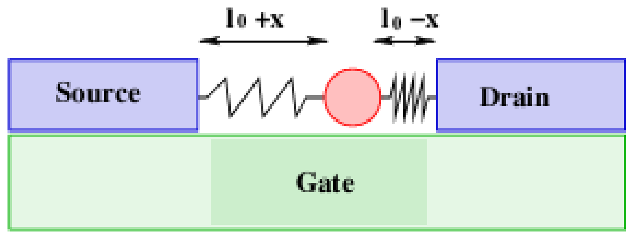
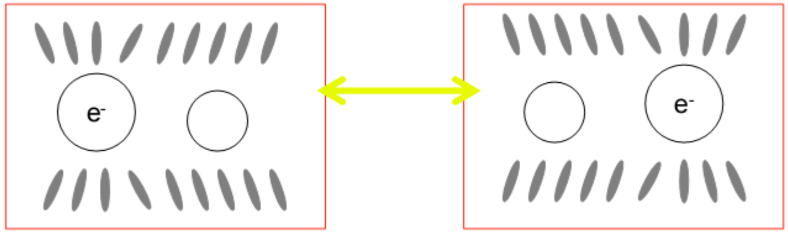
NRG with Bosons II: The Better, the Worse, and the Computationally Uglier

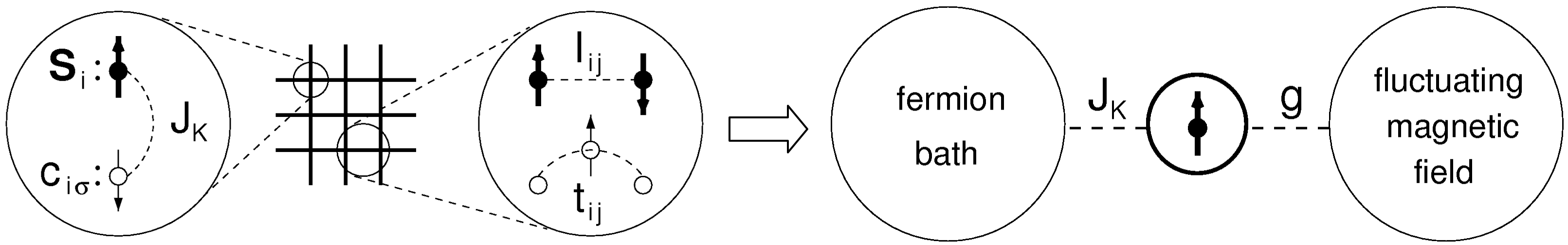
Kevin Ingersent (U. of Florida)



Al-Hassanieh et al., PRL (2005)



S. Tornow



Si et al., Nature (2001)

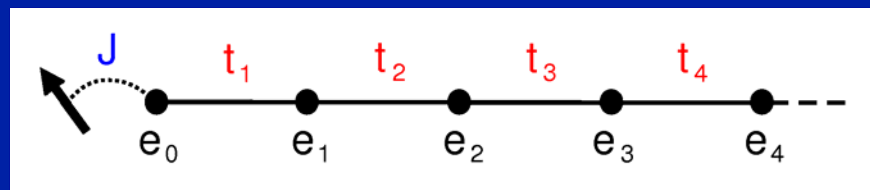
Supported by NSF under DMR-0312939 and DMR-0710540

Outline

- Classify problems by host type: $H = H_{\text{imp}} + H_{\text{imp-host}} + H_{\text{host}}$
- Fermionic NRG: brief review
- Adding bosons to NRG: the challenges
- Fermionic NRG + local bosons (Hewson et al.)
  - e-ph interactions in strongly correlated metals
  - molecular devices with vibrations
- Bosonic NRG (Bulla et al.)
  - spin-boson model
  - more complicated impurities, e.g., donor-acceptor systems
- Bose-Fermi NRG (KI & Glossop)
  - quantum dot in a dissipative environment
  - mean-field treatment of heavy-fermion quantum criticality
- Scorecard: the good, the bad, and the ugly

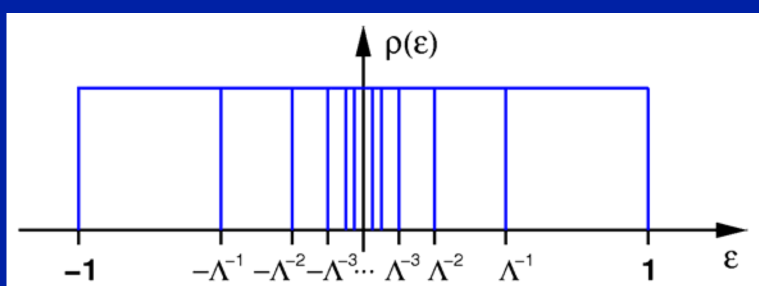
Review: Fermionic NRG

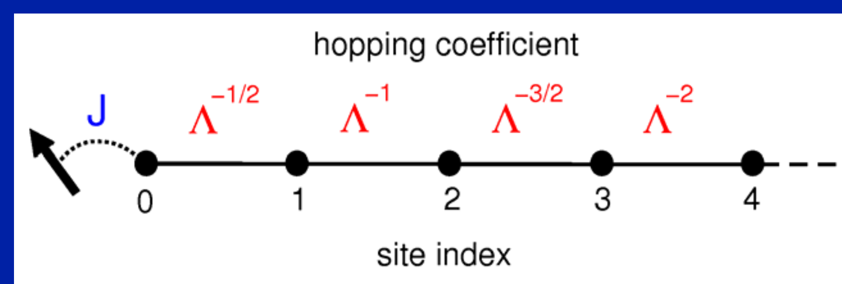
- Any quantum impurity problem can be mapped **exactly** to chain form:



But, tight-binding coefficients are all of same order $\Rightarrow$ ground state for length L is not built solely from low-lying states of length $L-1$.

- Wilson conceived the logarithmic discretization of a fermionic band to introduce an artifical separation of energy scales:

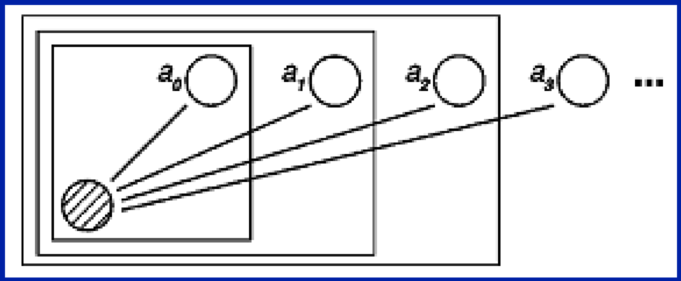




This energy separation allows iterative solution by sequential diagonalization on chains of lengths $L = 1, 2, 3, \ldots$

Band discretization

- Impurity couples only to $f_0 = \int d\varepsilon\, w(\varepsilon)\, c_\varepsilon$ (dropping spin indices).
- Define bins $m = \pm 1, \pm 2, \pm 3, \ldots$ spanning $\Lambda^{-|m|} < \varepsilon\, \mathrm{sgn}(m) < \Lambda^{1-|m|}$.
- Within bin m, define a complete basis of operators $a_{mp},\ p = 0, 1, 2, \ldots$
- Choose $a_{m0} = A_m^{-1} \int_{\text{bin } m} d\varepsilon\, w(\varepsilon)\, c_\varepsilon$ such that the impurity couples precisely to $f_0 = F^{-1} \sum_m A_m a_{m0}$.



- The approximation comes in the description of the host:

$$H_{\text{host}} = \int d\varepsilon\, \varepsilon\, c_\varepsilon^\dagger\, c_\varepsilon$$

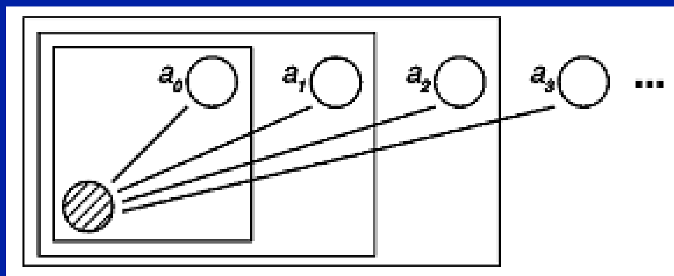
$$= \sum_{m,p} \varepsilon_{mp}\, a_{mp}^\dagger\, a_{mp} + \sum_{m,p,p'} t_{mpp'}\, a_{mp}^\dagger\, a_{mp'}$$

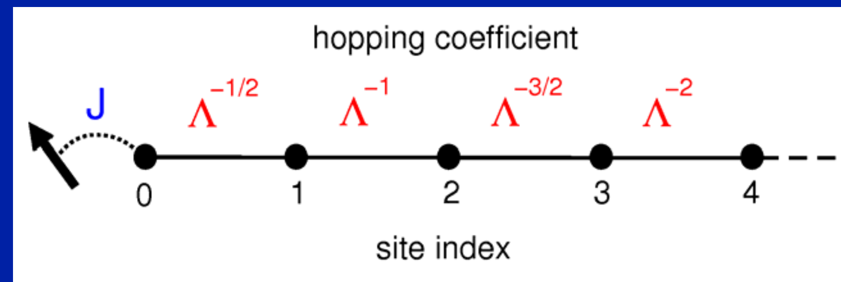
$$\approx \sum_m \varepsilon_{m0}\, a_{m0}^\dagger\, a_{m0} + \text{ decoupled terms.}$$

The resulting discretization error $\propto 1 - \Lambda^{-1}$, vanishes for $\Lambda \to 1$.

Chain mapping and iterative solution

- The discretized band is mapped to a chain by the Lanczos method:





- The exponential decay of hoppings and on-site energies allows sequential solution of chains of length $L = 1, 2, 3, \ldots$
- For n_f species of fermion, the basis grows by 2^{n_f} at each step.
  $\Rightarrow$ It is feasible to keep only the lowest N_s many-body eigenstates.

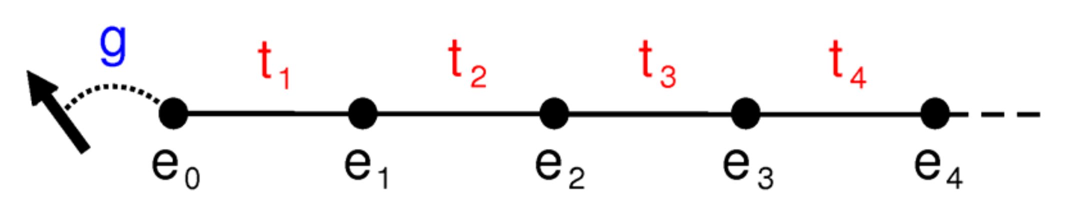
  For fixed N_s, and hence fixed CPU time, the resulting truncation error increases as $\Lambda \rightarrow 1$ (the reverse trend to the discretization error).
- The optimal Λ typically lies between 1.5 and 3. Impurity properties are generally captured very well and can be extrapolated to $\Lambda = 1$.

Adding Bosons to NRG: The Challenges

- Goal is to treat dispersive host baths: $H_{\text{host}} = \sum_q \omega_q a_q^\dagger a_q$.
- Typically, impurity couples to oscillator displacements:

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

- Chain mapping still yields asymptotically constant tight-binding coefficients [Evangelou & Hewson, J. Phys. C (1982)]:



  - It is desirable to introduce a separation of energy scales.
- Basis is infinite-dimensional even for chain length $L = 1$.
  - Truncation is necessary from the outset.
  - Choice of basis states may be important.

Step I: Fermionic NRG with Local Bosons

Hewson & Meyer, J. Phys. Condens. Matter (2002)

- Developed for the Anderson-Holstein model:

$$H_{\mathrm{imp}} = \left(\varepsilon_d + \tfrac{1}{2}U\right)n_d + \tfrac{1}{2}U\left(n_d - 1\right)^2 + \omega_0\, a^\dagger a\,, \qquad H_{\mathrm{host}} = \sum_{k,\sigma} \varepsilon_k\, c_{k\sigma}^\dagger c_{k\sigma}\,,$$

$$H_{\text{imp-host}} = \sum_{k,\sigma}\left(V_k\, d_\sigma^\dagger c_{k\sigma} + \mathrm{H.c.}\right) + \lambda\left(n_d - 1\right)\left(a + a^\dagger\right).$$

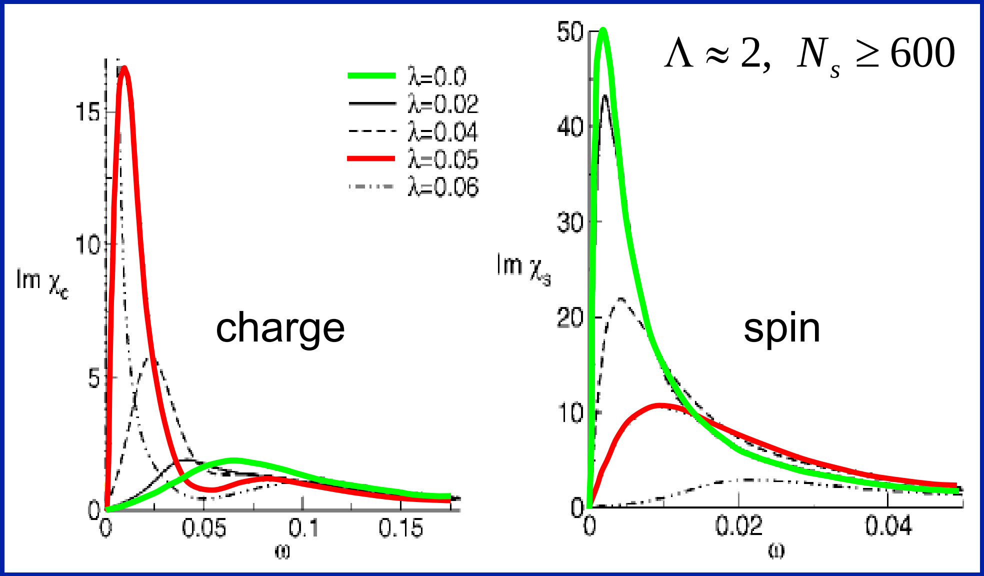
- For $V_k = 0$, define displaced oscillators $\tilde{a} = a + (\lambda/\omega_0)(n_d - 1)$, yielding $U_{\mathrm{eff}} = U - 2\lambda^2/\omega_0$. Have a Poisson distribution of $n_a = a^\dagger a$ with mean $\langle n_a \rangle = (\lambda/\omega_0)^2$. Need only states with $n_a \le 4\langle n_a\rangle$ in the $L = 1$ chain.

- Expect similar behavior for $V_k \neq 0$. Interesting physics occurs around $U_{\mathrm{eff}} \approx 0$ (where spin-Kondo → charge-Kondo effect), so need to include $n_a \le 4U/\omega_0$ for $L = 1$.

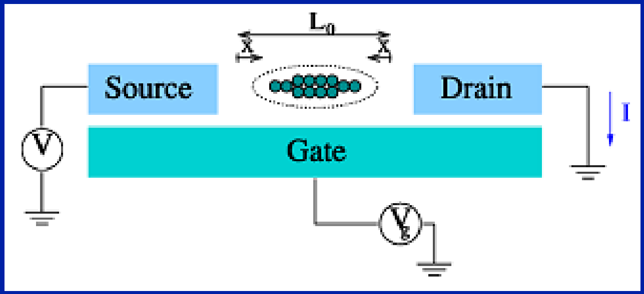
- At subsequent iterations, follow standard NRG truncation procedure.

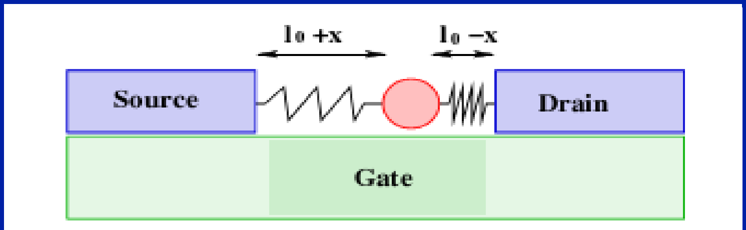
How well does it work?

- NRG with local bosons …
  - yields reliable dynamical properties [Hewson & Meyer; Jeon et al., PRB (2003)]:



  - works in DMFT [Meyer, Hewson & Bulla, PRL (2002)];
  - has been extended to treat molecular devices with vibrations [Cornaglia et al., PRB (2005), Dias & Dagotto, unpublished]:





Al-Hassanieh et al., PRL (2005)

- However, shows that care is needed in choosing the bosonic basis.

Step II: Bosonic NRG

Bulla, Tong & Vojta, PRL (2005); Bulla, Lee, Tong & Vojta, PRB (2005)

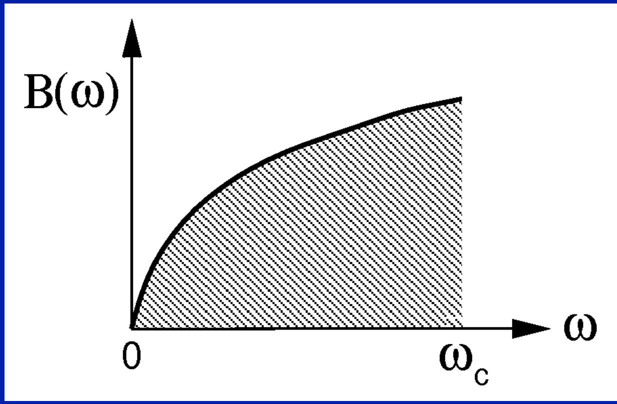
- Developed for the spin-boson model:

$$H_{\rm imp} = -\Delta S_x + \varepsilon S_z\,, \qquad H_{\rm host} = \sum_q \omega_q a_q^\dagger a_q\,,$$

$$H_{\rm imp-host} = S_z \sum_q \lambda_q \left(a_q + a_q^\dagger\right).$$

- ω_q and λ_q enter only through the bath spectral function

$$B(\omega) = \pi \sum_q \lambda_q^2\, \delta\left(\omega - \omega_q\right)$$
$$= 2\pi\;\alpha\;\omega_c\left(\omega/\omega_c\right)^s \quad \text{for}\;\; 0 < \omega < \omega_c\,.$$



- Impurity couples only to

$$b_0 \propto \int d\omega\, \sqrt{B(\omega)}\; a_\omega\,.$$

- In the spirit of NRG, want to discretize the bath, introducing a separation of energy scales into $H_{\rm host} = \int d\omega\, \omega\, a_\omega^\dagger\, a_\omega\,.$

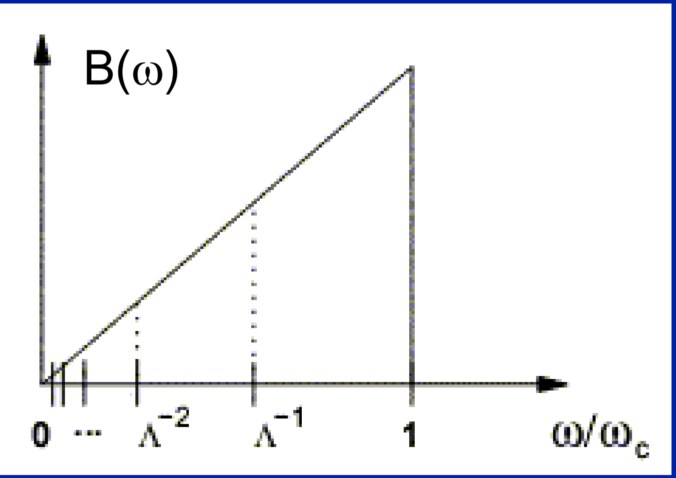
Discretization and chain mapping

- Use logarithmic bins as for fermions.
- 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

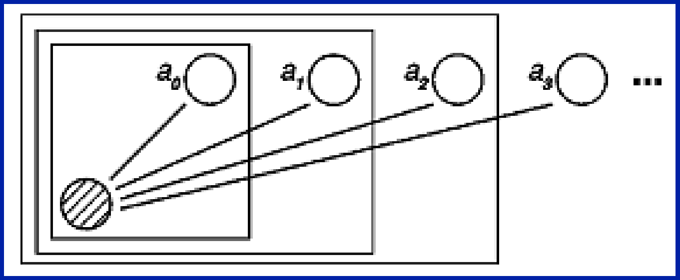
$$H_{\text{host}} \approx \sum_{m=0}^{\infty} \omega_m\, a_m^\dagger\, a_m \,.$$



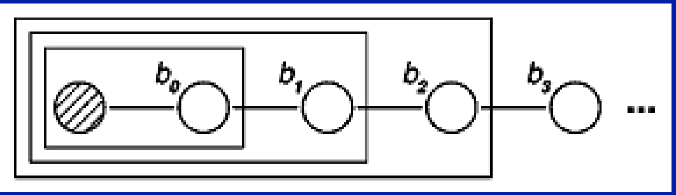
- The impurity interacts with all bins:

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

(We'll return to this "**star**" configuration shortly.)

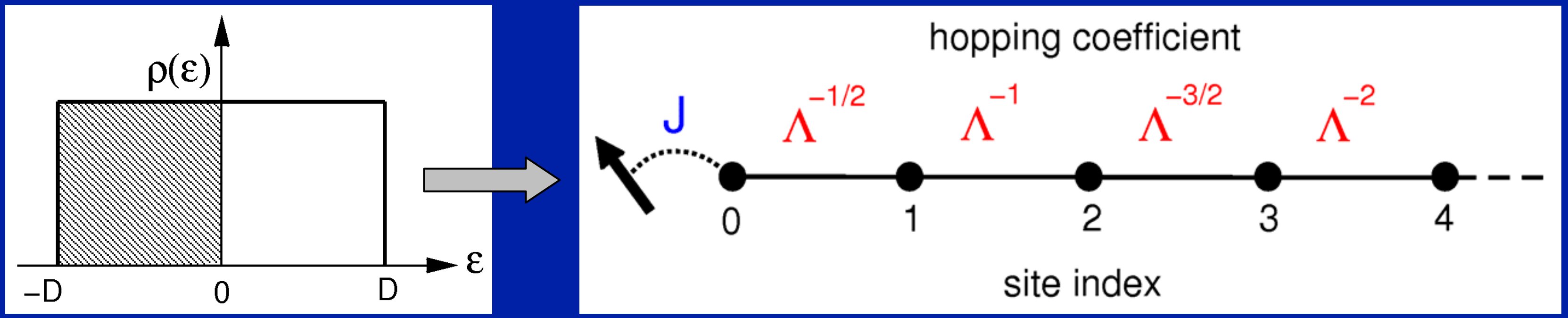


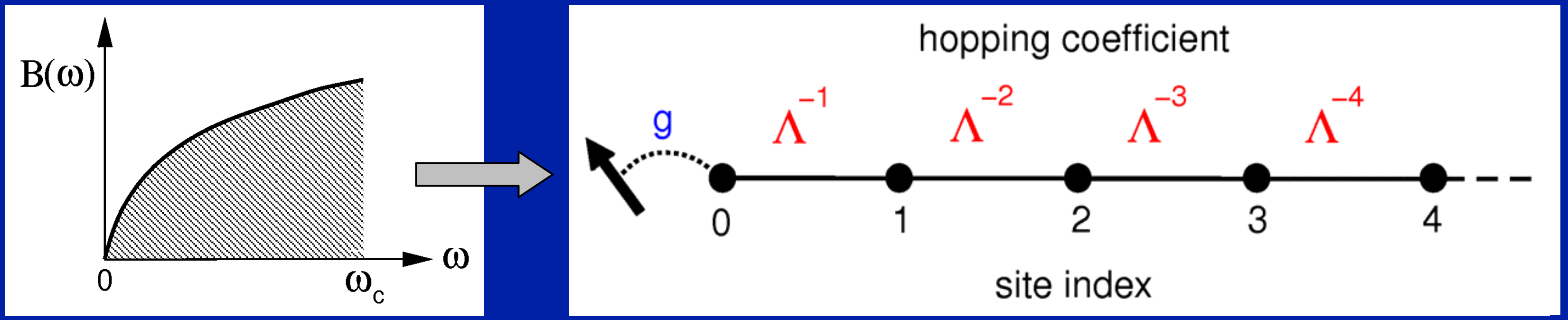
- Lanczos maps the problem to a "**chain**" configuration.



Separation of energy scales

- Tight-binding coefficients decay faster than in the fermionic case:





⇒ Logarithmic discretization achieves the desired energy separation.

- Iterative solution of chains of length $L = 1, 2, 3, \ldots.$ will be practical provided one can restrict each bosonic site to just N_b basis states.

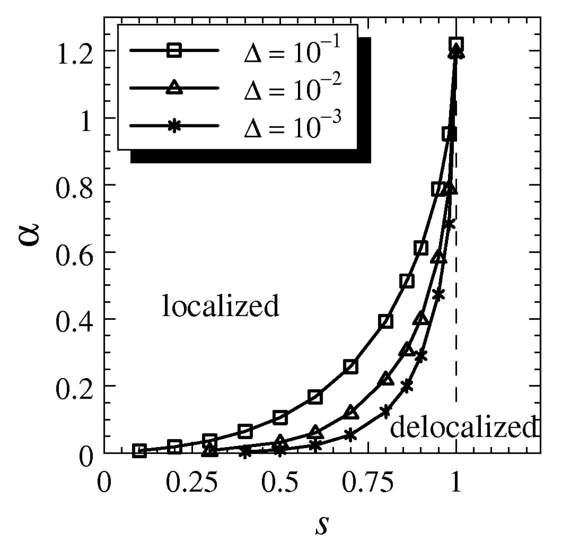
Does bosonic chain-NRG work?

- The method has been tested extensively on the spin-boson model at zero bias [Bulla et al., PRL (2003); PRB (2005)]:

$$H_{\text{imp}} = -\Delta S_x, \qquad H_{\text{imp-host}} = S_z \sum_q \lambda_q \left(a_q + a_q^\dagger \right),$$

with bath $$B(\omega) = \pi \sum_q \lambda_q^2 \, \delta\left(\omega - \omega_q\right) = 2\pi \, \alpha \, \omega_c \left(\omega/\omega_c\right)^s.$$

- For $0 < s < 1$, there is a quantum-critical point at $\alpha = \alpha_c$; for $s = 1$, have a Kosterlitz-Thouless-type quantum phase transition.



- Main conclusions:
  - Generally get good results using a basis of the N_b lowest eigenstates of $b_n^\dagger b_n$.
  - For $\alpha > \alpha_c$ with $s < 1$, $\langle b_n^\dagger b_n \rangle$ diverges for large n, and bosonic chain-NRG fails.

Bosonic star-NRG

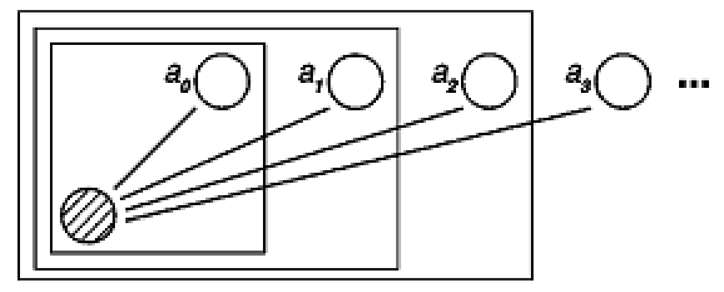
Bulla, Lee, Tong & Vojta, PRB (2005)

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

$$H = \sum_m \omega_m a_m^\dagger a_m + \pi^{-1/2} S_z \sum_m A_m \left(a_m + a_m^\dagger \right)$$
$$= \sum_{\sigma=\pm 1} |\sigma/2\rangle\langle\sigma/2| \sum_{m=0}^{\infty} \omega_m a_{m\sigma}^\dagger a_{m\sigma} + \text{constant} ,$$

where $a_{m\sigma} = a_m + \sigma A_m / \left(2\sqrt{\pi}\omega_m \right)$ (displaced oscillator state).

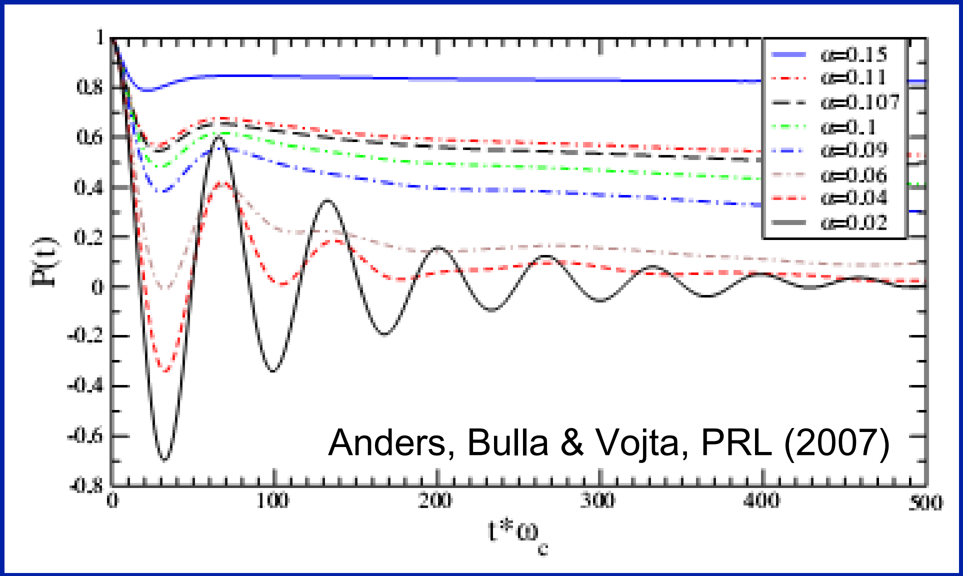
- Since $\omega_m \propto \Lambda^{-m}$, $A_m \propto \Lambda^{-(1+s)m}$, can diagonalize iteratively for $\Delta \neq 0$, using the appropriate displaced-oscillator basis for the end site:



- Main conclusion: works well in localized phase, but not in delocalized.

Bosonic NRG: Successes for the spin-boson model

- With reasonable effort, bosonic NRG yields **thermodynamics**, **dynamics**, **phase boundaries** & **critical exponents** that are well-converged w.r.t. boson basis size N_b & number of retained states N_s.
- Indicates that QCP is interacting for $0 < s < ½$, unlike the corresponding classical long-range Ising model. **(But see later!)**
- Now being combined with time-dependent NRG, e.g., probability of impurity spin being in up state vs time:



Bosonic NRG: Application to electron transfer problems

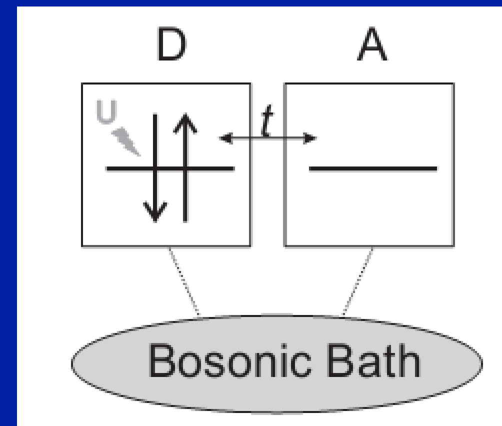
Tornow, et al., Europhys. Lett. (2006); PRB (2008).

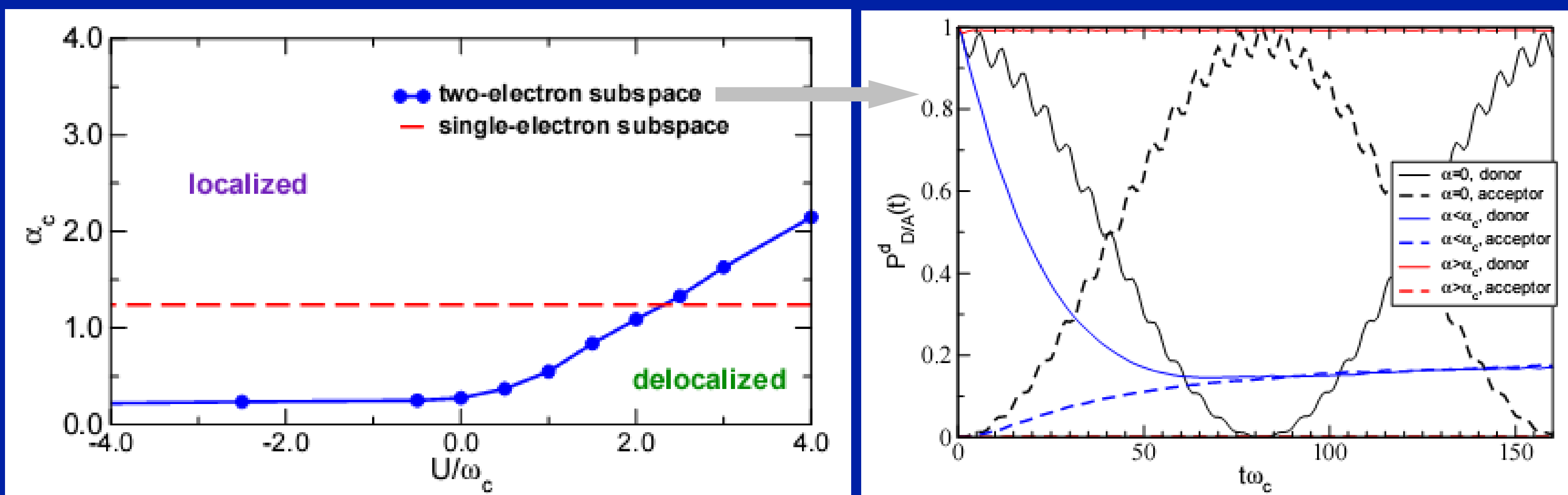
Model processes in DNA or protein complexes:

$$H_{\text{imp}} = \sum_{i=A,D}\left(\varepsilon_i n_i + U_i n_{i\uparrow} n_{i\downarrow}\right) - t\sum_{\sigma}\left(A_\sigma^\dagger D_\sigma + \text{H.c.}\right),$$

$$H_{\text{imp-host}} = \left(n_A - n_D\right)\sum_q \lambda_q\left(a_q + a_q^\dagger\right),$$

Bosonic bath: $J(\omega) = 2\pi\alpha\omega, \quad 0 < \omega < \omega_c.$





Step III: Bose-Fermi NRG

Glossop & KI, PRL (2005); PRB (2007)

- Developed for the Bose-Fermi Kondo model of a local spin-half $\mathbf{S}$ coupled to a conduction band **and** to one-three dissipative baths.
- Isotropic model has the Hamiltonian

$$H = \underbrace{J\mathbf{S}\cdot\mathbf{s} + H_{\text{band}}}_{H_{\text{Kondo}}} + \underbrace{g\mathbf{S}\cdot\mathbf{u} + H_{\text{bath}}}_{H_{\text{spin-boson}}}$$

where (for $\alpha = x, y, z$)

$$s_\alpha = \tfrac{1}{2}\sum_{\sigma,\sigma'} c_{0\sigma}^\dagger \sigma_{\sigma\sigma'}^\alpha c_{0\sigma'} \qquad u_\alpha = a_{0\alpha} + a_{0\alpha}^\dagger$$

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

- Anisotropic versions distinguish between

$$J_z \quad \text{and} \quad J_x = J_y = J_\perp \qquad g_z \quad \text{and} \quad g_x = g_y = g_\perp$$

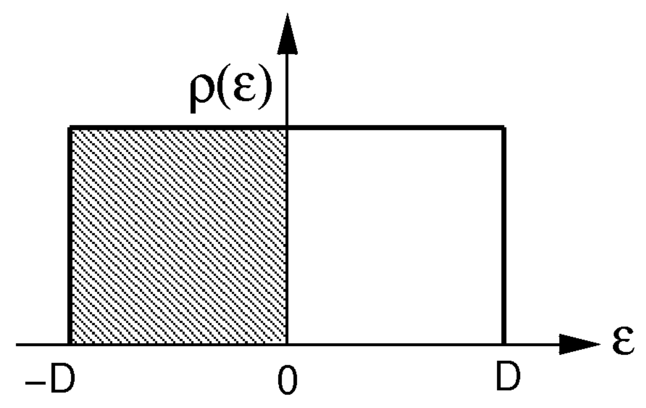
- To date, have focused on the **Ising-symmetry** case

$$J_z = J_\perp \qquad g_\perp = 0$$

Bose-Fermi Kondo model: Bath spectra

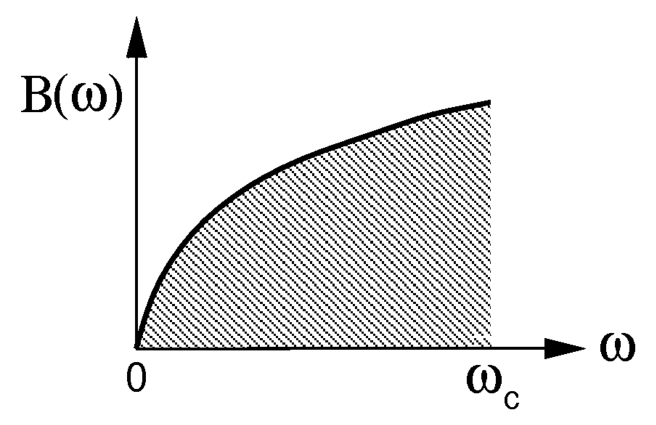
- Take a flat conduction band density of states:

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



- Assume a power-law bosonic spectrum:

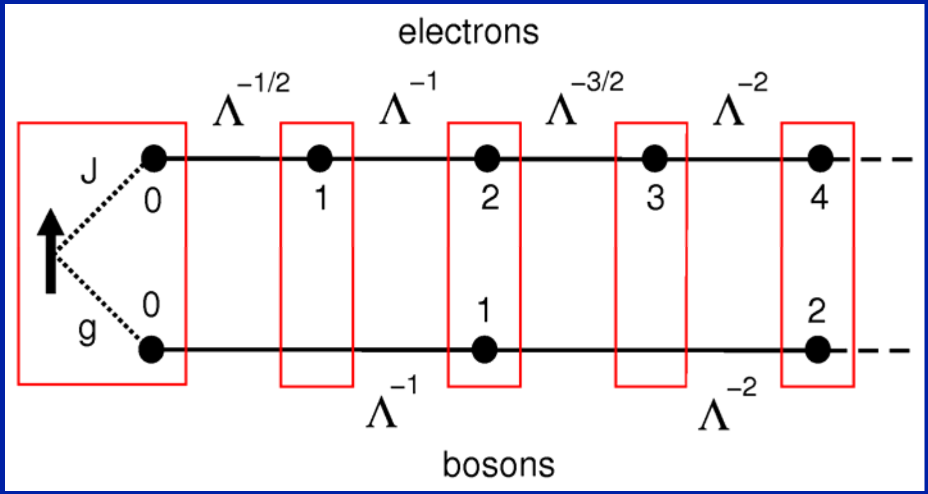
$$B(\omega) = K_0^2\, \omega_c \left(\omega/\omega_c\right)^{s}$$



- Dimensionless parameters: $\rho_0 J$ and $K_0 g$.

Strategy for Bose-Fermi NRG

- Seek an iterative procedure that treats simultaneously fermionic and bosonic degrees of freedom of the same energy.
- Guided by spin-boson model, focus on the **chain-boson formulation**.
- 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**:



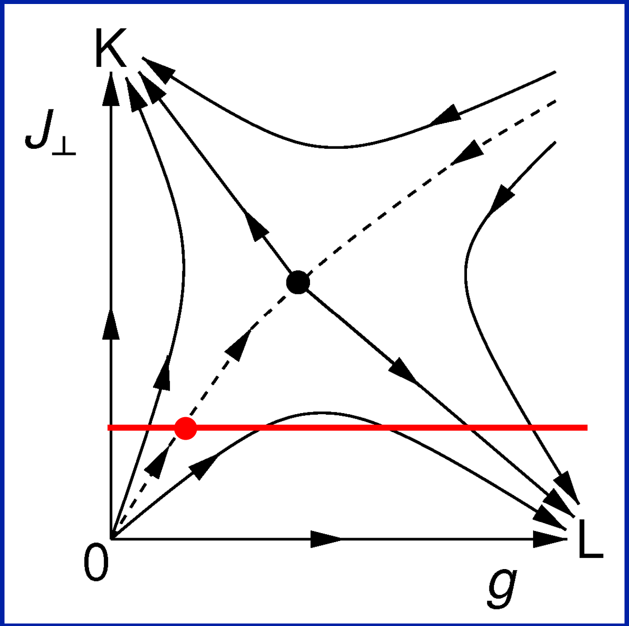
Testing the Bose-Fermi NRG

- 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

$$B(\omega) \propto \omega^{\min(1,\, s)}.$$

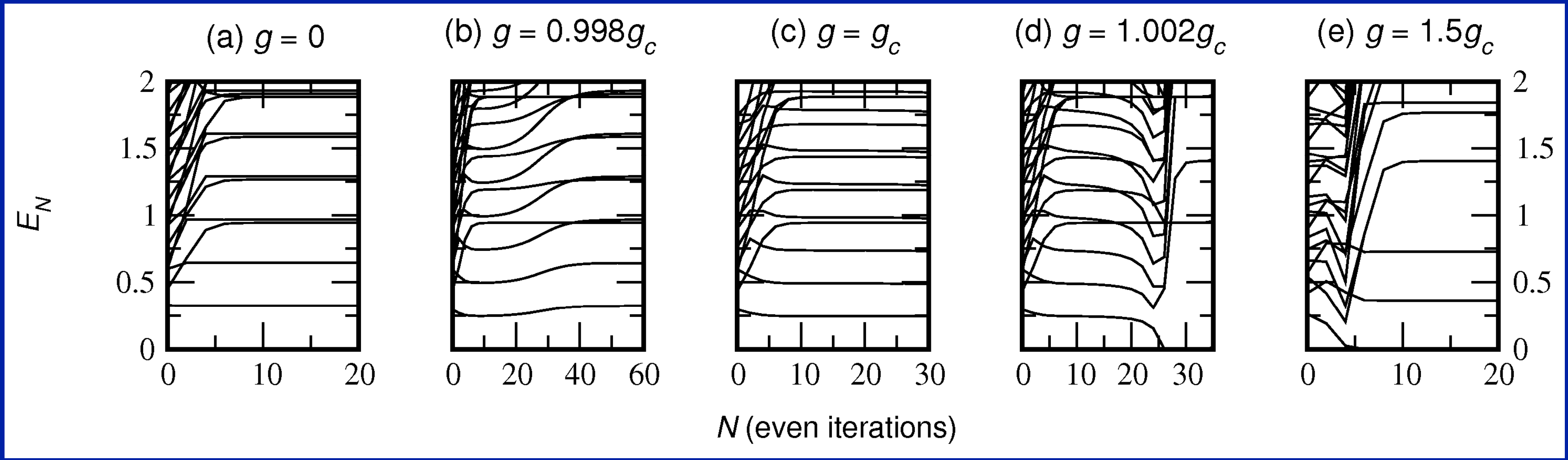
Quantum phase transition should lie in the $s_{\text{spin-boson}} = \min(1, s)$ universality class (studied via bosonic NRG).

- We have studied critical properties by varying the bosonic coupling g at fixed Kondo J.



NRG many-body energy spectrum

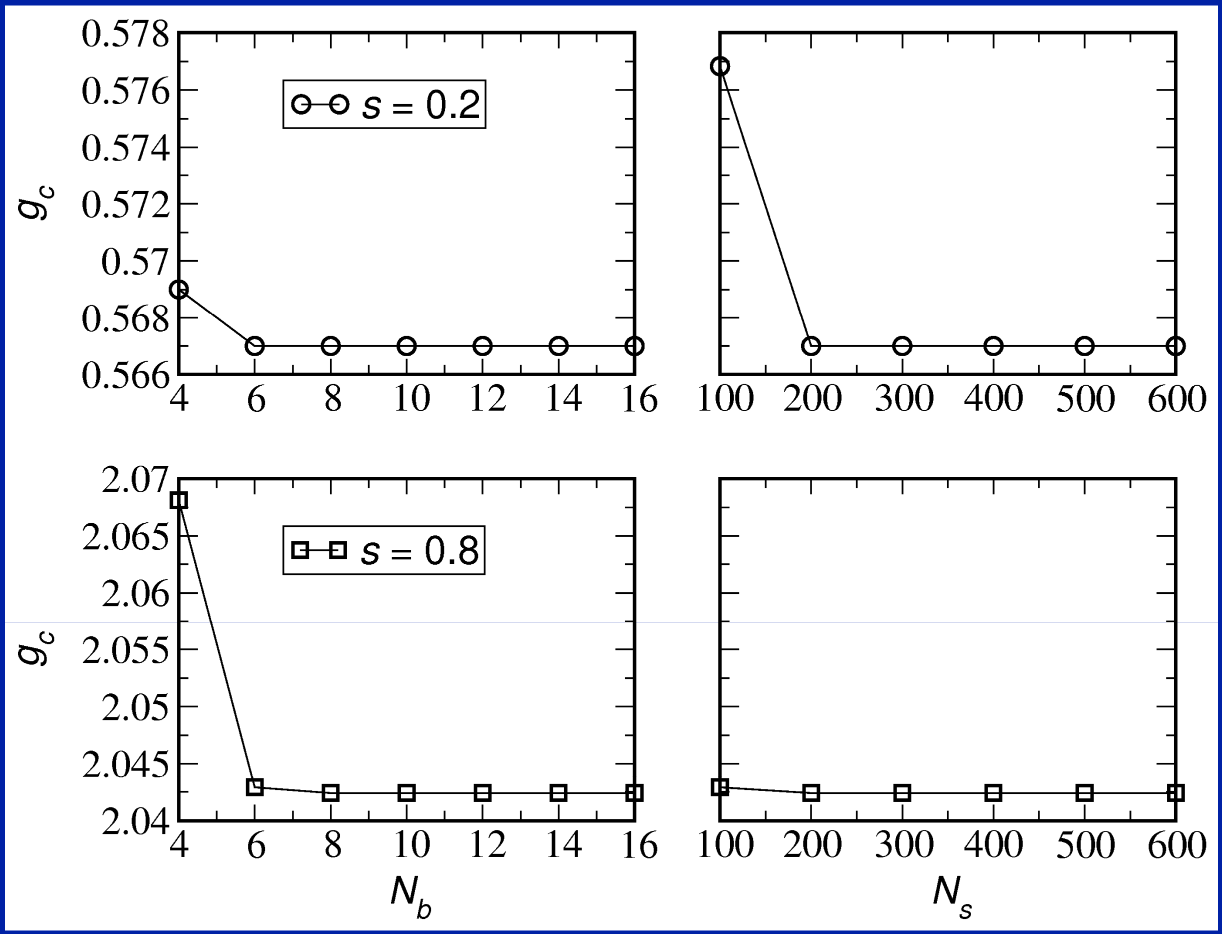
- NRG energy eigenvalues reveal existence of critical point:



- **Low-lying many-body spectrum**
  = (fermionic spectrum) ⊗ (bosonic spectrum).
  - Bosonic spectrum is identical to that of spin-boson model.
  - Fermionic spectrum corresponds to $J_z^* = J_\perp^* = \infty$ in Kondo phase, to $J_z^* \propto (g-g_c)^{-\beta}$, $J_\perp^* = 0$ for $g \geq g_c$.

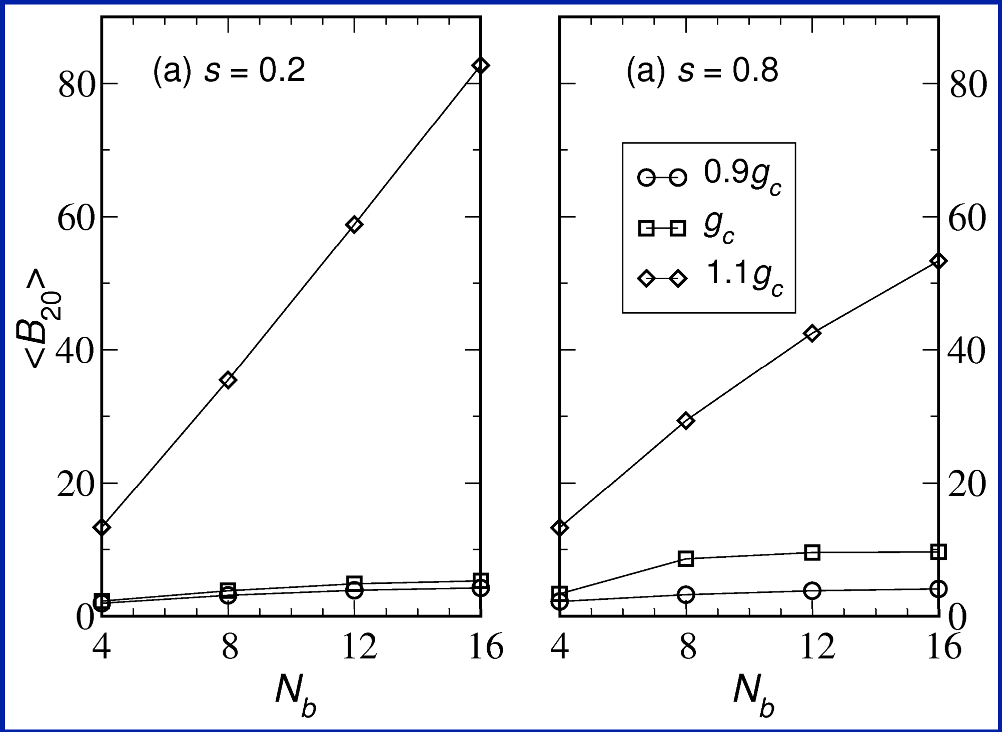
Truncation effects?

- Critical couplings are well converged w.r.t. boson basis size N_b & number of retained states N_s .



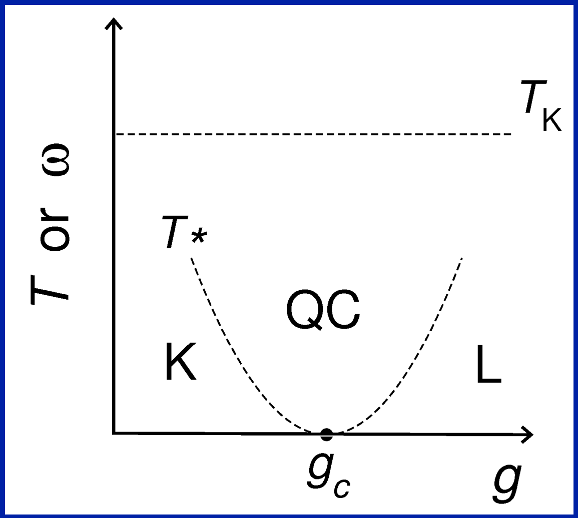
Truncation effects?

- Boson-number eigenbasis works well for $g \leq g_c$:

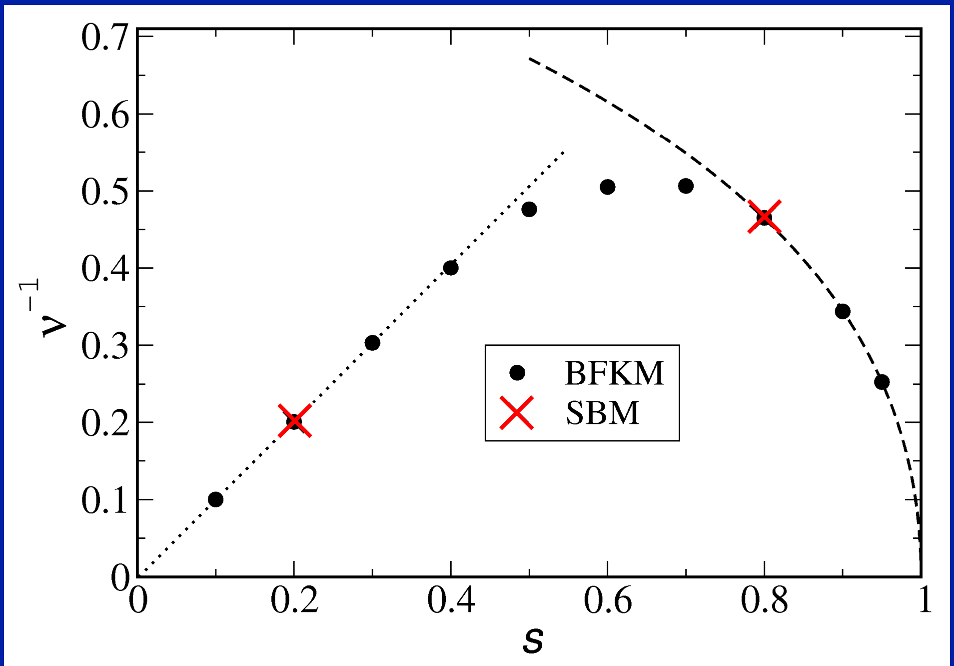


Critical behavior

- Can extract the correlation length exponent from the NRG energies:



$$T_* \propto |g - g_c|^{\nu}$$



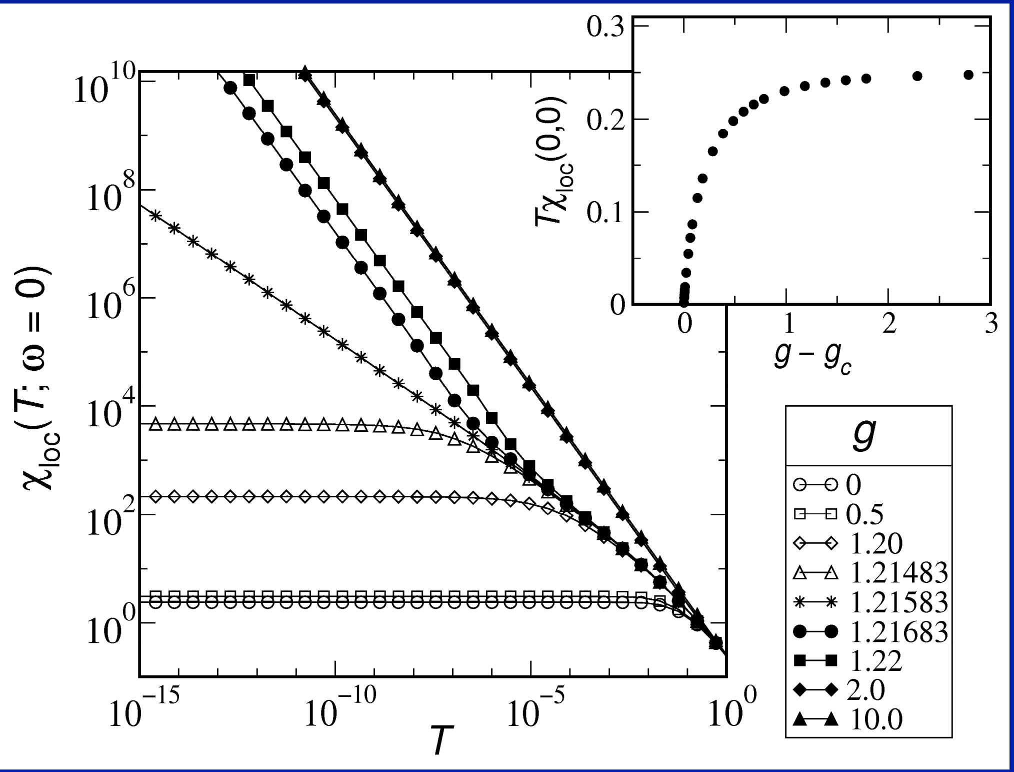
- Exponent agrees with that of spin-boson model for all $0 < s < 1$.

Response χ_{loc} to a local magnetic field *h*

- Probe QCP using $\chi_{\text{loc}}(\omega) = i\int_0^\infty dt\, e^{-i\omega t} \langle [S_z(t), S_z(0)] \rangle$,

  which should satisfy

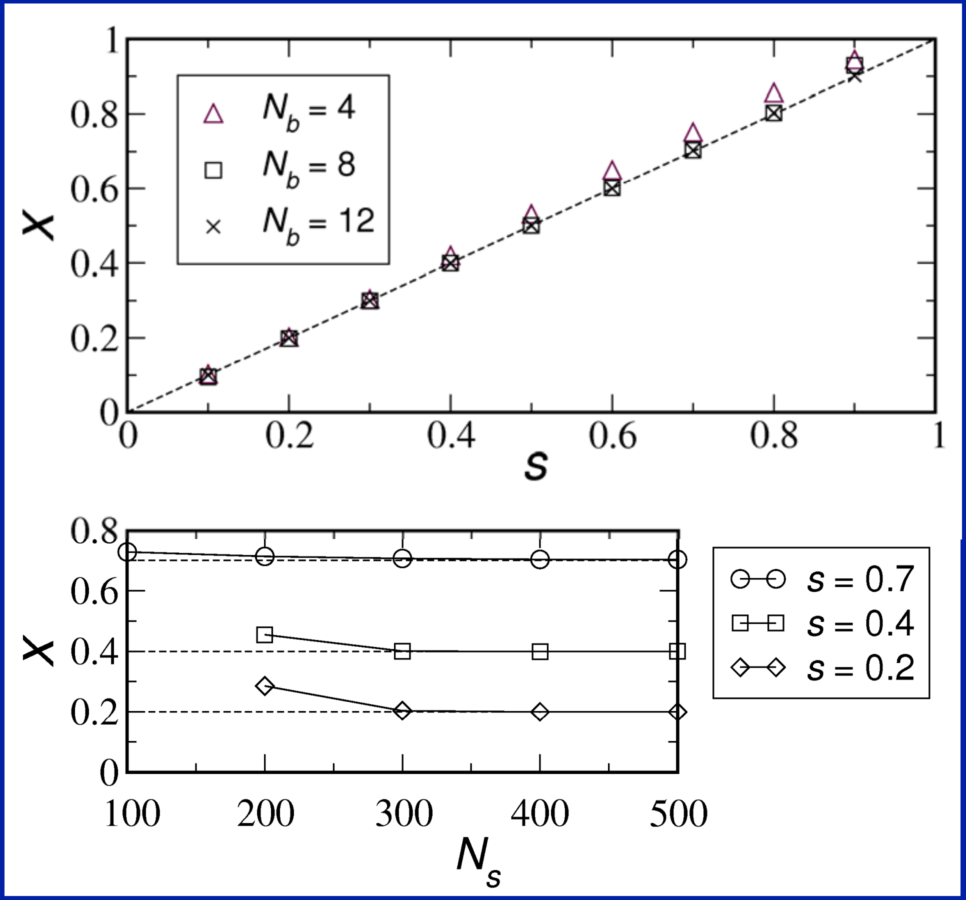
$$\chi_{\text{loc}}(0) = \lim_{h\to 0} -\frac{\langle S_z \rangle}{h} .$$



$\chi_{\text{loc}}(\omega = 0, g = g_c) \sim T^{-x}$ with $x = s$ (exact result of $1-s$ expansion)

Truncation effects on critical exponents?

- Exponent x converges rapidly with increasing boson basis size N_b & number of retained states N_s :



Scaling behavior near the critical point

- All critical exponents agree with those for the spin-boson model.

  $\Rightarrow$ Ising BFKM and SBM belong to same universality class.

- Static exponents are consistent with a critical free energy

$$F_{\text{imp}} = T\, f\left(\frac{g-g_c}{T^{1/\nu}}, \frac{h}{T^b}\right)$$

h = local magnetic field

i.e., exponents obey hyperscaling $\Rightarrow$ QCP is interacting.

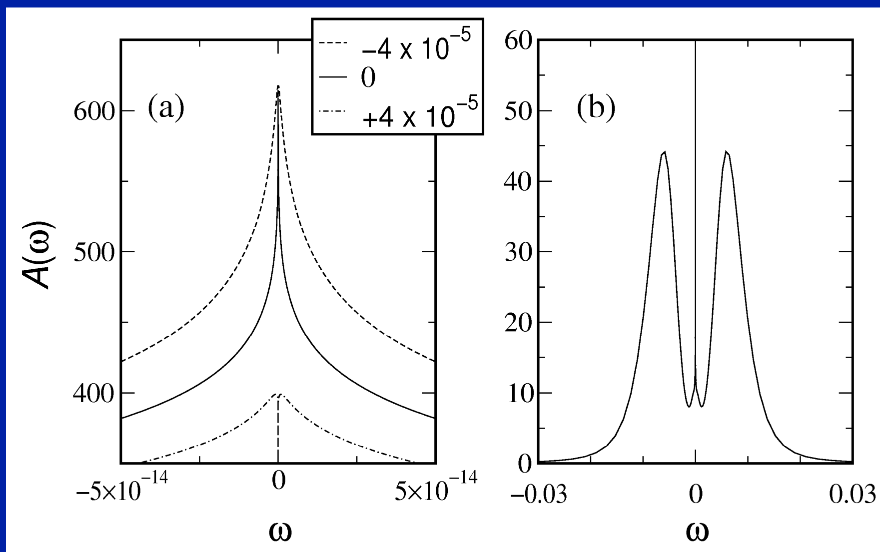
- Local spin dynamics obey

$$\chi''_{\text{loc}}(\omega, T=0, g=g_c) \sim |\omega|^{-y}\,\text{sgn}\,\omega \qquad \text{with} \qquad y = x = s$$

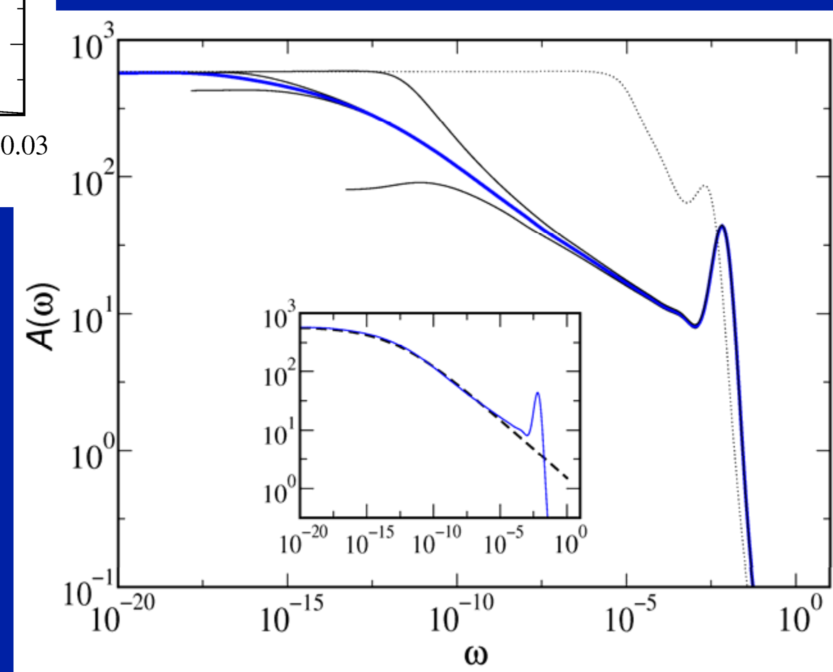
consistent with ω/T scaling.

Impurity spectral function

- Work with the Bose-Fermi Anderson model.



Dissipation collapses the Kondo resonance

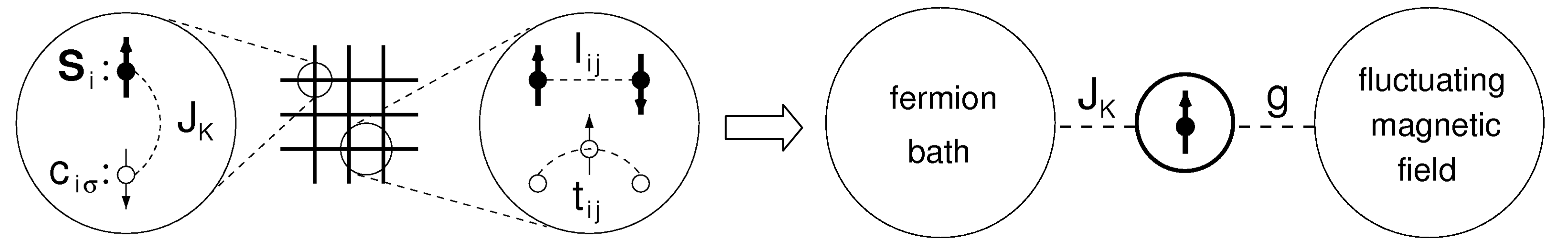


One puzzle: $A(0) \neq 0$

in the localized phase

Bose-Fermi NRG beyond the Ising BFKM

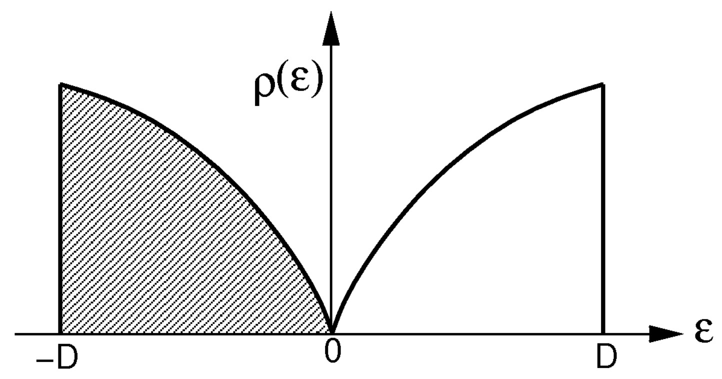
- We have applied Bose-Fermi NRG to a range of other problems:
  - Self-consistent Bose-Fermi Kondo model arising in the EDMFT treatment of the Kondo lattice.



Si et al., Nature (2001)

NRG provides nonperturbative confirmation of "**local criticality**" [Glossop & KI, PRL (2007)].

  - Problems with bosons and a Singular fermionic density of states: Pseudogap allows escape from the "SBM black hole" [Glossop et al, Physica B (2008)].



Bose-Fermi NRG beyond the Ising BFKM

- Charge-coupled Bose-Fermi Anderson model: a generalization of the Anderson-Holstein model [Cheng & KI, in preparation]
- Frustration of decoherence in a two-bath spin-boson model:

$$H_{\text{imp}} = -\Delta S_z , \qquad H_{\text{host}} = \sum_q \omega_q \left(a_q^\dagger a_q + b_q^\dagger b_q \right),$$

$$H_{\text{imp-host}} = \sum_q \lambda_q \left[S_x \left(a_q + a_q^\dagger \right) + S_y \left(b_q + b_q^\dagger \right) \right].$$

- Bose-Fermi Kondo model with XY anisotropy:

$$H = J\mathbf{S} \cdot \mathbf{s} + H_{\text{band}} + g_\perp \left(S_x u_x + S_y u_y \right) + H_{\text{baths}}$$

- Such two-bath problems are computationally very challenging because the basis grows by a large factor at each NRG step.

Recent Controversy

- Continuous-time QMC for the sub-Ohmic spin-boson model finds that the localization-delocalization transition is mean-field-like for bath exponents $0 < s < ½$ [Winter, Rieger, Vojta & Bulla, arXiv:0807.4716].
- This result contradicts the bosonic NRG [Vojta, Tong & Bulla, PRL **94**, 070604 (2005)]. Winter et al. suggest that NRG is failing on the localized side of the quantum phase transition.
- In a path-integral formulation, the SBM maps onto a transverse Ising chain with nearest-neighbor and long-range $|i-j|^{-(1+s)}$ interactions. The effective classical system is periodic with length $L = \beta = 1/T$.
- Kirchner and Si [arXiv:0808.0916] have pointed out that for $0 < s < ½$, it is important in the QMC whether the long-range interaction is evaluated just for the shortest distance $|\Delta\tau|$ around the ring, or obtained as a sum of contributions from all distances $|\Delta\tau \pm n\,\beta|$. Mean-field exponents only arise in the latter case. But "wrapping" should become insignificant in the limit $\beta \to \infty$.

Scorecard

- The good

  With the appropriate choice of basis states, bosonic NRG and Bose-Fermi NRG provide 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.

  The NRG’s validity for strongly sub-Ohmic bosonic baths is a matter of current debate.

- The computationally ugly

  With bosons, the basis grows very rapidly upon NRG iteration.

  This impedes extension to multi-impurity and multi-bath models, may prove problematic for time-dependent problems.

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