Theory of Extremely Correlated Fermions (I-II)

Sriram Shastry
University of California
Santa Cruz, CA

Collège de France
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Collaborators/ Inspirers

- Edward Perepelitsky,
- Daniel Hansen,
- Ehsan Khatami (UCSC),
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- Alex Hewson (London)
- Marcos Rigol (U Penn)

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- Phil Anderson
- Tom Banks
- Gabi Kotliar

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Middle way possible
Dyson (Maleev) type theory
& Inconvenience of non Hermitean QFT

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t-J model
& the
Hubbard model

(I)

ECFL
Schwinger Dyson method
Exact equations (2011)

(III)

Product expression of Greens function
i.e. non- Dysonian representation
with two self energies! (2011)

An approximate implementation
λ-expansion (2013)

Low energy long wavelength expansion of
the two self energies. (2013)
Motivated by DMFT comparison

(IV)

Shift identities-
problems with slave representations
Second chemical - potential (2013)

(V)

Checks of ECFL: (2013)
- High D- DMFT Comparison
- Anderson Impurity Model Comparison
- High T expansion Comparison

Experimental tests of ECFL:
(2011-14)
- ARPES line shapes
- Casey Anderson
- Asymmetry
- ARPES Kinks-
  - High energy kinks
  - Low energy kinks (2014)
- AIS/STM predictions

(VI)

Dyson-Maleev type
Non Hermitean representation
Path integral representation
λ-Fermions as a new option (2014)

(II)

- OPEN ISSUES-In progress
- Insulating phase
- Superconducting phase
- Magnetic phases

(VII)

Formalism papers

- `` Extremely Correlated Fermi Liquids '', B. S. Shastry, arXiv:1102.2858 (2011),Phys. Rev. Letts. 107, 056403 (2011); 108, 029702 (2012).
- `Anatomy of the Self Energy'', B. S. Shastry, arXiv:1104.2633; Phys. Rev. B 84, 165112 (2011); Phys. Rev. B 86, 079911(E) (2012).
- ``Extremely Correlated Fermi Liquids: Self consistent solution of the second order theory'', D. Hansen and B. S. Shastry, arXiv:1211.0594, (2012), Phys. Rev. B 87, 245101 (2013).
- ``Extremely Correlated Fermi Liquids: The Formalism'', B. S. Shastry, arXiv:1207.6826 (2012); Phys. Rev. B 87, 125124 (2013).
- ``ECFL in the limit of infinite dimensions'', E. Perepelitsky and B. S. Shastry, arXiv:1309.5373 (2013), Anns. Phys. 338, 283-301 (2013).
- Theory of extreme correlations using canonical Fermions and path integrals'', B. S. Shastry, arXiv:1312.1892 (2013), Ann. Phys. 343, 164-199 (2014).

Benchmarking papers

DMFT and AIM related papers

- ``Extremely correlated Fermi liquid theory meets Dynamical mean-field theory: Analytical insights into the doping-driven Mott transition'', R. Zitko, D. Hansen, E. Perepelitsky, J. Mravlje, A. Georges and B. S. Shastry, arXiv:1309.5284 (2013), Phys. Rev. B 88, 235132 (2013).
- ``Extremely Correlated Fermi Liquid study of the $U=\infty$ Anderson Impurity Model'', B. S. Shastry, E. Perepelitsky and A. C. Hewson, arXiv:1307.3492 [cond-mat.str-el], Phys. Rev. B 88, 205108 (2013).

High T Expansion comparison papers

- ` Linked-Cluster Expansion for the Green's function of the Infinite-U Hubbard Model'', E. Khatami, E. Perepelitsky, M. Rigol and B. S. Shastry, arXiv: 1310.8029 (2013).
- ``Electronic spectral properties of the two-dimensional infinite-U Hubbard model'', E. Khatami, D. Hansen, E. Perepelitsky, M. Rigol, B. S. Shastry, arXiv:1303.2657 [cond-mat.str-el] (2013), Phys. Rev. B 87, 161120 (R) (2013).

Experimentally relevant papers

- `` Dynamical Particle Hole Asymmetry in Cuprate Superconductors'', B. S. Shastry, arXiv:1110.1032 (2011), Phys. Rev. Letts. 109, 067004 (2012).
- ``Extremely Correlated Fermi Liquid Description of Normal State ARPES in Cuprates'', G.-H. Gweon, B. S. Shastry and G. D. Gu, arXiv:1104.2631 (2011), Phys. Rev. Letts. 107, 056404 (2011).
- Phenomenological Model for the Normal-State Angle-Resolved Photoemission Spectroscopy Line Shapes of High-Temperature Superconductors Kazue Matsuyama and G.-H. Gweon Phys. Rev. Lett. 111, 246401 (2013).

- Low energy Kinks and ECFL (Shastry 2014 Annals of Physics)
- Line Shapes: P.A. Casey, P. W. Anderson, Phys. Rev. Letts. 106, 097002, (2011), Nature Physics, 4, 210 (2008) { Hidden Fermi Liquid Theory}-
- S Doniach and M Sunjic (1970), P. Noizeres and C. De Dominicis (1969) X-ray edge singularity.

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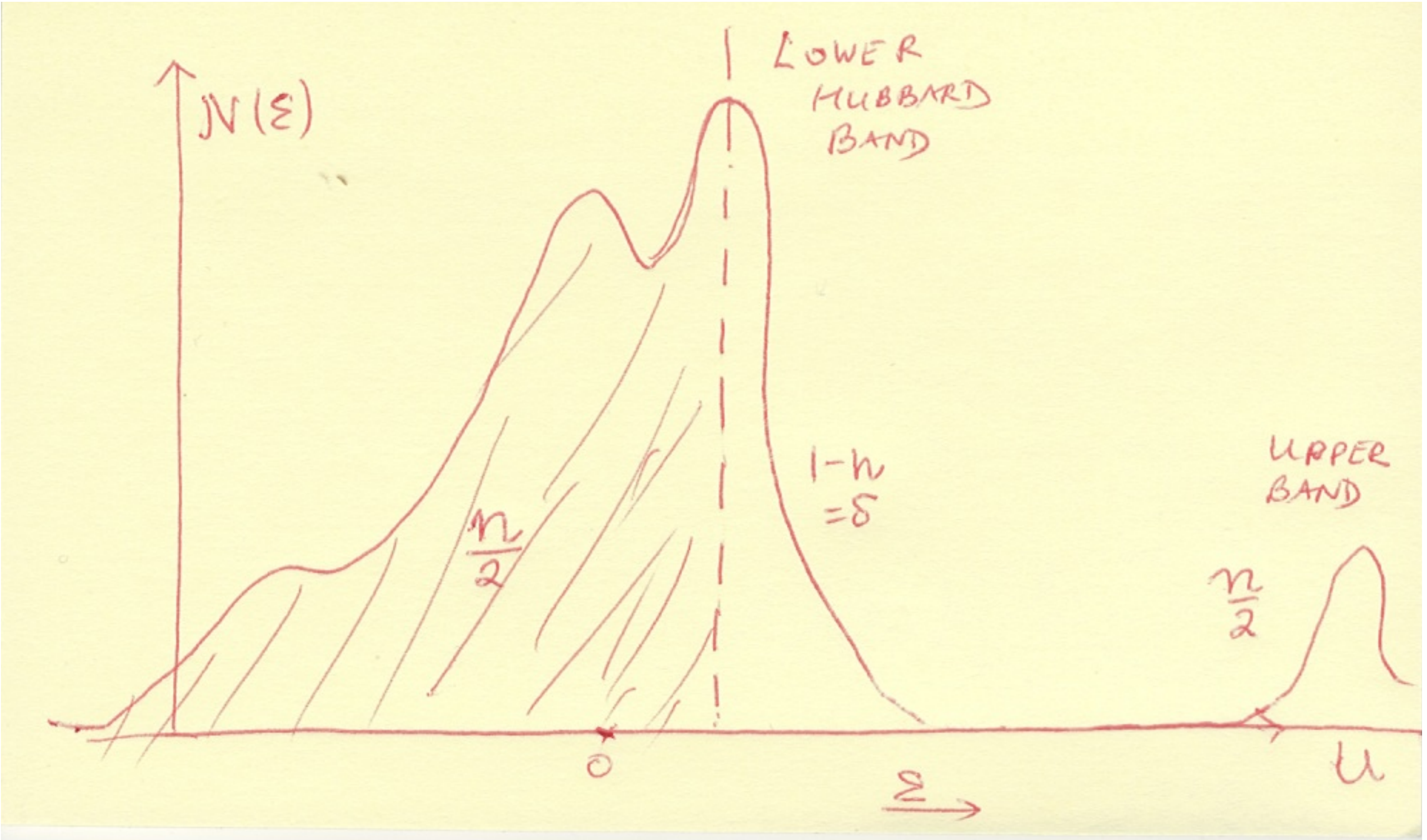

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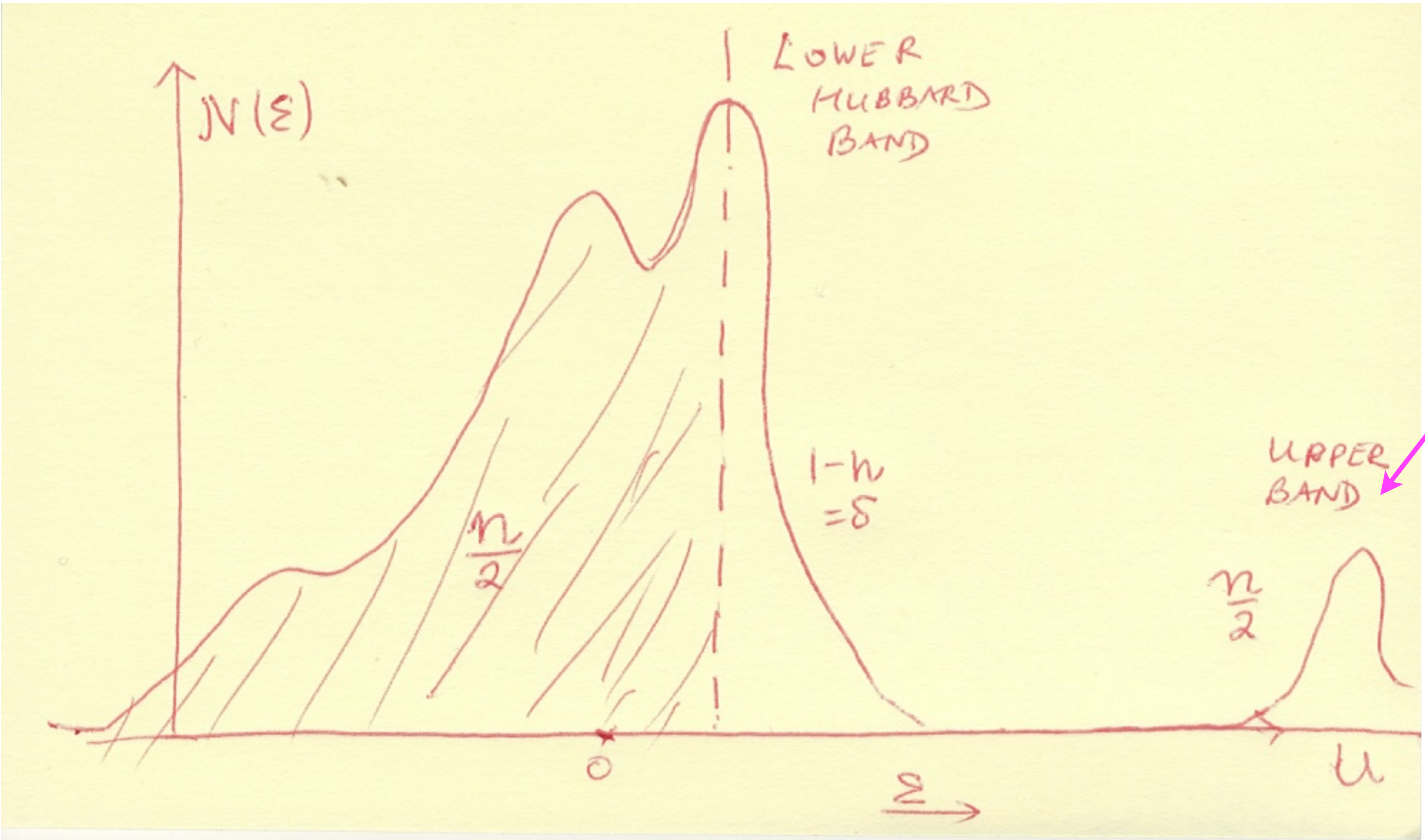

Eliminate using Gutzwiller Projection

Theoretical setting of the ECFL methodology for systematically studying the t J model.

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$$|a> \;\; a=\uparrow, a=\downarrow, a=0$$

$$a \neq \uparrow\downarrow$$

X's are Fermions with built in projection ops.
The hatted Fermions are equivalent to X's

$$X_i^{ab} = |a><b|$$

$$\hat{C}^\dagger_\sigma = (1-n_{-\sigma})C^\dagger_\sigma$$

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X's satisfy a Lie algebra (with anticommuting objects i.e. grading) as opposed to simple canonical Fermi operators.

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$$\{ X_i^{0\sigma}, X_j^{\sigma' 0} \} = \delta_{ij} (\delta_{\sigma\sigma'} - \sigma\sigma' X_i^{\bar{\sigma}'\bar{\sigma}})$$

$$\bar{\sigma} = -\sigma$$

What does extreme correlations mean?

$$H = -\sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Hubbard model (t,U)

(1) Weak Correlations $U \ll t$

Semiconductors

(2) Intermediate Correlations $U \leq t$

DFT (Band theory), Wide band free electron like metals

(3) Strong Correlations $U \geq t$

Transition metal magnetism, Dense Kondo Heavy Fermi systems, Iron arsenide superconductors etc

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Non Dysonian representation of Greens functions
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Reconstruction of Σ_{DM} possible but
Physics better captured by ECFL pair.

$$\{\Phi, \Psi\} \rightarrow \Sigma_{DM}$$

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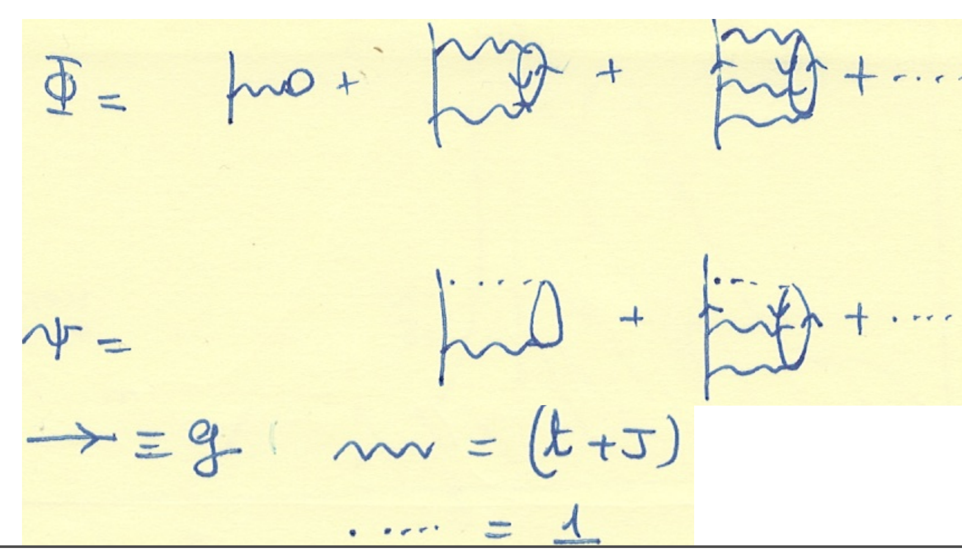

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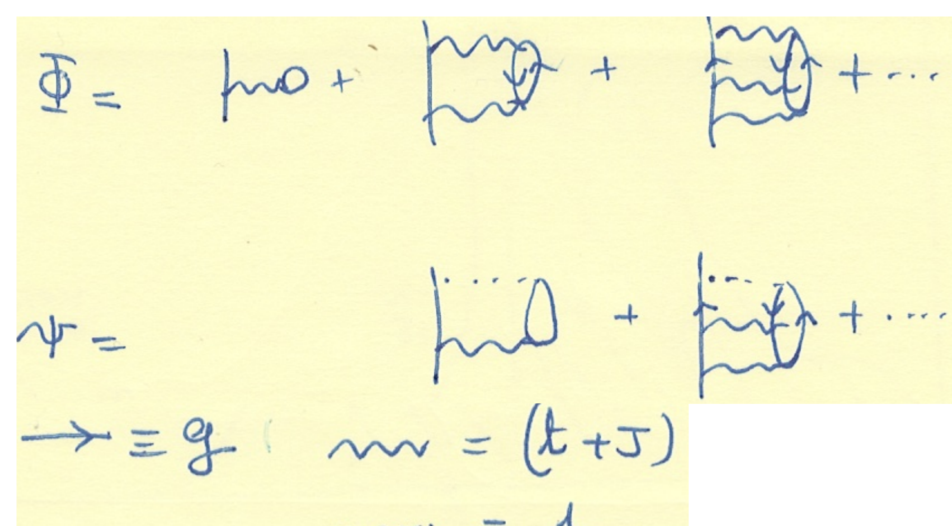

$\{\Phi,\Psi\}$ are BOTH generically ideal Fermi liquid like, but not so with Σ_{DM}

Why is the extreme correlation problem (t J model) so difficult?

- Non canonical field theory- Cannot consult existing text books!
    - Absence of Wicks theorem and Feynman series
    - Absence of any obvious small parameter.
- Gutzwiller projection is a ``singular perturbation", hence a major stumbling block for the dynamics.
- ECFL approach uses an adaptation of Schwinger's method.
    - Bypass Wicks theorem.
    - Uses extra time dependent potentials and magnetic fields to generate exact equations of motion (EOM).
- Freedom intrinsic to the Schwinger Dyson method + shift identities+ insights from spectral sum rules helps us to make progress.
- Connects with with Dyson Maleev approach invented for the spin problem
- ECFL describes a new **framework** for calculation with twin self energies and vertices.
- Obtain analytical results that are useful-novel and have experimental consequences. Also helpful in building bridges with DMFT and other approaches

A quick overview of "why things are so". Work in the liquid state (no broken symmetry)

$$\boxed{\mathcal{G}_{\sigma\sigma'}(i\tau_i, f\tau_f) = -\frac{\langle T_\tau e^{-\hat{\mathcal{A}}_S}\left(X_i^{0\sigma}(\tau_i) X_f^{\sigma'0}(\tau_f)\right)\rangle}{\langle T_\tau e^{-\hat{\mathcal{A}}_S}\rangle}}$$

Added time dependent potentials, finally set to zero.

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Hat Removal Theorem: (2013)

Provided Gutzwiller projector supplied at initial time

$$X_i^{0\sigma} \to C_{i\sigma},\ X_i^{\sigma 0} \to \widetilde{C}_{i\sigma}^\dagger = C_{i\sigma}^\dagger(1-N_{i\bar{\sigma}}),\ X_i^{\sigma\sigma'} \to C_{i\sigma}^\dagger C_{i\sigma'}.$$

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$$\boxed{\mathcal{G}_{\sigma\sigma'}(i\tau_i, f\tau_f) = -\frac{\langle T_\tau e^{-\hat{\mathcal{A}}_S}\left(X_i^{0\sigma}(\tau_i)X_f^{\sigma'0}(\tau_f)\right)\rangle}{\langle T_\tau e^{-\hat{\mathcal{A}}_S}\rangle}}$$

Added time dependent potentials, finally set to zero.

$$A = \sum_i \int_{\tau'} \mathcal{V}_i^{\sigma\sigma'}(\tau')\ \hat{C}^\dagger_{i\sigma}(\tau')\hat{C}_{i\sigma'}(\tau')$$

Double Hat Theorem: (1963)

$$X_i^{\sigma 0} = \tilde{C}^\dagger_\sigma = (1-n_{-\sigma})C^\dagger_\sigma$$
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Hat Removal Theorem: (2013)

Provided Gutzwiller projector supplied at initial time

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$$\langle\langle A(\tau_1)B(\tau_2)\ldots\rangle\rangle = \frac{1}{Z}\mathrm{Tr}\ e^{-\beta\hat{H}_{eff}}T_\tau\left(e^{-\hat{A}_S}A(\tau_1)B(\tau_2)\ldots\hat{P}_G(0^-)\right)$$

Leads to straightforward path integral rep, with Gutzwiller projector ONLY at initial time.

$$\hat{A}_S = T_{eff} + JS.S + A$$

$$\hat{T}_{eff} = -\sum_{ij\sigma} t_{ij}\widetilde{C}^\dagger_{i\sigma}C_{j\sigma}$$

Proof of Theorem:
Upper Triangular Representation

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t-J basis of states

$$[\psi]'_{final} = Q'_M \ldots Q'_2 . Q'_1 . [\psi]'_{initial} \qquad Q'_j \sim e^{-it_j H_{tJ}}$$

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Next we study the Canonical basis of states

$$[\psi] = \begin{bmatrix} \psi^{ph} \\ \psi^{un} \end{bmatrix} ; \quad \hat{P}_G = \begin{bmatrix} \mathbb{1}^{ph} & 0 \\ 0 & 0 \end{bmatrix}$$

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Theorem: Product of upper triangular matrices remains upper triangular. QED

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$$\boxed{\mathcal{G}_{\sigma_i\sigma_f}(i\tau_i, f\tau_f) = -\langle\langle C_{i\sigma_i}(\tau_i)\widetilde{C}^{\dagger}_{f\sigma_f}(\tau_f)\rangle\rangle}$$

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Reminder from last page: definition of hatted operators

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Notice the <<>> are still non trivial

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Second self energy by analogy with HM self energy defined through analogous ratio.
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“The Notorious”
Caparison function
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"The Notorious"
Caparison function
μ= (1- <N> +ψ

This "explains" how the Product form arises

Caparison= elaborate decoration (*Ye Olde English*).

Idea is that the auxiliary "g(k,ω)" is already dressed by Fermi liquid renormalization, G requires a second layer of decoration!!

$$S_i^+ = (2s)\ b_i^\dagger\ (1 - \frac{n_i}{2s}\ )$$

$$S_i^- = b_i$$

$$S_i^z + s = n_i,$$

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Dyson Maleev

Harris, Kumar, Halperin and Hohenberg

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Dyson Maleev

Harris, Kumar, Halperin and Hohenberg

	Spins: The Dyson–Maleev mapping		Fermions: The non-Hermitian mapping	
Destruction operator	S_i^-	b_i	$X_i^{0\sigma}$	$C_{i\sigma}$
Creation operator	S_i^+	$(2s)\ b_i^\dagger(1 - \frac{n_i}{2s})$	$X_i^{\sigma 0}$	$C_{i\sigma}^\dagger(1 - \lambda N_{i\bar\sigma})$
Density operator(s)	$S_i^z + s$	$n_i = b_i^\dagger b_i$	$X_i^{\sigma\sigma'}$	$C_{i\sigma}^\dagger C_{i\sigma'}$
Projection operator	$\hat{P}_D$	$\prod_i\{\sum_{m=0}^{2s}\delta_{n_i,m}\}$	$\hat{P}_G$	$\prod_i(1 - N_{i\uparrow}N_{i\downarrow})$, for $\lambda = 1$
Vacuum	$\vert\downarrow\downarrow\ldots\downarrow\rangle$	$\vert 00\ldots 0\rangle$	$\vert Vac\rangle$	$\vert 00\ldots 0\rangle$
Small parameter & its range	$\frac{1}{2s}$	$\frac{1}{2s}\in[0,1]$	λ	$\lambda\in[0,1]$
Auxiliary Green's function		$\mathbf{g}(i,j) = -\langle\langle b_i b_j^\dagger\rangle\rangle$		$\mathbf{g}(i,j) = -\langle\langle C_{i\sigma}C_{j\sigma}^\dagger\rangle\rangle$
Caparison function		$\mu(i,j) = \delta_{ij}(1 - \frac{1}{2s}\langle n_j\rangle) + \frac{1}{2s}\Psi(i,j)$		$\mu(i,j) = \delta_{ij}(1-\lambda\gamma)+\lambda\Psi(i,j)$
Second Self energy Ψ		$\Psi(i,j) = \mathbf{g}^{-1}(i,\mathbf{a})\langle\langle b_\mathbf{a} b_j^\dagger n_j\rangle\rangle_c$		$\Psi(i,j) = \mathbf{g}^{-1}(i,\mathbf{a})\langle\langle C_{\mathbf{a}\sigma}C_{j\sigma}^\dagger N_{j\bar\sigma}\rangle\rangle_c$

This table summarizes the parallel between spins and extreme Fermions.
We have anticipated the parameter λ in analogy to the semiclassical parameter 1/(2 S) in D-M

Summary: With Fourier transforms, and
with auxuliary "g" having its own self energy,
and expand the caparison function μ

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$G(k) = \frac{1}{i\omega - \varepsilon_k - \Sigma(k)}$	$\mathcal{G}(k) = \frac{1 - \frac{n}{2}}{i\omega - c\ \varepsilon_k - \Sigma_{DM}(k)}$	$\mathcal{G}(k) = \frac{(1 - \frac{n}{2} + \Psi(k))}{i\omega - c\ \varepsilon_k - \Phi(k)} = \mathbf{g}(k) \times \mu(k)$

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$$t_{ij} \sim \frac{1}{\sqrt{D}}$$

$$H = \sum_{\sigma} \epsilon_d X^{\sigma\sigma} + \sum_{k\sigma} \widetilde{\epsilon}_k n_{k\sigma} + \sum_{k\sigma} (V_k \, X^{\sigma 0} \, c_{k\sigma} + V_k^* \, c_{k\sigma}^{\dagger} \, X^{0\sigma}),$$

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We also obtain an independent solution of the tJ as well as the AIM model as an expansion in λ. Here λ is related to the density of particles or the filling of the d-level in the AIM. Will discuss the explicit solution to 2nd order later.

Simplest approach is to expand both the self energies at small (k, ω) assuming a Fermi liquid structure.

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Long wavelength expansion

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

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Spectral function with 5 parameters

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Scaling property near half filling

$z_0\rightarrow\overline{z}_0\times\delta;\quad \Delta_0\rightarrow\overline{\Delta}_0\times\delta;\quad \Omega_\Phi\rightarrow\overline{\Omega}_\Phi\times\delta$

$\nu_0\rightarrow\overline{\nu}_0\times\delta;\quad \nu_\Phi\rightarrow\overline{\nu}_\Phi\times\delta;$

$$A(\hat{k},\omega|T,\delta)\sim A\left(\hat{k},\,\omega\frac{\delta_0}{\delta}\middle|\,T\frac{\delta_0}{\delta},\delta_0\right)$$

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Calculation in brief: liquid state
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$$\boxed{\mathcal{G}\,(a,b) = \mathbf{g}(a,\bar{\mathbf{b}}) \cdot \mu(\bar{\mathbf{b}}, b),}$$

The caparison function appears here.
Motivation is to get rid of a crucial
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Next we use the chain rule for functional derivatives

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Turning off sources, $\gamma(i) \to n/2$ (n= density)

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Using chain rule for functional derivatives get exact equation

$$\boxed{[\mathbf{g}_0^{-1}(i,\mathbf{j}) - \mu\delta_{i\mathbf{j}} - t_{i\mathbf{j}} - \Phi(i,\mathbf{j})].\mathbf{g}(\mathbf{j},\mathbf{k}).\mu(\mathbf{k},\mathbf{f}) = \delta(\mathbf{i},\mathbf{f})(\mathbf{1} - \gamma(\mathbf{i})) + \mathbf{\Psi}(\mathbf{i},\mathbf{f})}$$

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Exact so far.
It is a formal solution and how do we make sense of it?
Can we devise an approximate solution, valid in some limit?

- Devise a small parameter λ between 0,1 related to particle density and also to double occupancy.

- At $\lambda=0$, get the Fermi gas, and at $\lambda=1$ get the full tJ model.

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Theory of λ Fermions
Lot of promise- but in infancy.
Hence will not purse in these lectures

Introducing λ expansion

Symbolic notation makes things simpler

Y represents the hopping matrix element broken into a static and dynamic parts.

$$Y \to (-t + \frac{J}{2}) + Y_1 \quad \left\{ \begin{aligned} X &= [-t + \frac{1}{2}J]\ D \\ Y_1 &= -[-t + \frac{1}{2}J]\ \gamma \\ \hat{G}_0^{-1}(\boldsymbol{\mu}) &\equiv (\boldsymbol{\mu} - \partial_\tau - \mathcal{V})\mathbb{1} - [-t + \frac{1}{2}J] \end{aligned} \right.$$

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Parameter λ introduced here

Set λ=1 at the end.
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It plays the role of double occupancy- see this explicitly in atomic limit.

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$$\boxed{G = (\hat{G}_0^{-1} - UG - U\frac{\delta}{\delta v})^{-1}\ .\ \mathbf{1}}$$

Inspiration comes from the symbolic EOM for Hubbard model (Canonical theory. Notice how the Hubbard U enters this eqn.

Start from exact EOM

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EOM continues to bifurcate exactly defining the auxiliary FL etc at a given λ. At λ=0 Fermi gas, while at λ=1 the exact tJ eqns.

$$(\hat{G}_0^{-1} - \lambda\ Y_1 - \lambda\ \Phi).\ \mathbf{g} = \mathbf{1}$$ *Auxiliary Fermi liquid*

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Hence low order theory in λ is expected to be a VERY GOOD start. (since unlike U, the range of λ is [0,1].)

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$$t_{ij} \to t_{ij} - u_t\ \delta_{ij},\ \ J_{ij} \to J_{ij} + u_J\ \delta_{ij},$$

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- *Shift theorem-(I):* A shift of either t or J can be absorbed into suitable parameters, leaving the physics unchanged.
- *Shift theorem-(II):* The two shifts of t and J cancel each other when $u_J = -4 \times u_t$.

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H_{eff} &= -\sum_{ij} t_{ij} f^{\dagger}_{i\sigma} f_{j\sigma} + \sum_{i} (\frac{1}{4} J_0 - \mu) f^{\dagger}_{i\sigma} f_{i\sigma} + V_{eff}, \\
V_{eff} &=_{\lambda} \frac{1}{4} \sum_{ij} t_{ij}(\sigma_1\sigma_2) \ \left[\left(f^{\dagger}_{i\sigma_1} f^{\dagger}_{i\bar{\sigma}_1} + f^{\dagger}_{j\sigma_1} f^{\dagger}_{j\bar{\sigma}_1} \right) f_{i\bar{\sigma}_2} f_{j\sigma_2} + (h.c.) \right] - \frac{1}{4} \sum_{ij} J_{ij}(\sigma_1\sigma_2) \ f^{\dagger}_{i\sigma_1} f^{\dagger}_{j\bar{\sigma}_1} f_{j\bar{\sigma}_2} f_{i\sigma_2} \\
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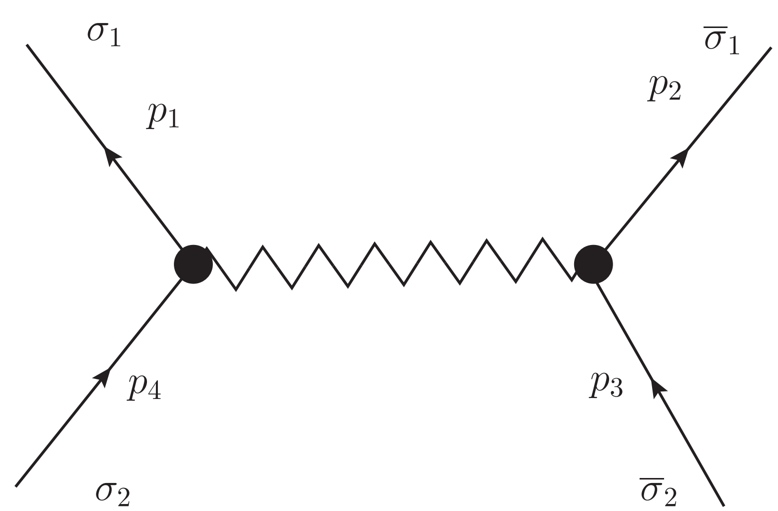

$$W_{eff} = -\delta_{p_1+p_2.p_3+p_4} \ \ \{\Sigma_j \, \varepsilon_j + J_{p_2-p_3} - u_0 \ \}$$

End Lectures 1&2

SUMMARY OF THE $O(\lambda^2)$ THEORY

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End Lectures 1&2

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- Leads to insight about Fermi liquid behaviour of the two self energies ~ g g g. This is as in 2nd order perturbation of Fermi liquids.

End Lectures 1&2