Single Particle Excitation From Correlated Materials: The Phenomenological Approach

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Photoemission photon in electron out $\Delta N = -1$

« Rigorous access to the energy spectrum of a hole - like excitation from a system, in which correlations of arbitrary strength are present »

ARPES Translational invariance parallel to surface $\Delta k_{II} = \kappa$

Wavenumber k_{II} of photoelectron is a symmetry label

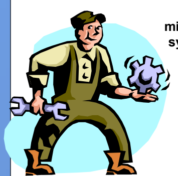
«Rigorous access to parallel momentum (modulo Umklapp κ) »

The **Hedin-Lundquist** formula
for the energy and momentum resolved photocurrent

$$< f_k \, I \, \mathbf{I} \, (k,\varepsilon) \, I \, f_k > = I \, M_k \, I^2 \, A^<(k,\varepsilon)$$

implements these rigorous principles within the sudden approximation: $A^<(k,\varepsilon)$, the Fourier spectrum of the correlation function $<c_k^+(t)c_k(0)>$ for the fermionic destruction operator that makes the photohole, is then evaluated in the equilibrium state. M_k is the matrix-element for photo-ionisation.

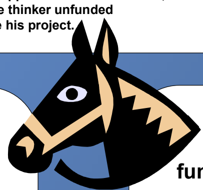
« After the instant of photo-ionisation, the out-going photo-electron in the orbital f_k undergoes no further inelastic, only multiple elastic scattering »



The "doer"says :
ARPES gives me access to the "intrinsic" $A^<(k,\varepsilon)$ and, from there, to the microscopic properties of correlated electron systems. Empirically, the connection seems well established. Without it, only a few specialists would be interested in ARPES.

Cooperation needed
(K. Matho,JESRP 117-118 pp 27-29 (2001))
New challenges are posed: Unexplained material properties involving correlations. New many-body techniques. ARPES at both higher and lower photon energy. The Hedin-Lundquist formula has enormous, unexploited possibilities. Complementary knowhow is required to implement these. Let's go with the "doer" and find out empirically how many of the challenges can be taken up within a properly evaluated framework of the sudden approximation. Meanwhile, let's not leave the thinker unfunded to advance his project.

The "thinker" says:
We need to go beyond the sudden approximation. Three-current-correlation function and Keldysh formalism are necessary to describe the steady state of the photocurrent, particularly at the low photon energies for which ARPES is possible



Hedin-Lundquist formula: a workhorse for ARPES

The unexploited possibilities can be realized when the hole operator is expanded in a complete one-particle basis

$$c_k = \Sigma \, \alpha_{fi}(k) \, a_i$$

Only operators with the same symmetry label k participate. Other labels are lumped together in i, in particular a real space label for layer dependence. The amplitudes $\alpha_{fi}(k)$ are proportional to the photo-ionisation matrix elements, multiplied by the elastic escape probability, as calculated e.g. by the inverse LEED method.

See the consequences

- **Diagonal and non-diagonal removal spectra $A^<_{ij}(k,\varepsilon)$ participate in the above autocorrelation function of the photohole**
- **Added amplitudes ≠ added intensities. The photocurrent of a multiorbital system with strong correlations is poorly approximated by a trace formula.**
- **Fano like interference is predicted, not only as function of photon energy ν, but also binding energy ε.**
- **Changes in the shape of an "EDC" as function of light polarisation can be modeled and controlled.**
- **Effects wiped out at poor angular resolution**
- **Layer dependence of the amplitudes, to lowest order reflected in the so called intrinsic lifetime broadening Δk_z, also influences the interferences.**

Excitations above the initial state, embodied in the removal spectra $A^<_{ij}(k,\varepsilon)$ can beobtained from a matrix Dyson equation, block diagonal in k, for the one electron Green function

$$\{\mathbf{G}^{-1}(k,\omega)\}_{ij} = \omega\delta_{ij} - \Sigma_{ij}(k,\omega)$$

Where does the phenomenological approach come in ?

- For most microscopic models, the elements Σ_{ij} are not known in a closed form. Information from numerical work: RNG, DMRG, QMC, ED represents valuable input.
- Our phenomenology combines sumrules (spectral moments) with generic low energy behaviour (known or conjectured) in a single continued fraction Ansatz.
- The analytical structure is in agreement with baqic causality requirements (position of poles or branchcuts in the complex ω -plane, Herglotz property).
- In high dimensions, the elements $\Sigma_{ij}(k,\omega=0)$ are unrenormalized, up to chemical shifts. This enables schemes like DMFT+LDA. In low dimensions, k-renormalization in $\Sigma_{ij}(k,\omega=0)$ as well as non-FL behaviour in ω can be incorporated.
- Explicit miocroscopic contact was made to a DMFT solution of the Hubbard model. Work on the periodic Anderson model in the charge-transfer regime is in progress.
- Even without an underlying microscopic model, sumrules are strikingly efficient to parametrise the partial spectra $A_{ij}(k,\varepsilon)$ for fitting of dazta. When comparing to an Ansatz with Lorentzians, an important reduction in the number of parameters occurs.

Two examples of phenomenological low energy scenarios

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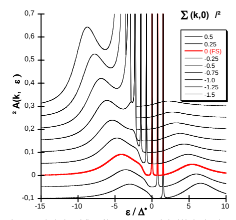

Phenomenological modeling of low energy Fermi Liquid behaviour in a hole-doped Hubbard model. Quasiparticle resonances and incoherent background. Fermi surface crossing defined by the vanishing of (k,0)Σ The quasiparticle weight equals the ratio of energy scales / Δ• Δ

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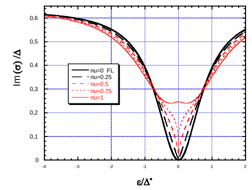

Destruction of FL behaviour tuned by a power-law exponent nu. Vanishing residue, but finite resonance weight Δ•/Δ distributed along branchcuts. For nuŠ0.25 => marginal FL. Scenario used to interprete lineshapes in Bi-2212. Andreas Müller, PhD Thesis, Shaker Verlag Aachen (2000). Computer programs for linefitting can be found there.