Computational Many-Body Physics

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Sheet 6: return on: Monday, July 4, 2016, 14:00

Exercise 1: entanglement entropy for one-dimensional spin models

(8 points + 4 bonus points)

The entanglement entropy $S_{\rm e}$ has been introduced in exercise 4 on sheet 5 and applied to various states $|\psi\rangle$ for a system of M spins, with a bi-partitioning into parts A (with $M_{\rm A}$ sites) and B. In this exercise, the state $|\psi\rangle$ is taken as the ground state of the spin models defined in exercise 3 on sheet 4, i.e.

$$H = -\sum_{i=1}^{M-1} \sum_{\alpha} J_i^\alpha S_i^\alpha S_{i+1}^\alpha \ ,$$

and different choices for the J_i^α.

Calculate $S_{\rm e}$ as a function of $M_{\rm A}$ ($M_{\rm A} = 1, 2, \ldots, M-1$) for fixed M and the state $|\psi\rangle$ given as the ground state of the following three models:

a) $J_i^\alpha = J\delta_{\alpha z}$, (4 points)

b) $J_i^\alpha = J$, (4 points)

c) $J_i^\alpha = \begin{cases} J\delta_{\alpha x} & : i \text{ even,} \\ J\delta_{\alpha z} & : i \text{ odd.} \end{cases}$ (4 bonus points)

The total number of sites can be fixed to $M = 8$; consider both $J = +1$ and $J = -1$. If the ground state happens to be degenerate, the calculations should be performed for one of the ground states.

Exercise 2: integral representation of the single-impurity Anderson model

(8 points)

The Hamiltonian of the single-impurity Anderson model in the 'integral representation' has the following form:

$$H = H_{\rm imp} + H_{\rm bath} + H_{\rm imp-bath} \ ,$$

with

$$H_{\mathrm{imp}} = \sum_\sigma \varepsilon_{\mathrm{f}} f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow \ , \tag{1}$$

$$H_{\mathrm{bath}} = \sum_\sigma \int_{-1}^{1} \mathrm{d}\varepsilon \, g(\varepsilon) a_{\varepsilon\sigma}^\dagger a_{\varepsilon\sigma} \ , \tag{2}$$

$$H_{\mathrm{imp-bath}} = \sum_\sigma \int_{-1}^{1} \mathrm{d}\varepsilon \, h(\varepsilon) \Big(f_\sigma^\dagger a_{\varepsilon\sigma} + a_{\varepsilon\sigma}^\dagger f_\sigma \Big). \tag{3}$$

a) Use the equation of motion method to show that the impurity Green function $G_\sigma(z) = \langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle_z$ for the case $U = 0$ is given by

$$G_\sigma(z) = \frac{1}{z - \varepsilon_{\mathrm{f}} - \bar{\Delta}(z)} \ , \quad \text{with} \ \ \bar{\Delta}(z) = \int_{-1}^{1} \mathrm{d}\varepsilon \frac{h(\varepsilon)^2}{z - g(\varepsilon)} \ . \tag{4}$$

(The derivation is analogous to the one shown in Sec. 2.2.4 in the lecture.)
(5 points)

b) Starting from the expression for $\bar{\Delta}(z)$ in eq. (4), show that the hybridization function $\Delta(\omega) = -\lim_{\delta\to 0} \mathrm{Im}\bar{\Delta}(z = \omega + i\delta)$ is given by

$$\Delta(\omega) = \pi h(g^{-1}(\omega))^2 \frac{\mathrm{d}}{\mathrm{d}\omega} g^{-1}(\omega) \ .$$

(One can assume here that the function $f(\varepsilon) = \omega - g(\varepsilon)$ is zero for a single value of ε only.)
(3 points)

Exercise 3: logarithmic discretization of the single-impurity Anderson model

(4 points)

The conduction electron part of the Hamiltonian, H_{bath} (see eq. (2) in exercise 2), can be written in the form

$$\begin{aligned} H_{\mathrm{bath}} &= \sum_{np\sigma} \Big(\xi_n^+ a_{np\sigma}^\dagger a_{np\sigma} + \xi_n^- b_{np\sigma}^\dagger b_{np\sigma} \Big) \\ &+ \sum_{n,p\neq p',\sigma} \Big(\alpha_n^+(p,p') a_{np\sigma}^\dagger a_{np'\sigma} - \alpha_n^-(p,p') b_{np\sigma}^\dagger b_{np'\sigma} \Big) \ , \end{aligned} \tag{5}$$

with the definitions of the operators $a_{np\sigma}$ and $b_{np\sigma}$ given in the lecture. For a constant hybridization function $\Delta(\omega) = \Delta$ we can simply set the dispersion as $g(\varepsilon) = \varepsilon$. Show that in this case the quantities $\xi_n^\pm$ and $\alpha_n^\pm$ are given by:

$$\xi_n^\pm = \pm \frac{1}{2} \Lambda^{-n} (1 + \Lambda^{-1}) \ ,$$

$$\alpha_n^\pm(p,p') = \frac{1 - \Lambda^{-1}}{2\pi i} \frac{\Lambda^{-n}}{p' - p} \exp\left[\frac{2\pi i (p' - p)}{1 - \Lambda^{-1}} \right] \ .$$

Exercise 4: flow diagrams for the tight-binding model

(5 points + 3 bonus points)

Consider the following quantum impurity model defined on a chain with $N+1$ sites:

$$H = \varepsilon f^\dagger f + V\left(f^\dagger c_1 + c_1^\dagger f\right) + \sum_{n=1}^{N-1} t_n \left(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n\right) \ . \tag{6}$$

This model corresponds to a tight-binding model of spinless fermions with a special choice of parameters, in particular, the hoppings t_n are assumed to fall off exponentially: $t_n = \Lambda^{-n/2}$ with $\Lambda = 2$. As the Hamiltonian eq. (6) is non-interacting, it can be diagonalized via an orthogonal transformation (see Sec. 2.1 in the lecture). This gives the single-particle spectrum from which the many-particle energies can be constructed.

The lowest-lying many-particle energies $E_N(r)$ ($r = 1, \ldots, r_{\rm max}$ and we assume $E_N(r) \leq E_N(r+1)$) for a chain with N bath sites can now be used to plot the energy-level flow diagram, i.e. $\Lambda^{N/2} E_N(r)$ as a function of N.

a) Plot the five ($r_{\rm max} = 5$) lowest-lying many-particle energies in this way for $\varepsilon = 0$, $V = 0.1$, and N in the range $N = 3, \ldots, 20$. (5 points).

b) Investigate the effect of the value of ε on the flow diagram by varying ε in the range [-2,2]. (3 bonus points).

Exercise 5: flow diagrams for the one-dimensional Heisenberg model

(5 points + 3 bonus points)

Now consider a somewhat artificial model, the one-dimensional Heisenberg model with nearest-neighbour interactions decaying exponentially:

$$H = -\sum_{n=1}^{N-1} \sum_{\alpha} J_n^\alpha S_n^\alpha S_{n+1}^\alpha \ ,$$

with $J_n^\alpha = J \Lambda^{-n/2}$.

a) Calculate the energy-level flow diagram, i.e. plot $\Lambda^{N/2} E_N(r)$ for the lowest-lying energies $E_N(r)$ as a function of N for $2 \leq N \leq 10$, $\Lambda = 2$, $J = \pm 1$ via the full diagonalization of the Hamilton matrix for each N separately (not via an iterative diagonalization scheme as in the NRG). (5 points)

b) Investigate the effect of a local perturbation of the form

$$H' = -\gamma S_1^x S_2^x \ ,$$

on the flow diagram for various values of γ. (3 bonus points)