X-ray edge and Kondo problems: A unified diagrammatic approach

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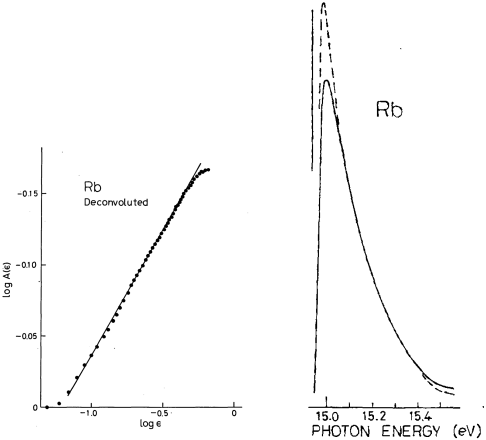
X-ray experimental motivation

- Light absorption in alkali metals
- Core electron excitation above the Fermi level
- Power-law divergence of intensity near the threshold
- Mechanism?



Simple theory

- Noninteracting conduction electrons, one core level

$$H_0 = \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \varepsilon_0 b^\dagger b$$

- Dipole interaction

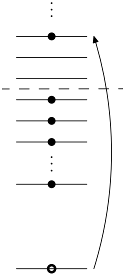
$$H_I = \sum_{\boldsymbol{k}} W_{\boldsymbol{k}} a_{\boldsymbol{k}}^\dagger b e^{-\boldsymbol{i}\omega t} + \text{h.c.}$$

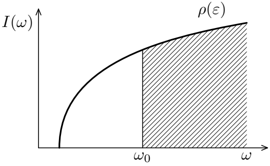
- Intensity — Fermi Golden Rule

$$I(\omega) = 2\pi \sum_{\boldsymbol{k}} |\langle 0; \boldsymbol{k}|H_I|1; 0\rangle|^2 \, \delta(\varepsilon_{\boldsymbol{k}} - \varepsilon_0 - \omega)$$

Simple theory fails!

- One electron transitions only
- Intensity proportional to the density of states
- Intensity does not diverge!





What is missing?

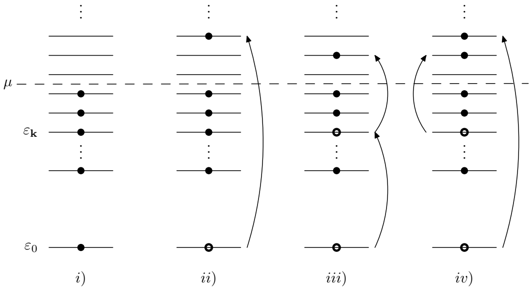
- Excitation of electron produces a charged deep hole!
- Deep hole scattering
- Improved hamiltonian (MND = Mahan–Nozières–de Dominicis)

$$H_{MND} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a^{\dagger}_{\mathbf{k}} a_{\mathbf{k}} + \varepsilon_0 b^{\dagger} b + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} a^{\dagger}_{\mathbf{k}} a_{\mathbf{k}'} b b^{\dagger}$$

- Fermi Golden Rule allows many electron transitions

Heuristics

- Typical transitions



Anderson Orthogonality Catastrophe

- Overlap of N-particle states with/without core hole $\sim N^{-\frac{1}{2}\alpha}$
- α proportional to the square of the phase shift on Fermi surface, $\alpha \approx 0.1$
- Ovelap ≈ 0.95 for molecules
- Overlap almost zero for metal
- Tends to suppress the edge singularity
- Higher order in interaction strength
- Needs nontrivial core hole selfenergy

Quantification

- Rewrite the Golden Rule to a Kubo like form

$$I(\omega) = 2\Re \sum_{\mathbf{k},\mathbf{k}'} W_{\mathbf{k}} W^*_{\mathbf{k}'} \int_0^\infty dt e^{i\omega_+ t} \left\langle \left| T \left\{ b^\dagger(t) a_{\mathbf{k}'}(t) a^\dagger_{\mathbf{k}}(0) b(0) \right\} \right| \right\rangle$$

- Near threshold behavior $\Leftrightarrow$ Long time behavior
- Task: long time (low frequency) asymptotic of dynamical susceptibility

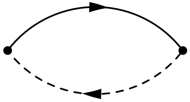
$$\chi_{\mathbf{k},\mathbf{k}'}(t-t') = \left\langle \left| T \left\{ a^\dagger_{\mathbf{k}}(t) b(t) b^\dagger(t') a_{\mathbf{k}'}(t') \right\} \right| \right\rangle$$

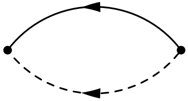
Many-body theory

- Equilibrium diagrammatic perturbation theory
- Scattering potential

$$-U \sum_{\mathbf{k},\mathbf{k}'} a^\dagger_{\mathbf{k}} a_{\mathbf{k}'} b b^\dagger$$

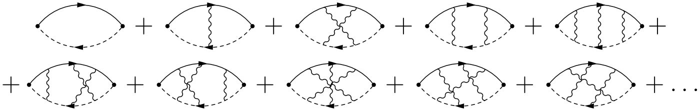
- Relevant sub-diagrams — logarithmic divergence (as $T \to 0$ and $\Delta\omega \to 0$)





Diagrams

- Mahan: Divergence anticipated from three lowest orders



- Result

$$I(\omega) \sim \left(\frac{\xi}{\omega - \omega_0}\right)^{2\rho_0 U} \Theta(\omega - \omega_0).$$

Kondo effect

- Single Impurity Anderson Model (SIAM)
- Free hamiltonian

$$\sum_{\boldsymbol{k}\sigma} \varepsilon_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma} + \varepsilon_0 \sum_{\sigma} b^\dagger_\sigma b_\sigma + \sum_{\boldsymbol{k}\sigma} (V_{\boldsymbol{k}} b^\dagger_\sigma a_{\boldsymbol{k}\sigma} + V^*_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}\sigma} b_\sigma)$$

- Spin up–spin down scattering

$$U\, b^\dagger_\uparrow b_\uparrow b^\dagger_\downarrow b_\downarrow$$

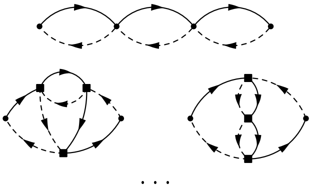
- Kondo scale $a \to 0$
- Characteristic divergent quantity $\log a$

Common features

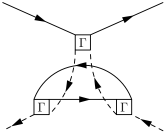
- We want to find a critical behavior
- Diagrams of all orders needed
- Specific class of diagrams of the same type (parquet)
- The same origin of the divergence: singularity in Bethe-Salpeter equations
- Two different models — difference?
- Just different one particle propagators!

Parquet diagrams

- Parquet type diagrams

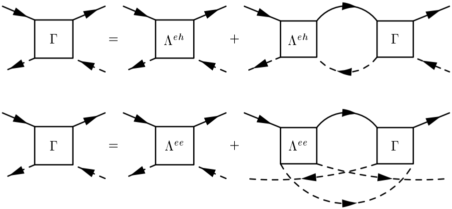


- Non-parquet diagram



Resummation

- How to sum relevant diagrams? Use two particle Green's functions!
- Find two particle vertex Γ
- Bethe-Salpeter equation in two channels



- Both channels needed

Parquet equations

- Diagram reducible in one channel is irreducible in the other
- Decomposition

$$\Gamma = \Lambda^{eh} + \Lambda^{ee} - I$$

- Totally irreducible vertex $I \approx U$
- Parquet equations for irreducible vertices Λ^{α}

$$\Lambda^{\alpha'} = I + \left\langle \Lambda^{\alpha} G\mathcal{G}[\Lambda^{\alpha} + \Lambda^{\alpha'} - I] \right\rangle_{\alpha}$$

- Nonlinear integral equations
- Analytic solution in the critical regime only

- Λ^α depends on one frequency only
- Inconsistency of parquet equations: Getting rid by specific averaging
- Averaged parquet equations

$$\Lambda^{ee} = U - \frac{\left\langle \Lambda^{eh} \mathscr{G}_c \mathscr{G} \right\rangle_{eh}^2}{\chi_{eh}\left[1 + \langle \Lambda^{eh} \mathscr{G}_c \mathscr{G} \rangle_{eh}\right]} \quad \Lambda^{eh} = U - \frac{\left\langle \Lambda^{ee} \mathscr{G}_c \mathscr{G} \right\rangle_{ee}^2}{\chi_{ee}\left[1 + \langle \Lambda^{ee} \mathscr{G}_c \mathscr{G} \rangle_{ee}\right]}$$

- χ — simple bubbles

$$\chi_{ee}(i\nu_m) = \frac{1}{\beta} \sum_n \mathscr{G}_c(i\omega_n) \mathscr{G}(i\nu_m - i\omega_n)$$

$$\chi_{eh}(i\nu_m) = \frac{1}{\beta} \sum_n \mathscr{G}_c(i\omega_n) \mathscr{G}(i\nu_m + i\omega_n)$$

Approximation 2

- Λ^{ee} is finite — replace it with a constant $\bar{U}$
- Λ^{eh} is divergent, keep the divergent part only

$$\Lambda^{eh}(\boldsymbol{i}\nu_m) \approx -\frac{\bar{U}^2 \chi_{ee}(\boldsymbol{i}\nu_m)}{1 + \bar{U}\chi_{ee}(\boldsymbol{i}\nu_m)}$$

- Taylor series near zero frequency (threshold)

$$\chi(z) \approx \chi(0) + \chi'(0)z$$

- "Kondo" scale

$$a \equiv 1 + \bar{U}\chi_{ee}(0) \to 0$$

Solution (model specific – X-ray)

- Use proper propagators, calculate $\chi_{eh}(0) = -\rho_0 \log \frac{\xi}{\Delta\omega}$
- SIAM — $\chi(0)$ not divergent
- Selfconsistent solution

$$\bar{U} \approx U - \frac{|\log a|}{\chi_{eh}(0)}$$

$$a = \exp\left[-(U\chi_{eh}(0) - 1)\right] \approx \left(\frac{\Delta\omega}{\xi}\right)^{U\rho_0}$$

- Power law divergence in Γ, hence in $I(\Delta\omega)$
- Kondo — exponential behavior

Conclusion

- Absorption intensity diverges as power law, confirming Mahan's result
- Common origin of the divergence—singularity in a BS equation
- Input to parquet equations is different
- Exponential $\times$ algebraic behavior