EXERCISES

Computational Materials Science

Prof. K. Held

SHEET 3

Exercise 3: Anderson impurity model

1) Write an exact diagonalization code for the Anderson impurity model (AIM)

$$H = \sum_{\sigma k=1}^{N_b} \epsilon_k n_{k\sigma} + U n_\uparrow n_\downarrow + (\epsilon - eV_G) \sum_\sigma n_\sigma + \sum_{\sigma k=1}^{N_b} V_k c^\dagger_{k\sigma} c_\sigma + h.c. \qquad (1)$$

in the computer language of your choice. Here, N_b is the number of bath sites; $n_x = c^\dagger_x c_x$.

2) Apply it to calculate the average number of electron $n_0 = \langle n_\uparrow + n_\downarrow \rangle$ on the impurity vs. applied gate voltage V_G at zero temperature, and from that the conductance through the quantum dot. Use a parameteritzation of the bath that (as far as this is possible with a few discrete levels) describes a flat conduction electron density of states (DOS).

To this end you can use the Friedel sum rule which states at zero temperature (s. Hewson, *The Kondo problem to Heavy Fermions*)

$$A(\omega = 0) = \frac{\sin^2(\pi/2 \times n_0)}{\pi\Gamma/2} \qquad (2)$$

where n_0 is the average number of electrons on the impurity, $\Gamma = \Gamma_L + \Gamma_R$; $\Gamma_\lambda = 2\pi V_\lambda^2 \rho_\lambda$ the scattering rate; ρ_λ the (supposedly ω-independent) DOS of the conduction electrons in lead λ.

Deliverables (per email to held@ifp.tuwien.ac.at): Program-Code, figure n_0 vs. eV_g, txt-file describing parameters used etc.

You can explore your own paths beyond:
For example, you can (i) study different number of bath sites and parameterizations thereof and analyze the stability of the results, (ii) calculate the full Green's function of the AIM, (iii) calculate other expectation values such as the impurity spin-spin correlation function $\langle S^z_{00}(t) S^z_{00}(0) \rangle$, or (iv) study a non-interacting model with impurity energy levels obtained from random matrix theory.