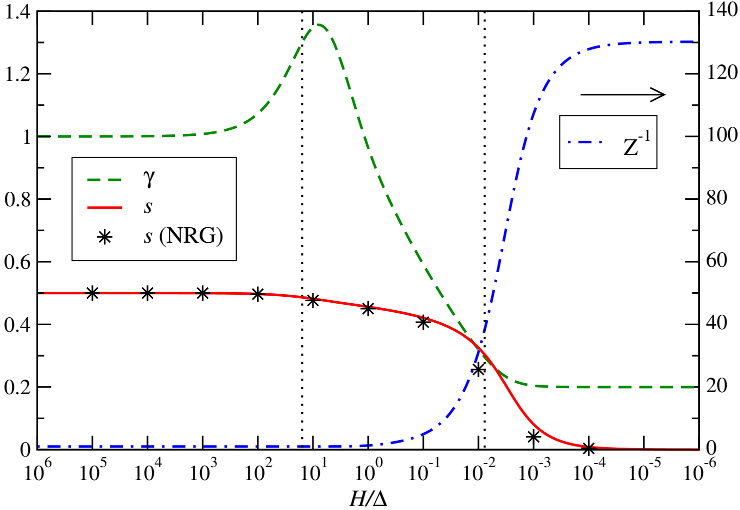
$$u \equiv U/(\pi\Delta)$$

- matching exact weak- and strong-coupling limits $\rightarrow$ $\alpha_0 \approx 0.36, \quad \alpha_2 \approx 1.4$, $\beta_1 \approx 0.19, \quad \beta_2 \approx 5.4$

Quasiparticle residue and spin-susceptibility at $H = 0$



Magnetic field behavior at strong-coupling, $U/(\pi\Delta) = 5$



Summary and Outlook

- FRG approach with external magnetic field as physical flow parameter
- bosonization of transverse spin fluctuations
- interaction vertices constrained by Ward identities
- correct Kondo scale in the quasiparticle residue and spin susceptibility
- magnetic field dependence of physical observables in agreement with Bethe-ansatz
- next:generalization to non-equilibrium [Yamada-Yoshida Ward identities: Oguri, Phys. Rev. B **64**, 153305 (2001)]
- apply to pseudogap-AIM