Renormalisation Group Approaches to Strongly Correlated Electron Systems

Numerical Renormalisation Group (NRG)

Impurity Models : Anderson and Kondo models –magnetic impuri ties, quantum dots Lattice Models (infinite dimension): Hubbard, Holstein and H-H models

- MIT, Polarons, Bipolarons, Antiferromagnetism, Superconductivity

Renormalised Perturbation Theory (RPT)

Low energy behaviour interpreted in terms of a model with renormalised parameters

Spin and Charge Fluctuations in the Hubbard Model

DMFT-NRG Results and their interpretation in terms of RPT

Brief Summary of the RPT Approach

- Definition of Renormalised Parameters
- Exact Results in terms of Renormalised Parameters
- Ways of calculating the Renormalised Parameters
- Perturbation theory in terms of the Renormalised Parameters

Renormalised Parameters: Anderson Model

Four parameters define the model ϵ_d , Δ , U, $\eta = g\mu_B/2$

Local Green's function
$$G_{d,\sigma}(\omega) = \frac{1}{\omega - \epsilon_{d,\sigma} + i\Delta - \Sigma_{\sigma}(\omega)}, \quad \epsilon_{d,\sigma} = \epsilon_d + \sigma h$$

Renormalised parameters defined by

$$\begin{split} \tilde{\epsilon}_{d,\sigma} &= z_{\sigma}(\epsilon_{d,\sigma} + \Sigma_{\sigma}(0)), \qquad \tilde{\Delta}_{\sigma} = z_{\sigma}\Delta, \qquad \tilde{U} = z_{\downarrow}z_{\uparrow}\Gamma_{\uparrow,\downarrow,\downarrow,\uparrow}(0,0,0,0) \\ \tilde{\epsilon}_{d} &= 0.5(\epsilon_{d,\uparrow} + \epsilon_{d,\downarrow}) \qquad \tilde{\eta} = 0.5(\epsilon_{d,\downarrow} - \epsilon_{d,\uparrow}) \end{split}$$

$$G_{d,\sigma}(\omega) = z_{\sigma} \tilde{G}_{d,\sigma}(\omega) = \frac{z_{\sigma}}{\omega - \tilde{\epsilon}_{d,\sigma} + i\tilde{\Delta}_{\sigma} - \tilde{\Sigma}_{\sigma}(\omega)},$$

 $\tilde{G}_{d,\sigma}(\omega)$ is the quasiparticle Green's function

$$z_{\sigma} = 1/(1 - \Sigma_{\sigma}'(0)) \quad \tilde{\Sigma}_{\sigma}(\omega) = z_{\sigma}(\Sigma_{\sigma}(\omega) - \Sigma_{\sigma}(0) - \omega\Sigma_{\sigma}'(0))$$

Exact Results

Friedel Sum Rule
$$n_{d,\sigma} = \tilde{n}_{d,\sigma} = \int_{-\infty}^{0} \tilde{\rho}(\omega) d\omega = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left(\frac{\tilde{\epsilon}_{d,\sigma}}{\tilde{\Delta}_{\sigma}} \right)$$

Spin and charge susceptibilities
$$\chi_{s,c} = \frac{1}{4} \sum_{\sigma} \tilde{\rho}_{\sigma}(0) \pm \frac{\tilde{U}}{2} \tilde{\rho}_{\downarrow}(0) \tilde{\rho}_{\uparrow}(0)$$

Non-interacting quasiparticle density of states

$$\tilde{\rho}_{\sigma}(\omega) = \frac{\tilde{\Delta}_{\sigma}/\pi}{(\omega - \tilde{\epsilon}_{d,\sigma})^2 + \tilde{\Delta}_{\sigma}^2}$$

Specific Heat coefficient
$$\gamma = \frac{\pi^2}{3} \sum_{\sigma} \tilde{\rho}_{\sigma}(0)$$
 $1/\tilde{\rho}(0) = 4T^*$

Kondo limit
$$\tilde{U}\tilde{\rho}(0) \rightarrow 1 \quad T^* \rightarrow T_K$$

Calculation of Renormalised parameters from NRG



Non-interacting single particle excitations correspond to poles of

non-interacting Green's function

$$G_d^{(0)}(\omega) = \frac{1}{\omega - \epsilon_d - V^2 g_0(\omega)} = 0$$

We substitute lowest single particle excitations Ep and Eh for interacting model

to determine effective values of V and ϵ_d



 $\pi \Delta = 0.05, \, \epsilon_d = -0.2, \, U = 0.3.$

Renormalised Interaction Term \tilde{U}

We look at two-particle excitations:

Epp Ehh Eph

Look at the difference with two single particle excitations:

Epp - 2Ep used to define an interaction term $\widetilde{U}pp$

Similar effective interaction terms between holes Uhh \sim Particles and holes Uph

We require
$$\lim_{N \to \infty} \tilde{U}_{hh}(N) = \lim_{N \to \infty} \tilde{U}_{hh}(N) = \lim_{N \to \infty} \tilde{U}_{ph}(N) = \tilde{U}$$

 \sim



Exact Results

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The plot shows how the renormalised parameters vary as the impurity level moves from below the Fermi level to above the Fermi level for a fixed value of U with $U = 2\pi\Delta$.

In the Kondo regime $\tilde{U} = \pi \tilde{\Delta} = 4T_K$ ACH, Oguri, Meyer Eur. Phys. J. B 40, 177–189 (2004)



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Renormalised Perturbation theory

Perturbation expansion in powers of \widetilde{U} for $\widetilde{\Sigma}_{\sigma}(\omega)$

1. The free quasiparticle Green's functions are the propagators

2. The counter terms cancel off renormalisations already included

Advantages?

Low order results correspond to Fermi liquid theory—asymptotically exact

First order diagrams give exact results given earlier for $\chi_{s,c}$

Second Order

$$\sigma_{\rm imp}(T) = \sigma_0 \left\{ 1 + \frac{\pi^2}{3} \left(\frac{T}{\tilde{\Delta}} \right)^2 \left(1 + 2 \left(\frac{\tilde{U}}{\pi \tilde{\Delta}} \right)^2 \right) + \mathcal{O}(T^4) \right\} \qquad \qquad \checkmark$$

Spin and Charge Dynamics

Repeated scattering of a quasiparticle and a quasihole gives a good description of low energy spin and charge dynamic susceptibilities



where $\tilde{\pi}^{(0)}(\omega)$ is a convolution of qp-qh pair ω





 $U/\pi\,\Delta=3.0$



Relation between vertices and Fermi liquid parameters:

$$F_0^a = -\tilde{u}_s \tilde{\rho}(0) = -\frac{\tilde{U}\tilde{\rho}(0)}{1 + \tilde{U}\tilde{\rho}(0)}, \qquad F_0^s = \tilde{u}_c \tilde{\rho}(0) = \frac{\tilde{U}\tilde{\rho}(0)}{1 - \tilde{U}\tilde{\rho}(0)},$$

Exact Fermi liquid relation:

$$\sum_{l} \left[\frac{F_{l}^{s}}{1 + F_{l}^{s}/(2l+1)} + \frac{F_{l}^{a}}{1 + F_{l}^{a}/(2l+1)} \right] = 0$$

If scattering is purely s-wave then $F_l^{a,s} = 0, l \neq 0$ and the relation is satisfied exactly

Localised limit: $\tilde{u}_c \to \infty$ then $F_0^a \to -1/2$

N.D. Mermin, Phys. Rev. 159, 161 (1967)

Renormalised Parameters: Hubbard Model

Bare parameters
$$\epsilon_{\mathbf{k}}, \quad \mu, \quad U, \quad \eta = g\mu_{\mathrm{B}}/2$$

One-electron
Green's function
$$G_{\sigma}(\omega, \mathbf{k}) = \frac{1}{\omega + \mu_{\sigma} - \epsilon_{\mathbf{k}} - \Sigma_{\sigma}(\omega)}, \qquad \mu_{\sigma} = \mu + \sigma h$$

Renormalised Parameters:

$$\begin{split} \tilde{\mu}_{\sigma} &= (z_{\sigma}(\mu - \Sigma_{\sigma}(0)), \qquad \tilde{\epsilon}_{\mathbf{k},\sigma} = z_{\sigma}\epsilon_{\mathbf{k},\sigma}, \qquad \tilde{U} = z_{\downarrow}z_{\uparrow}\Gamma_{i\uparrow,i\downarrow,i\downarrow,i\uparrow}(0,0,0,0) \\ \tilde{\mu} &= 0.5(\mu_{\uparrow} + \mu_{\downarrow}) \qquad \tilde{\eta} = 0.5(\mu_{\downarrow} - \mu_{\uparrow}) \\ G_{\sigma}(\omega,\mathbf{k}) &= z_{\sigma}\tilde{G}_{\sigma}(\omega,\mathbf{k}) = \frac{z_{\sigma}}{\omega + \tilde{\mu}_{\sigma} - \tilde{\epsilon}_{\mathbf{k},\sigma} - \tilde{\Sigma}_{\sigma}(\omega)}, \qquad \text{on-site} \end{split}$$

Quasiparticle Green's function

$$z_{\sigma} = 1/(1 - \Sigma_{\sigma}'(0)) \quad \tilde{\Sigma}_{\sigma}(\omega) = z_{\sigma}(\Sigma_{\sigma}(\omega) - \Sigma_{\sigma}(0) - \omega\Sigma_{\sigma}'(0))$$

Exact Results:

Luttinger's Theorem
$$n_{d,\sigma} = \tilde{n}_{d,\sigma} = \int_{-\infty}^{0} \tilde{\rho}_{\sigma}(\omega) d\omega$$

Bethe lattice
$$\rho_{\omega,\sigma}(\omega) = \frac{2}{\pi D_{\sigma}^2} \sqrt{D_{\sigma}^2 - (\omega + \mu_{\sigma})^2}$$

Quasiparticle DOS
$$\tilde{\rho}_{\omega,\sigma}(\omega) = \frac{2}{\pi \tilde{D}_{\sigma}^2} \sqrt{\tilde{D}_{\sigma}^2 - (\omega + \tilde{\mu}_{\sigma})^2} \qquad \tilde{D}_{\sigma} = z_{\sigma} D$$

Occupation Number
$$\tilde{n}_{\sigma} = \frac{1}{\pi} \left[\sin^{-1} \left(\frac{\tilde{\mu}_{\sigma}}{\tilde{D}} \right) + \frac{\pi}{2} + \frac{\tilde{\mu}_{\sigma}}{\tilde{D}^2} \sqrt{\tilde{D}^2 - \tilde{\mu}_{\sigma}^2} \right]$$

Specific Heat $\gamma = \frac{\pi^2}{3} \Sigma \tilde{\rho}_{\sigma}(0)$. Define energy scale $1/\tilde{\rho}(0) = 4T^*$

Half filling



Is \tilde{U} the on-site quasiparticle interaction of any use in lattice calculations?

For the infinite dimensional lattice $\Sigma_{\text{lattice}}(\omega) = \Sigma_{\text{impurity}}(\omega)$ We also have $\tilde{\Sigma}_{\sigma}(\omega) = z_{\sigma}(\Sigma_{\sigma}(\omega) - \Sigma_{\sigma}(0) - \omega\Sigma'_{\sigma}(0))$ Hence we deduce $\text{Im}\Sigma_{\text{lattice}}(\omega) = \frac{1}{z}\text{Im}\tilde{\Sigma}_{\text{impurity}}(\omega)$

$$\frac{1}{z} \text{Im} \tilde{\Sigma}_{\text{impurity}}^{(2)}(\omega)$$



We deduce asymptotic form $\text{Im}\Sigma_{\text{lattice}}(\omega) \sim -\frac{\pi\omega^2}{2z}\tilde{\rho}(0)^3\tilde{U}^2$

Strong correlation limit $T^* \rightarrow 0$

Im
$$\Sigma_{\text{lattice}}(\omega) \sim -\frac{\pi C_0^2}{32\rho(0)} \left(\frac{\omega}{T^*}\right)^2 \qquad C_0 = 0.816.$$

We can derive the asymptotically exact T^2 term from the same diagram

Local Dynamic Spin Susceptibility



Local Dynamic Charge Susceptibility



Good agreement over low energy range ---charge excitations suppressed

Beyond the NRG $\chi(\omega, \mathbf{q})$

As the irreducible vertices for the infinite dimensional model are only frequency dependent we can use the same vertices in the calculation of $\chi(\omega, \mathbf{q})$



This gives for the static susceptibility:

$$\chi_s = \frac{1}{2} \frac{\tilde{\rho}(0)}{1 - \tilde{u}_s \tilde{\rho}(0)}$$

Condition for on-set of ferromagnetism $\tilde{u}_s \tilde{\rho}(0) = 1$.



This implies that the model never has spontaneous ferromagnetism

Relation to RPA

We can relate free quasiparticle 'bubble' to that of bare electrons

$$\tilde{\pi}^{(0)}(\omega,\mathbf{q}) = \frac{1}{z}\pi^{(0)}(\omega/z,\mathbf{q})$$

The result can then be related the the RPA form:

$$\chi_s(\omega, \mathbf{q}) = \frac{1}{2z} \frac{\pi^{(0)}(\omega/z, \mathbf{q})}{1 - \tilde{u}_s/z\tilde{\pi}^{(0)}(\omega/z, \mathbf{q})} = \frac{1}{z} \chi_s^{\text{RPA}}(\omega/z, \mathbf{q}),$$
scale factors

The effective interaction Ueff is given by \tilde{u}_s/z

Near Half-filling



Values of n deduced from direct NRG evaluation agree with formula to less then 1%

$$n = \frac{2}{\pi} \left[\sin^{-1} \left(\frac{\tilde{\mu}}{\tilde{D}} \right) + \frac{\pi}{2} + \frac{\tilde{\mu}}{\tilde{D}^2} \sqrt{\tilde{D}^2 - \tilde{\mu}^2} \right]$$

Near Half-filling



Again agreement with asymptotic form in range $\omega \sim T^*$. $\mathrm{Im}\Sigma_{\mathrm{lattice}}(\omega) \sim -\frac{\pi\omega^2}{2z}\tilde{\rho}(0)^3\tilde{U}^2$

Near Half-filling

Comparison of results for local dynamic spin susceptibility

New features in the presence magnetic field h

- 1. All renormalised parameters become field dependent.
- 2. Different response and interactions in longitudinal and transverse spin channels.
- 3. Away from particle-hole symmetry the effective masses become spin dependent.
- 4. For very large field strengths the quasiparticles revert to free particles.

Renormalised parameters a a function of the magnetic field value

Mean field regime

$\tilde{\epsilon}_{\rm d}(h) = h + U m_{\rm MF}(h), \, \tilde{\Delta}(h) = \Delta$

$$\tilde{U}(h) = \frac{U}{1 - U\tilde{\rho}_{dMF}(0, h)}$$

Parameters are not all independent:

$$1 + \tilde{U}(h)\tilde{\rho}_{\rm d}(0,h) = \frac{\partial\tilde{\epsilon}_{\rm d}(h)}{\partial h} - \frac{\tilde{\epsilon}_{\rm d}(h)}{\tilde{\Delta}(h)}\frac{\partial\tilde{\Delta}(h)}{\partial h}$$

FIG. 1. (Color online) Plots of the renormalized parameters, $\tilde{\Delta}_{\uparrow}(h)/\Delta$, $\tilde{\Delta}_{\downarrow}(h)/\Delta$, $\tilde{\varepsilon}_{d}(h)/\pi\Delta$, $\tilde{U}(h)/U$, and $\tilde{\eta}(h)$, for the asymmetric Anderson model, with $\pi\Delta=0.1$, $U/\pi\Delta=2$, and $\varepsilon_{d}/\pi\Delta=-0.3$, as a function of the logarithm of the magnetic field $h/\pi\Delta$. The ratio $\tilde{\Delta}_{\downarrow}(h)/\tilde{\Delta}_{\uparrow}(h)$ is also shown.

J. Bauer +ACH PHYSICAL REVIEW B 76, 035119 (2007)

Real and imaginary parts of dynamic spin susceptibilities

Note the difference in vertical scales

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Fully aligned state (U=6, h=0.26) at 5% doping.

Comparison of quasiparticle band with interacting DOS

Narrow spin down quasiparticle band predicted by Hertz and Edwards

Change of local spectral density with increase of magnetic field

U=6 x=0.95

Future Work?

• Further applications to lattice models?

Results already for infinite dimensional lattice models

• Others ways of calculating renormalised parameters?

Several new possibilities to be explored

• Inclusion of higher order diagrams for the self-energy?

Encouraging results already obtained extending the frequency range

• Application to QCP behaviour?

 $\chi(\omega, \mathbf{q})$ can be calculated ----see what happens as we approach an instability

Irreducible vertices, $\tilde{U}_{h\downarrow}^{p\uparrow}(h)$ (black), $\tilde{U}_{h\uparrow}^{p\uparrow}(h)$ (blue), and $\tilde{U}_{p\downarrow}^{p\uparrow}(h)$ (red) as a function of $\ln (h/T_{\rm K})$ for $U/\pi\Delta = 3.0$.

Antiferromagnetic instability (half-filling)

Broken Symmetry in Lattice Models

Studies using a combination of DMFT-NRG and RPT:

- Hubbard Model in a magnetic field
- Antiferromagnetism in Hubbard model
- Superconductivity in negative U Hubbard model

Hubbard model in a magnetic field

$$H_{\mu} = -\sum_{i,j,\sigma} (t_{ij} c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.}) - \sum_{i\sigma} \mu_{\sigma} n_{i\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

Magnetic field

Particle number

$$n_{\sigma} = \sum_{i} \langle n_{i,\sigma} \rangle / N$$

Magnetisation

$$m = (n_{\uparrow} - n_{\downarrow})/2$$

U=5 x=0.5

U=6 x=0.95

Change of effective mass with magnetic field.

Note the effective mass is spin dependent away from half-filling

Doped Antiferromagnetism in the Hubbard model

$$U=3$$

Quasiparticle weight

$$w_{\rm qp} = \sum_{\sigma} z_{\sigma} u_{-}^{\sigma}(\varepsilon_{k_{\rm F}}) = \frac{z_{\uparrow} + z_{\downarrow}}{2} + \frac{(z_{\uparrow} - z_{\downarrow})\Delta\tilde{\mu}}{2|\tilde{\mu}|}$$

Effective mass
$$\frac{m^*}{m} = \frac{1}{\sqrt{z_{\uparrow} z_{\downarrow}}} \frac{|\tilde{\mu}|}{\sqrt{\tilde{\mu}_{0,\uparrow} \tilde{\mu}_{0,\downarrow}}}$$