NRG with Bosons

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Outline

 Quantum impurity problems couple a local degree of freedom to an extended, noninteracting host:

$$H = H_{\rm host} + H_{\rm host-imp} + H_{\rm imp}$$



- The NRG provides controlled nonperturbative solutions of problems involving fermions (T. Costi's talk).
- Extension of the NRG to problems involving bosons ...
 - Inclusion of local bosons Anderson-Holstein model
 - Formulation for bosonic hosts spin-boson model
 - Combined approach for fermionic + bosonic hosts Bose-Fermi Kondo model

I. Review: Fermionic NRG

• The NRG was developed for problems with fermionic hosts, e.g.,

$$H_{\text{Kondo}} = H_{\text{host}} + J \mathbf{S}_{\text{imp}} \cdot \mathbf{s}_{\text{host}} (\mathbf{r}_{\text{imp}}),$$

where

$$H_{\text{host}} = \sum_{k,\sigma} \mathcal{E}_k c_{k\sigma}^{\dagger} c_{k\sigma}.$$

- A fundamental challenge of the Kondo model is the equal importance of spin-flip scattering of band electrons on every energy scale ε on the range $-D \le \varepsilon \le D$.
- Poor man's scaling attempts to tackle this, but it is perturbative in the renormalized Kondo coupling and thus limited to temperatures $T > T_K$ (A. Nevidomskyy's talk).
- The NRG was conceived to reliably reach down to T = 0.

Chain mapping of any host

 Any noninteracting host can be mapped exactly to a tightbinding form on one or more semi-infinite chains:



• Start with $|f_0\rangle = \text{host state entering } H_{\text{host-imp}}$ • Since $i\hbar \frac{d}{dt} |\Psi\rangle = H |\Psi\rangle$,

reach only host states given by repeated action of H_{host}

• Lanczos (1950): $H_{\text{host}} |f_0\rangle = e_0 |f_0\rangle + t_1 |f_1\rangle$ $H_{\text{host}} |f_1\rangle = e_1 |f_1\rangle + t_1 |f_0\rangle + t_2 |f_2\rangle$ $H_{\text{host}} |f_2\rangle = e_2 |f_2\rangle + t_2 |f_1\rangle + t_3 |f_3\rangle$ etc

Chain mapping of a conduction band

 Any noninteracting host can be mapped exactly to a tightbinding form on one or more semi-infinite chains:



• The conduction band in the Kondo model maps to $H_{\text{host}} = \sum_{\sigma} \sum_{n=0}^{\infty} \left[e_n f_{n\sigma}^{\dagger} f_{n\sigma} + t_n \left(f_{n\sigma}^{\dagger} f_{n-1,\sigma} + \text{H.c.} \right) \right] + \text{decoupled}$ part

- Since the basis grows by a factor of 4 for each chain site, we would like to diagonalize *H* on finite chains. But ...
 - Coefficients e_n , t_n are all of order the half-bandwidth.
 - No useful truncations: Ground state for chain length L is not built just from low-lying states for chain length L 1.

NRG's key feature: Band discretization

- Wilson (~1974) introduced a logarithmic discretization of the conduction band: $\Lambda > 1$
- Approximation: The impurity couples to just one state per bin $H_{\text{host},\Lambda} = \sum_{\sigma} \sum_{m=0}^{\infty} \omega_m \left(a_{m\sigma}^{\dagger} a_{m\sigma} - b_{m\sigma}^{\dagger} b_{m\sigma} \right) - \omega_m = \frac{1}{2} \left(1 + \Lambda^{-1} \right) \Lambda^{-m} D$
- Now apply Lanczos to the discretized band:



NRG iterative solution

• Wilson's artificial separation of bin energy scales $\propto \Lambda^{-m}$ gives exponential decaying tight-binding coefficients:

$$H_{\text{host},\Lambda} = \sum_{\sigma} \sum_{n=0}^{\infty} \left[e_n f_{n\sigma}^{\dagger} f_{n\sigma} + t_n \left(f_{n\sigma}^{\dagger} f_{n-1,\sigma} + \text{H.c.} \right) \right] \quad \left| e_n \right|, t_n \leq c D \Lambda^{-n/2}$$

$$\stackrel{\text{hopping coefficient}}{\stackrel{1}{\checkmark} 0 \quad 1 \quad 2 \quad 3 \quad 4} \quad (\text{not a } \Lambda^{-n} \text{ decay!})$$

$$\stackrel{\text{site index}}{\stackrel{\text{site index}}}$$

- Allows iterative solution on chains of length L = 1, 2, 3, ...
 - Ground state for chain length L is mainly built from lowlying states for chain length L - 1.
 - Thus, can truncate the Fock space after each iteration.

NRG iterative solution



What does NRG give?

- The solutions of $H_{\text{host},\Lambda}$ can be used to calculate the value X_{host} of a bulk property in the pure host (without impurity).
- Solutions of

$$H = H_{\text{host},\Lambda} + H_{\text{host-imp}} + H_{\text{imp}}$$

give the value X_{total} in the full system with the impurity.

- Both X_{host} and X_{total} vary strongly with the discretization Λ .
- <u>But</u> the value of

$$X_{\rm imp} = X_{\rm total} - X_{\rm host}$$

varies only weakly with Λ .

• Can use $2 \le \Lambda \le 10$ to estimate the physical ($\Lambda = 1$) value.

II. Fermionic NRG with Local Bosons

- Now want to extend the method to problems with bosons.
- Simplest: Impurity couples to a single local boson mode (e.g., an optical phonon).
- Example: the Anderson-Holstein model

$$H_{\text{host}} = \sum_{\mathbf{k},\sigma} \varepsilon_k c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma},$$
$$H_{\text{host-imp}} = \frac{V}{\sqrt{N_k}} \sum_{\mathbf{k},\sigma} \left(d_{\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \text{H.c.} \right),$$
$$H_{\text{imp}} = \varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} \left(+ \omega_0 a^{\dagger} a + \lambda (n_d - 1) (a + a^{\dagger}) \right)$$

Holstein coupling of impurity

charge to oscillator displacement x

Anderson-Holstein model

$$H = H_{\text{Anderson}} + \omega_0 a^{\dagger} a + \lambda (n_d - 1) (a + a^{\dagger})$$

1. Haldane (1977) proposed the model to describe mixedvalent rare-earth compounds, e.g. CeAl₃, YbAl₂.

Local boson describes fast changes in 3d charge distribution in response to slower fluctuations in 4f occupancy, e.g. Ce $4f^0(4+) \leftrightarrow 4f^1(3+)$.

It is also a one-impurity version of a model (Anderson, 1975) for enhanced superconductivity due to "negative-U" centers in amorphous semiconductors.

Local boson describes oscillations of a covalent bond length.

Anderson-Holstein model

$$H = H_{\text{Anderson}} + \omega_0 a^{\dagger} a + \lambda (n_d - 1) (a + a^{\dagger})$$

3. Over the last 20 years, the model has been applied to quantum dots (Li et al., 1995, and many since) and single-molecule devices.



• "Anderson-Holstein" name: Hewson and Meyer (2002).

Decoupled limit

- Let's specialize to the symmetric case $\varepsilon_d = -U/2$. Then can rewrite

$$H_{\rm imp} = \frac{1}{2}U(n_d - 1)^2 + \omega_0 a^{\dagger}a + \lambda(n_d - 1)(a + a^{\dagger}).$$

• Consider the decoupled limit of zero hybridization V = 0. Now n_d is fixed and can use a displaced oscillator mode

$$b = a + (\lambda / \omega_0)(n_d - 1)$$

to write

$$H_{\rm imp} = \frac{1}{2} U_{\rm eff} (n_d - 1)^2 + \omega_0 b^{\dagger} b$$

where

$$U_{\rm eff} = U - 2\lambda^2 / \omega_0.$$

Decoupled limit

• Since only states with $n_d \neq 1$ can benefit from the bosonic coupling, get a reduction in the effective on-site repulsion:



• For $\lambda > \lambda_0 = \sqrt{\omega_0 U/2}$, decoupled impurity has a chargedoublet ground state $n_d = 0, 2$.

Decoupled limit

• How many bosons are there in the ground state?

• From
$$H_{\rm imp} = \frac{1}{2}U_{\rm eff} (n_d - 1)^2 + \omega_0 b^{\dagger} b$$

it is obvious that in the displaced oscillator basis

$$\left\langle b^{\dagger}b
ight
angle _{GS}=0.$$

• What about the original bosons $a = b - (\lambda / \omega_0)(n_d - 1)$?

$$ig\langle a^{\dagger}aig
angle_{GS} = ig\langle b^{\dagger}big
angle_{GS} - (\lambda/\omega_0)(n_d-1)ig\langle b+b^{\dagger}ig
angle_{GS} + (\lambda/\omega_0)^2(n_d-1)^2 = (\lambda/\omega_0)^2(n_d-1)^2.$$

• $P(n_a)$ is a Poisson distribution with mean $(\lambda/\omega_0)^2$ and standard deviation λ/ω_0 .

Full problem

• For V > 0, n_d is no longer fixed. Tunneling of an electron to/from the band creates & destroys a cloud of bosons as the oscillator adjusts to the new dot occupancy:

$$V \rightarrow V \exp\left\{ (\lambda / \omega_0) (b - b^{\dagger}) \right\}$$
 [Lang & Firsov (1962)].

- Adiabatic limit $\omega_0 \ll \Delta = \pi \rho(\varepsilon = 0) V^2$: Bosons can't adjust to changes in n_d , so don't affect the Kondo physics of Anderson model.
- Instantaneous limit $\omega_0 \gg \Delta$: Bosons are always relaxed w.r.t. instantaneous value of n_d . For $\omega_0 \gg U$, recover Anderson model physics with $U \rightarrow U_{\rm eff} = U 2\lambda^2 / \omega_0$ and, for $U_{\rm eff} < 0$, $\Delta \rightarrow \Delta_{\rm eff} = \Delta e^{-(\lambda/\omega_0)^2}$.
- The most interesting regime for quantum dots, $\lambda \gg \Delta$ and $U \gg \omega_0$, is not susceptible to algebraic analysis.

NRG treatment of local bosons

Hewson & Meyer (2002)

• Since a local boson has a finite energy ω_0 , it can be included in

 $H_{\rm imp} = \varepsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + \omega_0 a^{\dagger} a + \lambda (n_d - 1) (a + a^{\dagger}),$

leaving untouched both $H_{\text{host-imp}}$ and H_{host} .

- Now $H_{\rm imp}$ has an infinite-dimensional Fock space that precludes exact diagonalization.
- But if we can find the right finite subset of eigenstates of

$$H_0 = H_{\rm imp} + H_{\rm host-imp} \left(f_{0\sigma}^{\dagger}, f_{0\sigma'} \right) + e_0 f_{0\sigma}^{\dagger} f_{0\sigma}$$

we should be able to use the conventional NRG approach to incorporate the conduction-band degrees of freedom.

NRG treatment of local bosons

• Based on the decoupled limit, expect the system to relax after each change in n_d toward a ground state with

$$\langle a^{\dagger}a \rangle_{GS} = (\lambda/\omega_0)^2 (n_d - 1)^2.$$

• To capture these states, Hewson & Meyer used a bosonic basis consisting of eigenstates of $a^{\dagger}a$ spanning

$$0 \le n_a \le n_{\max} = 4(\lambda/\omega_0)^2.$$

• To reach

$$U_{\rm eff} = U - 2\lambda^2 / \omega_0 \approx 0,$$

need

$$n_{\rm max} \approx 4U/\omega_0 \gg 1.$$



NRG treatment of local bosons

• In summary, can follow standard NRG iterative procedure

$$H_N = H_{N-1} + \sum_{\sigma} \left[e_N f_{N\sigma}^{\dagger} f_{N\sigma} + t_N \left(f_{N\sigma}^{\dagger} f_{N-1,\sigma} + \text{H.c.} \right) \right]$$

with a more complicated H_0 whose basis has dimension $4 \times 4 \times 4 U/\omega_0$.



• This poses no fundamental problem for $U/\omega_0 \sim 10$ (say), which allows access to the most interesting regime:

 $\lambda \gg \Delta$ and $U \gg \omega_0$.

Results: Spin Kondo to charge Kondo crossover

Conventional spin Kondo effect evolves smoothly with increasing λ into a charge Kondo effect where the impurity charge is collectively screened by band electrons.



Results: Spin Kondo to charge Kondo crossover

In a quantum-dot, linear conductance

$$G(T=0) = \frac{2e^2}{h} \pi \Delta \rho_d(\omega=0) = \frac{2e^2}{h} \sin^2 \frac{\pi \langle n_d \rangle}{2}$$



Results: Spin Kondo to charge Kondo crossover

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For $\lambda > \lambda_0$ (= ω_0 here) charge doublet g.s. is split by $|U + 2\varepsilon_d|$.

Kills Kondo effect for

$$egin{aligned} U+2arepsilon_d&|>\ &T_{_K}ig(arepsilon_d&=-U/2ig) \end{aligned}$$



II. Bosonic NRG

 Goals: Nonperturbative solutions of impurity problems with a gapless continuum of bosonic modes:

$$H_{\rm host} = \sum_{q} \omega_{q} a_{q}^{\dagger} a_{q}.$$

• Typically, impurity couples to oscillator displacements:

$$H_{\text{host-imp}} = \hat{O}_{\text{imp}} \sum_{q} \lambda_q \left(a_q + a_q^{\dagger} \right).$$

Again seek energy separation to allow iterative solution:



• Every bosonic chain site has an infinite basis, so ... basis choice and state truncation likely to be crucial.

Spin-boson model

• A canonical model for coupling of a local degree of freedom to a dissipative environment:

$$\begin{split} H_{\text{host}} &= \sum_{q} \omega_{q} a_{q}^{\dagger} a_{q}, \qquad \qquad H_{\text{imp}} = -\Delta S_{x}, \\ H_{\text{host-imp}} &= \frac{1}{\sqrt{N_{q}}} S_{z} \sum_{q} \lambda_{q} \left(a_{q} + a_{q}^{\dagger} \right). \end{split}$$

• ω_q and λ_q enter only through the bath spectral function

$$J(\omega) = \frac{\pi}{N_q} \sum_q \lambda_q^2 \,\delta(\omega - \omega_q)$$
$$= 2\pi \,\alpha \,\omega_c \,(\omega/\omega_c)^{S} \text{ for } 0 < \omega < \omega_c.$$



NRG discretization and chain mapping

Bulla et al. (2005)

- Define logarithmic bins.
- Retain one bath state in each bin:

$$a_m = A_m^{-1} \int_{\text{bin } m} d\omega \sqrt{B(\omega)} a_{\omega},$$

so that

$$H_{\rm host} \approx \sum_{m=0}^{\infty} \omega_m a_m^{\dagger} a_m$$
.

- The impurity interacts with all bins in a "star" configuration.
- Lanczos starting from

$$b_0 = B_0^{-1} \sum_{m=0}^{\infty} A_m a_m$$

maps to a "chain" configuration.







Separation of energy scales

• Chain coefficients decay faster than for band electrons:



 \Rightarrow Discretization achieves the desired energy separation.

• Iterative solution of chains of length L = 1, 2, 3, ... should work if can restrict each chain site to just N_h basis states.

Does bosonic chain-NRG work?

• The method has been tested very carefully on the spinboson model [Bulla et al. (2003, 2005)]:

$$\begin{split} H &= \sum_{q} \omega_{q} a_{q}^{\dagger} a_{q} - \Delta S_{x} + S_{z} N_{q}^{-1/2} \sum_{q} \lambda_{q} \left(a_{q} + a_{q}^{\dagger} \right). \end{split}$$
with bath $J(\omega) &= 2\pi \; \alpha \; \omega_{c} \left(\omega / \omega_{c} \right)^{S} \; \text{ for } \; 0 < \omega < \omega_{c} \,.$
using a basis of the N_{b} lowest eigenstates of $b_{n}^{\dagger} b_{n}$.

- As expected from other approaches,
 - for 0 < s < 1, there is a quantumcritical point at $\alpha = \alpha_c(\Delta)$
 - for s = 1, instead have a Kosterlitz-Thouless quantum phase transition.



Does bosonic chain-NRG work?

• In the delocalized phase and at the critical point ($\alpha \le \alpha_c$), results are stable and insensitive to choice of N_b .



• In the localized phase ($\alpha > \alpha_c$) with s < 1, $\langle b_n^{\dagger} b_n \rangle$ diverges for large *n*, and bosonic chain-NRG fails.

Bosonic star-NRG

Bulla et al. (2005)

• In the limit $\Delta = 0$, S_z provides a static potential for the bosons. Under the star formulation,

$$H = \sum_{m} \omega_{m} a_{m}^{\dagger} a_{m} + S_{z} \sum_{m} A_{m} \left(a_{m} + a_{m}^{\dagger} \right)$$

with $\omega_{m} \propto \Lambda^{-m}$, $A_{m} \propto \Lambda^{-(1+s)m/2}$



• Can transform to displaced oscillators (for $\sigma = \pm 1$) $a_{m\sigma} = a_m + \sigma A_m / (2\sqrt{\pi}\omega_m)$

such that
$$H = \sum_{\sigma=\pm 1} |\sigma/2\rangle \langle \sigma/2| \sum_{m=0}^{\infty} \omega_m a_{m\sigma}^{\dagger} a_{m\sigma}$$

• Then
$$\langle a_m^{\dagger} a_m \rangle \approx \frac{A_m}{4\pi\omega_m^2} \sim \Lambda^{(1-s)m/2}$$
 diverges for $s < 1$.

Bosonic star-NRG

• For $\Delta \neq 0$, don't know exact oscillator shifts, but can use variational optimization of basis, then work with small N_b .



• Main conclusion: bosonic-star NRG works well in localized phase, but not in delocalized phase.

Bosonic NRG: Successes and limitations

- With reasonable computational effort, bosonic NRG yields thermodynamics, dynamics, phase boundaries that are well-converged w.r.t. boson basis per site N_b and number of retained states N_s .
- Results are non-perturbative: not limited to small values of any model parameter.
- However, choice of bosonic basis is crucial:
 - Proper basis depends on location in phase diagram.
 - NRG described here is inefficient at basis optimization.
 - Variational product state NRG (Weichselbaum et al.) has advantages here.
- Critical behavior remains challenging (see lecture notes).

III: Bose-Fermi NRG

- Bose-Fermi Kondo model describes a spin-half S coupled to a conduction band and to 1-3 dissipative baths.
- Isotropic model has the Hamiltonian

$$H = \bigcup \mathbf{S} \cdot \mathbf{s} + H_{\text{band}} + \bigcup \mathbf{S} \cdot \mathbf{u} + H_{\text{bath}}$$

$$H_{\text{Kondo}} = \mathbf{M}_{\text{Kondo}} + \mathbf{M}_{\text{spin-boson}}$$
where (for $\alpha = x, y, z$)
$$s_{\alpha} = \frac{1}{2} \sum_{\sigma, \sigma'} c_{0\sigma}^{\dagger} \sigma_{\sigma\sigma'}^{\alpha} c_{0\sigma'} \qquad u_{\alpha} = a_{0\alpha} + a_{0\alpha}^{\dagger}$$

$$H_{\text{band}} = \sum_{k,\sigma} \varepsilon_{k} c_{k\sigma}^{\dagger} c_{k\sigma} \qquad H_{\text{bath}} = \sum_{q,\alpha} \omega_{q} a_{q\alpha}^{\dagger} a_{q\alpha}$$

Most studies have focused on one-bath case:

$$g\mathbf{S} \cdot \mathbf{u} \to gS_z u_z$$

Bose-Fermi Kondo model: Bath spectra

• Take a flat conduction band density of states:

$$\rho(\varepsilon) = \rho_0 \text{ for } |\varepsilon| < D$$

• Assume a power-law bosonic spectrum:

 $B(\omega) = K_0^2 \,\omega_c (\omega / \,\omega_c)^S$

• Dimensionless couplings: $\rho_0 J = K_0 g$



One-bath Bose-Fermi Kondo model

For any sub-Ohmic bath exponent 0 < s < 1, one-bath BFK model

$$H = J\mathbf{S} \cdot \mathbf{s} + H_{\text{band}} + gS_z u_z + H_{\text{bath}}$$

has a nontrivial critical point governing the boundary between Kondo and localized phases:



Embodies critical destruction of the Kondo effect, c.f. heavy fermions.

Bose-Fermi NRG

Glossop and KI (2005)

- Seek an NRG that treats simultaneously fermionic and bosonic degrees of freedom of the same energy.
- Guided by spin-boson model, use the chain NRG.
- Slightly complication: different Λ dependences of fermionic and bosonic tight-binding coefficients.
 - Could use different discretizations, $\Lambda_{\text{fermions}} = \Lambda^2_{\text{bosons}}$.
 - Instead, we add a bosonic site at every other iteration:



Testing the Bose-Fermi NRG

• The Ising-symmetry Bose-Fermi Kondo model is a good test ground: bosonization of the fermions maps problem onto the spin-boson model with an asymptotic bath spectrum $B(\omega) \propto \omega^{\min(1, s)}.$

QPT should lie in the $s_{\text{spin-boson}} = \min(1, s)$ universality class (studied via bosonic NRG).

• BF-NRG reproduces spin-boson results, including their flaws.



Bose-Fermi NRG beyond the BFK model

- Bose-Fermi NRG has been applied to a range of other problems:
 - Self-consistent Bose-Fermi Kondo model arising in the EDMFT treatment of the Kondo lattice.



 Problems with a singular fermionic density of states as well as a sub-Ohmic bath (see lecture notes).



NRG with bosons: A scorecard

- The good: With appropriate choices of bosonic basis, NRG provides robust, non-perturbative solutions to a variety of interesting problems.
- The bad: NRG with bosons is not a "black-box" tool that can be applied indiscriminately, because the basis must be chosen appropriately for the regime of interest. May be fundamental problems near some critical points.
- The computationally ugly: With bosons, the basis grows very rapidly upon NRG iteration.

Impedes extension to multi-impurity and multi-bath models, may be problematic for time-dependent studies.

• Key direction for future work: optimization of the bosonic basis.