Theory of Extremely Correlated Fermions (III-IV)

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Lightening Summary of last lecture

Usual Dyson type theory

$$\mathcal{G}(k,i\omega) \to \underbrace{\frac{1-\frac{n}{2}}{i\omega + \mu - c \ \varepsilon_k - \Sigma(k,i\omega)}}_{Dysonform}$$

ECFL form gives instead:

$$\mathcal{G}(k,i\omega) = \underbrace{\frac{1}{i\omega + \mu - c\varepsilon_k - \Phi(k,i\omega)}}_{g(k,i\omega)} \times \underbrace{\left[1 - \frac{n}{2} + \Psi(k,i\omega)\right]}_{\mu(k,i\omega)}$$

auxiliary Greens function

caparison function

Calculation of the two self energies proceeds by one of three methods.

 \mathbf{P} Expansion in parameter λ analogous to I/(2S) in spin wave theory, by a self consistent skeleton graph expansion (numerically implemented).

Formulas for self energies look like bubble graphs in Fermi liquid theory- self consistently lead to FL type behaviour

Solution Θ Phenomenological models for Ψ and Φ based on Fermi liquid type hypothesis from the λ expansion

Solution Ψ and Ψ and Φ , inspired by the comparison with DMFT-

$$\Psi(k) = -2\lambda \sum_{p,q} E(k,p) \mathbf{g}(p) \mathbf{g}(q) \mathbf{g}(q+p-k),$$

$$\Phi = \int_{p,q} \Phi(k) = -2\lambda \sum_{p,q} E(k,p) [E(p,k) + E(q+p-k,p)] \times \mathbf{g}(p) \mathbf{g}(q) \mathbf{g}(q+p-k).$$

$$\Psi = \int_{p,q} \Phi(k) = -2\lambda \sum_{p,q} E(k,p) [E(p,k) + E(q+p-k,p)] \times \mathbf{g}(p) \mathbf{g}(q) \mathbf{g}(q+p-k).$$

Phenomenological spectral function s-ECFL (Shastry PRL 2011, Gweon et al PRL 2011)

$$\begin{split} \Psi(\omega) \sim -\frac{1}{\Delta} \Phi(\omega) & \text{Dimensional/engineering approximation} \\ \sigma(\lambda^2) \text{ equations.} \\ \Phi(\omega) = \int dx \frac{\Gamma(x)}{i\omega - x} & 40 \\ \Gamma(\omega) = \frac{\omega^2 + \pi^2 T^2}{\omega_0} e^{-(\pi^2 T^2 + \omega^2)/\Omega_0^2} & h(\omega) = \mathcal{P} \int \frac{\Gamma(\omega')}{(\omega - \omega')} d\omega' = \text{error function} \\ A_{FL}(\omega) = \frac{\Gamma(\omega)}{\Gamma^2(\omega) + (\omega - \hat{k}v_F - h(\omega))^2} & \text{Fermi liquid spectral functions} \\ Lorentzian, shap, dispersive, T dependent with width as T^2 & -0.5 & -0.4 & -0.3 & -0.2 & -0.1 \\ A_{SECFL}(\omega) = \frac{1}{\pi} \frac{\Gamma(\omega)}{\Gamma^2(\omega) + (\omega - \hat{k}v_F - h(\omega))^2} \times (1 - \frac{\omega}{\Delta} + c\hat{k}v_F) \\ \end{array}$$

(needed for Laser vs synchrotron ARPES)

2) Ω_0 (strength of FL)

3) ω_0 (High frequency cut off of FL)

$$\Delta = \int d\omega f(\omega) \langle A_{FL}(k,\omega)(\epsilon - \mu - \omega) \rangle_k$$

Expand both the self energies at small (k, $\omega)$ assuming a Fermi liquid structure.

Long wavelength expansion

$$1 - \frac{n}{2} + \Psi(\vec{k}, \omega) = \alpha_0 + c_{\Psi}(\omega + \nu_{\Psi} \ \hat{k} \ v_f) + i\mathcal{R}/\gamma_{\Psi} + O(\omega^3)$$

$$\omega + \mu - \left(1 - \frac{n}{2}\right)\varepsilon_k - \Phi(k, \omega) = (1 + c_{\Phi})\left(\omega - \nu_{\Phi} \ \hat{k} \ v_f + i\mathcal{R}/\Omega_{\Phi} + O(\omega^3)\right)$$

$$\alpha_0 = 1 - \frac{n}{2} + \Psi_0 \to (1 - n)$$

$$\mathcal{R} = \pi \{ \omega^2 + (\pi k_B T)^2 \}$$
$$\hat{k} = (\vec{k} - \vec{k}_F) \cdot \vec{k}_F / |\vec{k}_F|$$

$$v_f = (\partial_k \varepsilon_k)_{k_F}$$
 is the *bare* Fermi velocity

Non Lorentzian Spectral function with **5** parameters

$$A(\vec{k}, \omega) = \frac{z_0}{\pi} \frac{\Gamma_0}{(\omega - \nu_{\Phi} \ \hat{k} \ v_f)^2 + \Gamma_0^2} \times \mu(k, \omega)$$

$$\Gamma_0(\hat{k}, \omega) = \eta + \frac{\pi(\omega^2 + (\pi k_B T)^2)}{\Omega_{\Phi}}$$

$$\mu(\hat{k}, \omega) = 1 - \frac{\omega}{\Delta_0} + \frac{\nu_0 \ \hat{k} \ v_f}{\Delta_0}$$

 $\{\Delta_0, z_0, \Omega_{\Phi}, \nu_0, \nu_{\Phi}\}$ $v_F \to \text{bare Fermi velocity}$

Comments:

 \mathbf{Q} Notable feature of all the ECFL spectral functions is the non Lorentzian nature- due to the multiplying factor (caparison factor) that depends on k and ω .

- \bigcirc As a result different "spectra"- locating the maxima of A(k, ω)-are definable:
 - Θ at fixed k scan various ω (EDC's)
 - Θ at fixed ω scan versus k (MDC's)

 Θ The MDC spectrum and EDC spectrum differ at very low energies in the spectral function A_{ECFL}(k, ω)- the caparison factor makes the difference.

See- the notorious case of spin waves in Iron above Tc, (1978-81).

 Θ Here locating spin waves from constant k scans is right, often constant ω scans were used to make dramatic, but ultimately incorrect claims.



Theoretical Results and Benchmarking

Short summary of second order results in 2-dimensions

- Secomparison with High T expansion results
- Comparison with DMFT
- Secomparison with Anderson Impurity Model

Experimental Benchmarking and predictions

ARPES Line shapes: ECFL
 ARPES Line shapes+ Casey Anderson theory
 ARPES High energy kinks- (t-t'-J model electron doped versus hole doping)
 ARPES Low energy kinks from ECFL

SYMMETRY- emergent energy scale- its identification and isolation as an urgent task

Open questions

Short summary of second order results in 2-dimensions

PHYSICAL REVIEW B 87, 245101 (2013)

Extremely correlated Fermi liquids: Self-consistent solution of the second-order theory

Daniel Hansen and B. Sriram Shastry





Wednesday, April 9, 2014

Comparison with High T expansion results

PHYSICAL REVIEW B 87, 161120(R) (2013)

Electronic spectral properties of the two-dimensional infinite-U Hubbard model

Ehsan Khatami,^{1,2} Daniel Hansen,¹ Edward Perepelitsky,¹ Marcos Rigol,³ and B. Sriram Shastry¹

Dynamics out to quite high (8th) order in hopping computed, using Metzner's series for G.

$$\varepsilon_1^0(k) = \frac{\langle \{ [\hat{C}(k), H], \hat{C}^{\dagger}(k) \} \rangle}{\langle \{ \hat{C}(k), \hat{C}^{\dagger}(k) \} \rangle}$$

Symmetric moment (EDC) can be compared with ECFL spectrum to $O(\lambda^2)$, and does quite well except at high energy (unoccupied) states near X point



← Here ECFL is the symbols and Pade results as solid/dashed lines- up to n~0.7. Beyond n~0.7 ECFL is not available and only series results are shown.

 $\varepsilon_1^>(k) = \frac{\langle [\hat{C}(k), H] \ \hat{C}^{\dagger}(k) \rangle}{\langle \hat{C}(k) \hat{C}^{\dagger}(k) \rangle}$

Particle addition type moment does much better. Essentially exact agreement with the actual QP peaks. Reason is that unoccupied Fermi function invoked here kills the long tails in the occupied side (see ECFL curves), and thereby focuses on the QP's.





Compare with DMFT in infinite D Formal preliminaries

Extremely correlated Fermi liquids in the limit of infinite dimensions

Edward Perepelitsky*, B. Sriram Shastry

Annals of Physics 338 (2013) 283-301

In high dimensions we can show that these are further related through

$$\Psi(k) = \Psi(i\omega_k),$$

$$\Phi(k) = \chi(i\omega_k) + \epsilon_k \Psi(i\omega_k).$$

$$\Sigma_{DM}(k) = \Sigma_{DM}(i\omega_k) = \frac{(i\omega_k + \mu)\Psi(i\omega_k) + (1 - \frac{n}{2})\chi(i\omega_k)}{1 - \frac{n}{2} + \Psi(i\omega_k)},$$

$$\Psi(i\omega_k) = -\lambda u_0 I_{000}(i\omega_k) + 2\lambda I_{010}(i\omega_k),$$

$$\chi(i\omega_k) = -\frac{u_0}{2}\Psi(i\omega_k) - u_0\lambda I_{001}(i\omega_k) + 2\lambda I_{011}(i\omega_k).$$

$$\mathbf{g}_{\text{loc},m}(i\omega_k) \equiv \sum_{\vec{k}} \mathbf{g}(k)\epsilon_{\vec{k}}^m,$$

$$I_{m_1m_2m_3}(i\omega_k) \equiv -\sum_{\omega_p,\omega_q} \mathbf{g}_{\text{loc},m_1}(i\omega_q)\mathbf{g}_{\text{loc},m_2}(i\omega_p)\mathbf{g}_{\text{loc},m_3}(i\omega_q + i\omega_p - i\omega_k),$$

$$\sum_k \mathbf{g}(k) = \frac{n}{2};$$

$$\sum_k \mathcal{G}(k) = \frac{n}{2}.$$



Extremely correlated Fermi liquid theory meets dynamical mean-field theory: Analytical insights into the doping-driven Mott transition

A comparison of ECFL and DMFT spectral function color plots after scaling the frequency by Z (the QP weight). In this rough representation, it is hard to tell the theories apart!



A comparison of ECFL and DMFT after scaling the frequency by Z (the QP weight).



Sec The O(λ^2) version of ECFL used here seems closer to U= 4D, consistent with the interpretation of λ .

The shapes of the functions are in excellent accord- out to unexpectedly high densities- (ECFL version arguably good for small densities, does impressively well at high densities.)

 \mathbf{Q} Note the strong particle hole assymmetry about ω =0.A strong bias in both theories- discussed later.



Momentum Occupation vs ε with DMFT and ECFL on left and right, respectively



2.0 Exciting because we obtain a promising synthesis between the analytical power of ECFL and the exact numerical power of DMFT. 1.5 Muchannese to learn from this joint approach..... $T_{MIR}^{(ECFL)} \approx .61 D$









$I_{ARPES} \sim |M|^2 \times A(k,\omega) \times f(w)$

Angle resolved photo emission ARPES (1990) Surprising.





C. G. Olson, R. Liu, and D. W. Lynch

$$A(k,\omega) = \sum_{\alpha,\nu} e^{-\beta\varepsilon_{\alpha}} |\langle \nu|C(k)|\alpha\rangle|^2 \ \delta(\omega + \varepsilon_{\nu} - \varepsilon_{\mu})$$

$$A_{FL}(k,\omega) \sim \frac{\Gamma/\pi}{\Gamma^2 + (\omega - E_k)^2}$$

$$\Gamma_{FL} \sim (\omega^2 + \pi^2 T^2)$$

$$E_k = \text{Quasi hole energy}$$

$$I_{15.5^{\circ}} = I_{15.5^{\circ}}$$

$$I_{14.75^{\circ}} = I_{14.75^{\circ}} = I_{14.75^{\circ}}$$

$$I_{14.75^{\circ}} = I_{14.75^{\circ}} = I_{14.$$

Fermi-Liquid Line Shapes Measured by Angle-Resolved Photoemission Spectroscopy on 1-T-TiTe2

0

-200

R. Claessen, R. O. Anderson, and J. W. Allen Randall Laboratory, University of Michigan, Ann Arbor, Michigan 48109-1120

C. G. Olson and C. Janowitz

P.W. Anderson and P Casey Hidden Fermi Liquid: Beautiful and compact idea based on X ray edge singularity work.

$$G(k,\omega) = \int \int dx \, dt \, e^{i(kx-\omega t)} t^{-p} / (x - v_F t).$$
$$= \int dt \, t^{-p} e^{i(v_F k - \omega)t} \propto (v_F k - \omega)^{-1+p}.$$
$$p = \frac{1}{4}n^2$$

$$A(k,\omega) = f(\omega/T) \frac{\sin[(1-p)(\pi/2 - \tan^{-1}[(\omega - v_{\rm F}k)/\Gamma])]}{[(\omega - v_{\rm F}k)^2 + \Gamma^2]^{(1-p)/2}}.$$

$$\Gamma = aT$$

At T=0 is a Non Fermi Liquid at any density n. At finite T looks a lot like ECFL because it has the right asymmetry built into it Accurate theoretical fits to laser-excited photoemission spectra in the normal phase of high-temperature superconductors

LETTERS

PHILIP A. CASEY¹, J. D. KORALEK^{2,3}, N. C. PLUMB², D. S. DESSAU^{2,3} AND PHILIP W. ANDERSON^{1*}



Simplified ECFL 3 parameter fn vs data:

$$A_{sECFL}(\omega) = \frac{1}{\pi} \frac{\Gamma(\omega)}{\Gamma^2(\omega) + (\omega - \hat{k}v_F - h(\omega))^2} \times (1 - \frac{\omega}{\Delta} + c\hat{k}v_F)$$
$$\Gamma(\omega) = \frac{\omega^2 + \pi^2 T^2}{\omega_0} e^{-(\pi^2 T^2 + \omega^2)/\Omega_0^2}$$
$$\Gamma \to (\Gamma + \eta)$$

Energy dispersion and the 10 chosen values of k to compare theory and experiment.



PRL 107, 056404 (2011)

Extremely Correlated Fermi-Liquid Description of Normal-State ARPES in Cuprates















Theory of extreme correlations using canonical Fermions and path integrals

B. Sriram Shastry

$$A(\vec{k},\omega) = \frac{z_0}{\pi} \frac{\Gamma_0}{(\omega - \nu_{\Phi} \ \hat{k} v_f)^2 + \Gamma_0^2} \times \mu(k,\omega)$$

$$\mu(\hat{k},\omega) = 1 - \frac{\omega}{\Delta_0} + \frac{\nu_0 \ k \ v_f}{\Delta_0},$$
$$\Gamma_0 = \eta + \frac{\pi^3 (k_B T)^2}{\Omega_\Phi}$$

$$Q(\hat{k}) = \Delta_0 + (\nu_0 - \nu_{\Phi}) \hat{k} \nu_f$$

$$r = \frac{\nu_0}{\nu_{\Phi}},$$

$$Recall that \Delta_0 \text{ is important asymmetry scale.}$$

$$E(k) = \frac{1}{2 - r} \left(\nu_{\phi} \hat{k} \nu_f + \Delta_0 - \sqrt{r(2 - r) \Gamma_0^2 + Q^2} \right),$$

$$E^*(k) = \left(\nu_0 \hat{k} \nu_f + \Delta_0 - \sqrt{\Gamma_0^2 + Q^2} \right).$$

$$E(k_{kink}) = -\frac{1}{r - 1} \Delta_0 - \Gamma_0 \sqrt{\frac{r}{2 - r}}$$

Low energy kinks and their electronic origin. (non Landau FL)

Explicit expressions for both kink energies.

E and E* are MDC and EDC peak energies found by max A w.r.t. $\omega \;\; \text{or } k.$

In MDC a clear maximum is not very robust. EDC more robust

Both spectra are hybrids of massless and massive Dirac spectra, - asymptotically $E(k) \sim \frac{1}{2-r}(v_{\Phi} + (v_0 - v_{\Phi}) sign(\hat{k})) \hat{k} v_f.$ $E^*(k) \sim (v_0 + (v_0 - v_{\Phi}) sign(\hat{k})) \hat{k} v_f$

Weights E Kink arises from role of caparison function.

Solution with the set of the set

Separate on n,T and η given explicitly here

$$(\hat{k} v_f)_{kink} = \frac{\Delta_0}{v_{\Phi}(1-r)},$$

Hence kink in occupied side provided r>1.



Identifying Asymmetry at lowest frequencies in ARPES data:

Main message:

Inverse intensity gives a better perspective for identifying asymmetry.

Intensity itself focusses attention elsewhere.

Doniach Sunjic 1969!!





Shastry, Phys. Rev. Letts (2011)



Construct object Q from intensity

$$\widetilde{\omega}_k = \omega - E_k^*,$$

energy shifted by peak position

$$\mathcal{Q}(\widetilde{\omega}_k) = A - B\,\widetilde{\omega}_k$$

A sloping Q factor pinpoints and quantifies asymmetry!

Some predictions re asymmetry

Dynamical Particle-Hole Asymmetry in High-Temperature Cuprate Superconductors

B. Sriram Shastry

PRL 109, 067004 (2012)

Dynamical P-H transformation
$$(\hat{k} \equiv \vec{k} - \vec{k}_F)$$

 $(\hat{k}, \omega) \rightarrow -(\hat{k}, \omega).$

$$\mathcal{S}_{\mathcal{G}}(\vec{k},\omega) \equiv f(\omega)f(-\omega)\rho_{\mathcal{G}}(\vec{k},\omega) = \frac{1}{|M(\vec{k})|}f(-\omega)I(\vec{k},\omega).$$

This is the Fermi symmetrized spectral function that focuses attention near chemical potential. Here I(k,w) is ARPES intensity and M is dipole matrix element

Construct symmetric and antisymmetric combinations under the above DPH transformation $\frac{1}{2} \left[S_{\mathcal{G}}(\vec{k}_F + \vec{\hat{k}}, \omega) \mp S_{\mathcal{G}}(\vec{k}_F - \vec{\hat{k}}, -\omega) \right]$

From these form the (dimensionless) asymmetry ratio R $\mathcal{R}_{\mathcal{G}}(\vec{k}_F | \vec{\hat{k}}, \omega) = \mathcal{S}_{\mathcal{G}}^{a-s}(\vec{k}_F | \vec{\hat{k}}, \omega) / \mathcal{S}_{\mathcal{G}}^s(\vec{k}_F | \vec{\hat{k}}, \omega)$

> Important ratio Can experimentally distinguish between two classes of theories.





Requires momentum resolution $\Delta k = .001$ Angstrom (perhaps just beyond current reach.)

Asymmetry related comments:

Prospects and Open issues

Superconductivity due to exchange J - this is very natural - (MS in preparation)

Selection of Mott insulating state?

Onderdoped phase?

Other broken symmetries (AFM- Quantum liquids..)?

Merci Beaucoup