Center for
Electronic Correlations and Magnetism
University of Augsburg

From Gutzwiller Wave Functions to Dynamical Mean-Field Theory

Dieter Vollhardt

Autumn School on Correlated Electrons
DMFT at 25: Infinite Dimensions
Forschungszentrum Jülich, September 15, 2014

Supported by DFG FOR 1346

Outline:

- Electronic correlations
- Approximation schemes: Mean-field theories, variational wave functions
- Gutzwiller wave functions, Gutzwiller approximation
- Derivations of the Gutzwiller approximation
- From one to infinite dimensions
- Simplification of many-body perturbation theory in $d = \infty$
- Dynamical mean-field theory (DMFT)
- Applications: LDA+DMFT for correlated electron materials

Correlations in fermionic matter

< 1950s - Mott insulators/metal-insulator transitions
- Ferromagnetism in 3*d* transition metals

Hubbard model (1963)

1950s Liquid Helium-3

1960s Kondo effect (1964)

1970s Heavy fermion systems

1980s - Fractional quantum Hall effect
- High-T_c superconductivity

1990s Colossal magnetoresistance

2000s Cold fermionic atoms in optical lattices

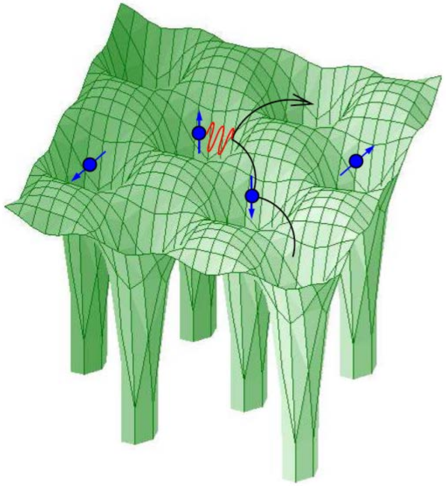
etc.

material

modeling

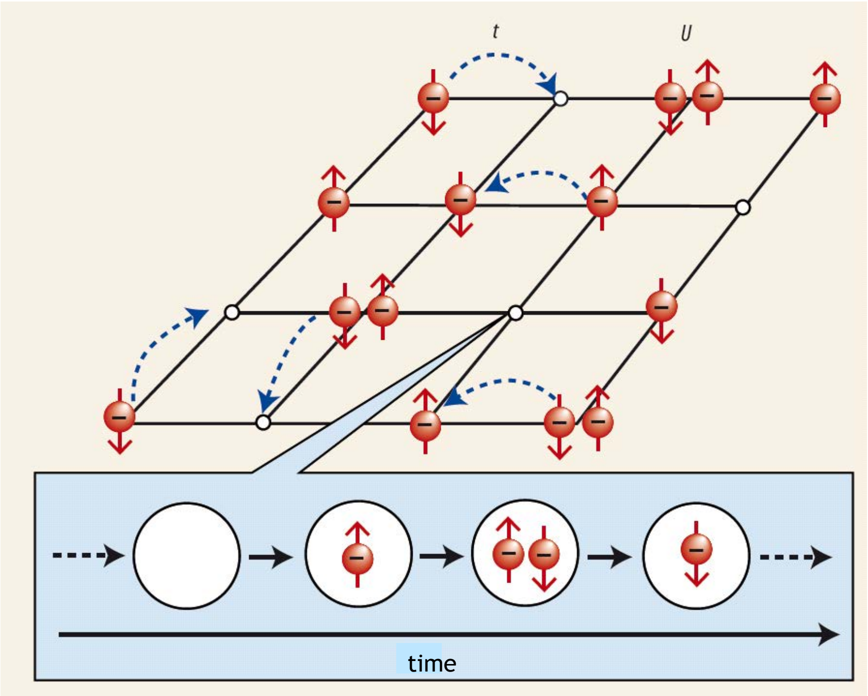
$\Rightarrow$

realistic model



$\Rightarrow$ maximal simplification ?

Hubbard model



Gutzwiller, 1963
Hubbard, 1963
Kanamori, 1963

$$\hat{H} = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} \hat{c}^\dagger_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow}$$

$$\boxed{\langle \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow} \rangle \neq \langle \hat{n}_{\mathbf{i}\uparrow} \rangle \langle \hat{n}_{\mathbf{i}\downarrow} \rangle}$$

Dimension of Hilbert space $\sim O(4^L)$
L: # lattice sites

Static (Hartree-Fock-type) mean-field theories generally insufficient

Computational time for N_2 molecule:
ca. 1 year with 50.000 compute nodes

Purely numerical approaches (d=2,3):
hopeless!

Best-known approaches:
- Mean-field theories
- Variational wave functions

Mean-field theory (MFT)

1) Construction by decoupling/factorization

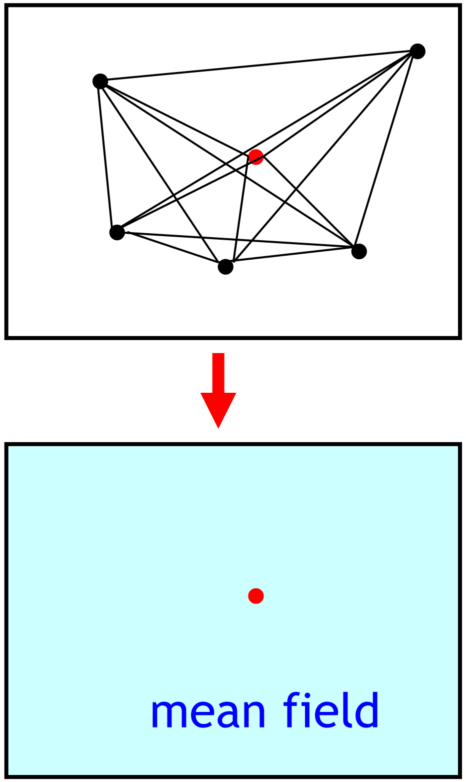
$$\langle AB \rangle \to \langle A \rangle \langle B \rangle$$

e.g., spins:

$$\langle S_i S_j \rangle \to \langle S_i \rangle \langle S_j \rangle$$

→ Weiss molecular field theory (1907)

Prototypical "single site" MFT



Mean-field theory (MFT)

2) Construction by continuum/infinity limit

$$\left.\begin{array}{l}\text{Spin } S \\ \text{Degeneracy } N \\ \text{Dimension } d \text{ /coordination number } Z\end{array}\right\} \rightarrow \infty$$

→ Weiss MFT for spin models

Variational Wave Functions

Applications, e.g.:
- Quantum liquids ^{3}He, ^{4}He
- Nuclear physics
- Correlated electrons
- Heavy fermions
- FQHE
- High-T_c superconductivity

$$\boxed{|\Psi_{\rm var}\rangle = \hat{C}|\Psi_0\rangle}$$

$|\Psi_0\rangle$ One-particle wave function

$\hat{C}(\lambda_1, \ldots, \lambda_n)$ Correlation operator reduces energetically unfavorable configurations in $|\Psi_0\rangle$

λ_i Variational parameters

$$\langle \hat{\mathcal{O}} \rangle_{\rm var} = \frac{\langle \Psi_{\rm var} | \hat{\mathcal{O}} | \Psi_{\rm var} \rangle}{\langle \Psi_{\rm var} | \Psi_{\rm var} \rangle}$$

Expectation value of some operator

$$E_{\rm var} = \langle \hat{H} \rangle_{\rm var} \geq E_{exact}$$

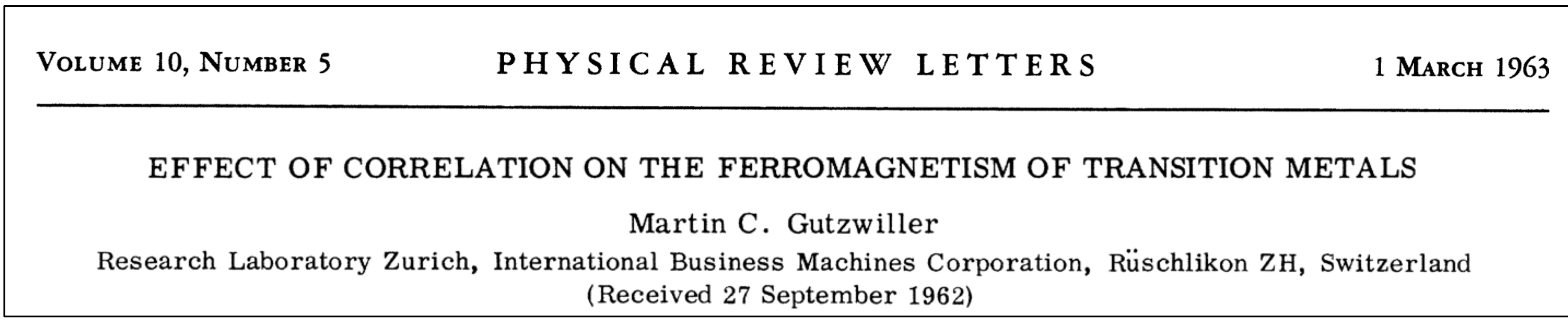
Energy expectation value

$$\left.\frac{\partial E_{\rm var}}{\partial \lambda_i}\right|_{\lambda_i^*} = 0 \Rightarrow \lambda_i^*$$

Minimization determines variational parameters

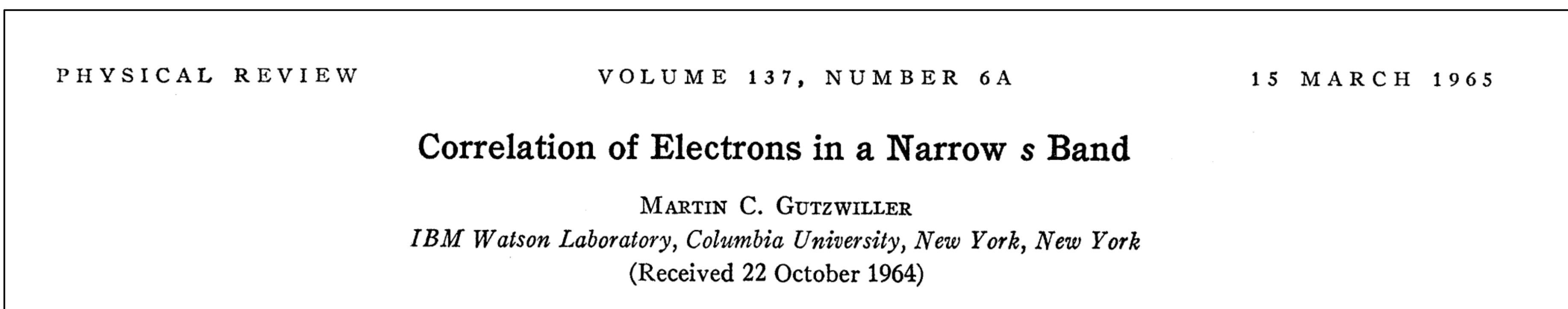
Martin Gutzwiller
(1925-2014)

Gutzwiller Wave Functions


VOLUME 10, NUMBER 5 PHYSICAL REVIEW LETTERS 1 MARCH 1963

EFFECT OF CORRELATION ON THE FERROMAGNETISM OF TRANSITION METALS

Martin C. Gutzwiller
Research Laboratory Zurich, International Business Machines Corporation, Rüschlikon ZH, Switzerland
(Received 27 September 1962)


PHYSICAL REVIEW VOLUME 137, NUMBER 6A 15 MARCH 1965

Correlation of Electrons in a Narrow *s* Band

MARTIN C. GUTZWILLER
IBM Watson Laboratory, Columbia University, New York, New York
(Received 22 October 1964)

Gutzwiller wave functions

$$\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{int}}$$

$$= \sum_{i,j,\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \underbrace{\sum_i \underbrace{\hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}_{\hat{D}_i}}_{\hat{D}}$$

$\hat{D}_i$ Op. of local double occupation

$\hat{D}$ Op. of total double occupation

Gutzwiller variational wave functions

$$\boxed{|\psi_G\rangle = \underbrace{e^{-\lambda \hat{H}_{\text{int}}}}_{\hat{C}} |\Psi_0\rangle}$$

Gutzwiller (1963)

One-particle (product) wave function

Gutzwiller wave function

$$\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{int}}$$

$$= \sum_{i,j,\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \underbrace{\sum_i \underbrace{\hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}_{\hat{D}_i}}_{\hat{D}}$$

$\hat{D}_i$ Op. of local double occupation

$\hat{D}$ Op. of total double occupation

Gutzwiller variational wave functions

$$\boxed{|\psi_G\rangle = \underbrace{e^{-\lambda \hat{H}_{\text{int}}}}_{\hat{C}} |FG\rangle}$$

Gutzwiller (1963)

Fermi gas

$$e^{-\lambda \hat{H}_{\text{int}}} = e^{-\lambda U \hat{D}} \overset{\boxed{e^{-\lambda U} \equiv g}}{=} g^{\hat{D}}, \quad 0 \le g \le 1$$

$$\boxed{\begin{array}{l} g = 1 \Leftrightarrow U = 0 \\ g = 0 \Leftrightarrow U = \infty \end{array}}$$

$$\boxed{\begin{aligned} |\Psi_G\rangle &= g^{\hat{D}} |\text{FG}\rangle \\ &= \prod_i [1 - (1-g)\hat{D}_i] |\text{FG}\rangle \end{aligned}}$$

Global reduction of configurations with too many doubly occupied sites

$$g^{\hat{D}} \Big|_{g=0} = \prod_i [1 - \hat{D}_i] \equiv \hat{P}_G$$

"Gutzwiller projection"

Gutzwiller wave function

$$|\Psi_G\rangle \quad = \quad g^{\hat{D}}|\mathrm{FG}\rangle$$ with $$|\mathrm{FG}\rangle = \sum_D \sum_{\{i_D\}} A_{i_D} |\Psi_{i_D}\rangle$$

$|\Psi_{i_D}\rangle$ Electronic configuration with D doubly occupied sites

$\{i_D\}$ Set of all different electron configurations with given D

$$\Rightarrow \quad \boxed{\langle\Psi_G|\Psi_G\rangle = \sum_D g^{2D} \sum_{\{i_D\}} |A_{i_D}|^2}$$

Probability of the electron configuration i_D

How to calculate?

Gutzwiller Approximation

Approximates quantum mechanical expectation values
by counting classical spin configurations

Gutzwiller approximation

$$|\Psi_G\rangle = g^{\hat{D}}|\mathrm{FG}\rangle$$ with $$|\mathrm{FG}\rangle = \sum_D \sum_{\{i_D\}} A_{i_D}|\Psi_{i_D}\rangle$$

$$\langle\Psi_G|\Psi_G\rangle = \sum_D g^{2D} \sum_{\{i_D\}} \underbrace{|A_{i_D}|^2}_{?}$$

Simplest approximation: Neglect correlations between electrons:

count classical configurations of ↑,↓ electrons

→ all probabilities $|A_{i_D}|^2$ equal

$$\boxed{|A_{i_D}|^2 = P_\uparrow P_\downarrow = \mathrm{const}}$$

$$P_\sigma = 1/\binom{L}{N_\sigma}$$ Probability for a configuration of electrons with spin σ

$$\Rightarrow \quad \boxed{\langle\Psi_G|\Psi_G\rangle = P_\uparrow P_\downarrow \sum_D g^{2D} N_D}$$

N_D : # electron configurations with given D

Gutzwiller approximation

$$\boxed{\langle\Psi_G|\Psi_G\rangle = P_\uparrow P_\downarrow \sum_D g^{2D} \boxed{N_D}}$$

L: # lattice sites

N_σ: # electrons with spin σ

D: # doubly occupied sites

$L_\sigma = N_\sigma - D$: # singly occupied sites with spin σ

$E = L - N_\uparrow - N_\downarrow + D$: # empty sites

$$\boxed{N_D} = \frac{L!}{L_\uparrow! L_\downarrow! D! E!}$$: # spin configurations with given D

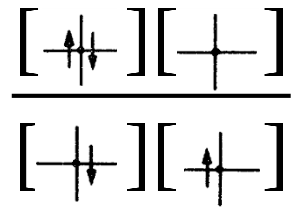
Thermodynamic limit: Sum over D determined by the largest term:

$$\frac{d}{dD}\left(g^{2D} N_D\right)\Big|_{\bar{D}} = 0 \xrightarrow{\bar{D}/L \equiv \bar{d}} g^2 = \frac{\bar{d}(1 - n_\uparrow - n_\downarrow + \bar{d})}{(n_\downarrow - \bar{d})(n_\uparrow - \bar{d})} \quad \Rightarrow \bar{d}(g)$$

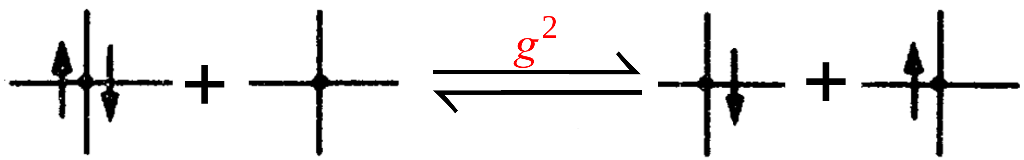
Physical meaning?

Gutzwiller approximation

$$g^2 = \frac{\bar{d}(1 - n_\uparrow - n_\downarrow + \bar{d})}{(n_\downarrow - \bar{d})(n_\uparrow - \bar{d})} =$$



Law of mass action for the “chemical reaction”



Quasi-chemical equilibrium:
Typical mean-field result!

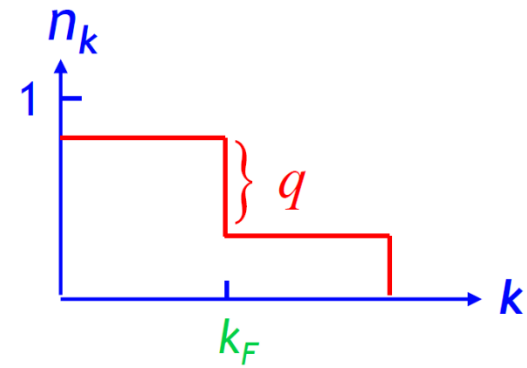
Norm $\boxed{\langle \Psi_G | \Psi_G \rangle = P_\uparrow P_\downarrow \, g^{2\bar{D}} N_{\bar{D}}}$, $\bar{D} = \bar{D}(g)$

Gutzwiller approximation

Similarly:

Kinetic energy

$$\left\langle \hat{H}_{\text{kin}} \right\rangle_G = \frac{\left\langle \psi_G \middle| \hat{H}_{\text{kin}} \middle| \psi_G \right\rangle}{\left\langle \psi_G \middle| \psi_G \right\rangle} \equiv E_{\text{kin}} = q(\bar{d}, n)\underbrace{E^0_{\text{kin}}}_{-L|\varepsilon_0|}$$



$$n_\uparrow = n_\downarrow = \frac{n}{2}$$

$$q = \frac{2(1-\delta-2\bar{d})(\sqrt{\bar{d}+\delta}+\sqrt{\bar{d}})^2}{1-\delta^2}, \quad \delta = 1 - n$$

Interactions→ multiplicative renormalization of kinetic energy

Interaction energy

$$\left\langle \hat{H}_{\text{U}} \right\rangle_G = \frac{\left\langle \psi_G \middle| U\hat{D} \middle| \psi_G \right\rangle}{\left\langle \psi_G \middle| \psi_G \right\rangle} \equiv E_{\text{int}} = U\bar{D}$$

→ Ground state energy

$$\frac{1}{L}\left\langle \hat{H} \right\rangle_G \equiv \frac{E_G(\bar{d}(g), n)}{L} = -q(\bar{d}, n)|\varepsilon_0| + U\bar{d}$$

$$\left.\frac{\partial E_G}{\partial \bar{d}}\right|_{\bar{d}^*} = 0 \Rightarrow g(\bar{d}^*)$$

In the following: $\bar{d}^* \equiv d$

Study origin of band ferromagnetism

Gutzwiller (1965)

Gutzwiller-Brinkman-Rice theory

Brinkman, Rice (1970)

PHYSICAL REVIEW B VOLUME 2, NUMBER 10 15 NOVEMBER 1970

Application of Gutzwiller's Variational Method to the Metal-Insulator Transition

W. F. Brinkman and T. M. Rice
Bell Telephone Laboratories, Murray Hill, New Jersey 07974
(Received 16 April 1970)

$$\boxed{n=1}$$

$$\boxed{d=\frac{1}{4}\left(1-\frac{U}{U_c}\right)}$$

$$\boxed{U_c=8\left|\varepsilon_0\right|}$$

$$\boxed{q=1-\left(\frac{U}{U_c}\right)^2}$$

$$\boxed{\frac{E_G}{L}=-\left|\varepsilon_0\right|\left(1-\frac{U}{U_c}\right)^2}$$

$$U\to U_c:\quad E_{\text{kin}}\to 0 \text{ and } E_{\text{int}}\to 0$$

Electrons localize
→ no charge current

Gutzwiller approximation describes a correlation induced ("Mott") metal-insulator transition as in V_2O_3

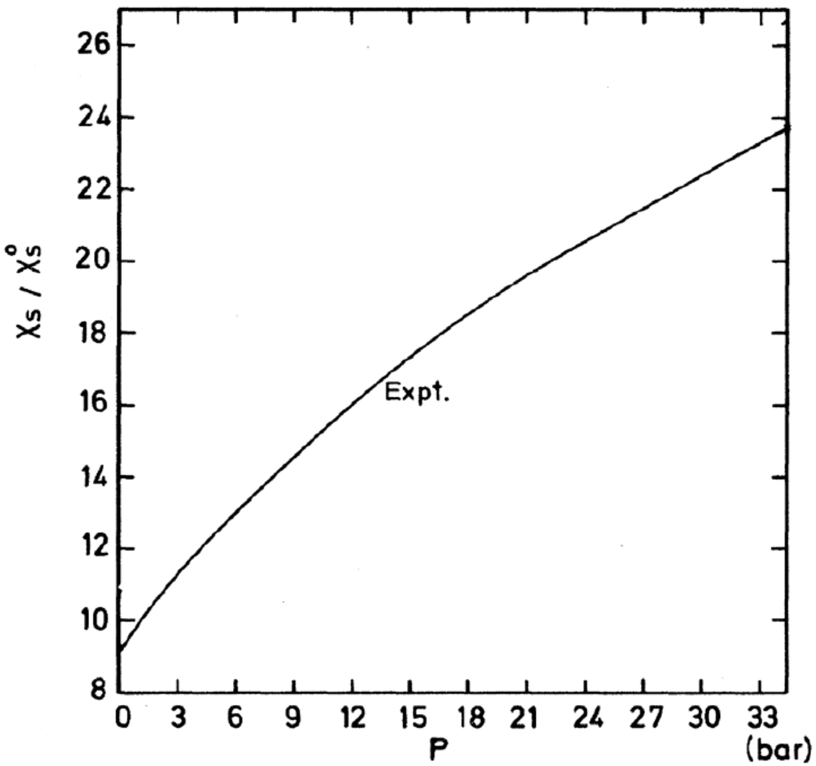
Applicable to normal liquid ^{3}He?

Anderson, Brinkman (1975)

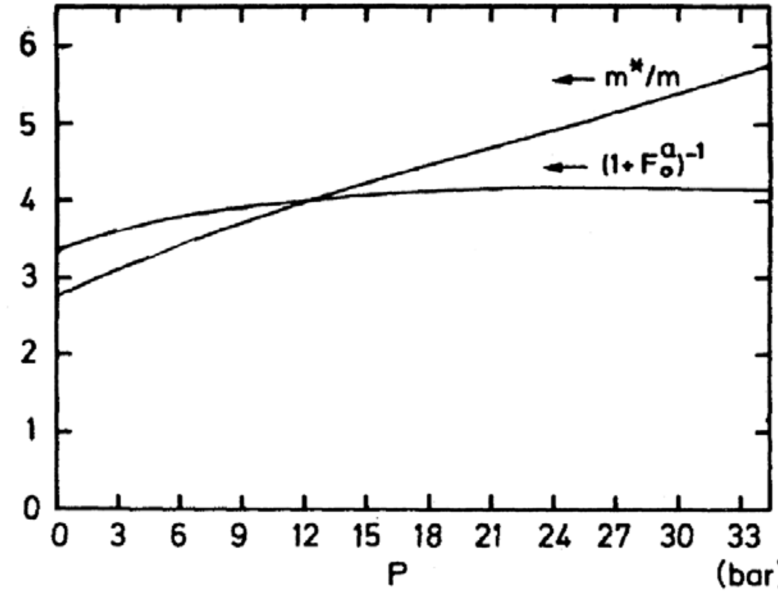
Properties of normal liquid ^{3}He

Greywall (1983)
DV (1984)

Strongly renormalized Fermi gas



Spin susceptibility



Effective mass m^*/m

Wilson ratio $\dfrac{\chi_s/\chi_s^0}{m^*/m} = \dfrac{1}{1+F_0^a}$

Why does χ_s become so large?

Anderson, Brinkman (1975)

Paramagnon theory: $\chi_s = \dfrac{\chi_s^o}{1-UN_F}$, $\quad U \to N_F^{-1}$ → ^{3}He close to ferromagnetic instability

Fermi liquid theory: $\chi_s = \chi_s^0 \dfrac{m^*/m}{1+F_0^a}$ → ^{3}He close to Mott (localization) transition?

Gutzwiller approximation and Fermi liquid theory

Change of the ground state energy

Brinkman, Rice (1970)
DV (1984)

$$\frac{E_G}{L} = q\varepsilon_0 + U\bar{d} \Rightarrow \frac{\delta E_G}{L} = \left(q\ \delta\varepsilon_0 + \delta q\ \varepsilon_0\right)\Big|_{\bar{d}^*}$$

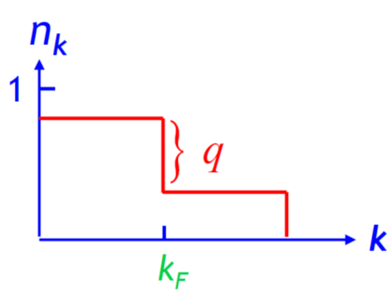
change of: particle energy, distribution of particles

Correspondence with
Landau Fermi liquid theory:

$$\delta E_{FL} = \frac{1}{V}\sum_{\mathbf{p}\sigma} \varepsilon^0_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma} + \underbrace{\frac{1}{2}\frac{1}{V^2}\sum_{\mathbf{p}\sigma}\sum_{\mathbf{p}'\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\delta n_{\mathbf{p}\sigma}\delta n_{\mathbf{p}'\sigma'}}$$

$$\Downarrow \quad l<1$$

$$\frac{1}{2N^*(0)}\left[F_0^s(\delta n_\uparrow + \delta n_\downarrow)^2 + F_0^a(\delta n_\uparrow - \delta n_\downarrow)^2\right]$$



$$N^*(0) = \frac{m^*}{m}N(0), \quad \varepsilon^0_{p\sigma} = \frac{m}{m^*}\varepsilon^0_{p\sigma}\Big|_{\text{bare}} \Rightarrow \boxed{q = \frac{m}{m^*}}$$

Gutzwiller approximation and Fermi liquid theory

Fermi liquid relations

Spin susceptibility $$\chi_s = \chi_s^0 \frac{m^*/m}{1+F_0^a}$$

Compressibility $$\kappa = \kappa^0 \frac{m^*/m}{1+F_0^s}$$

Gutzwiller approximation

$$\bar{U} = \frac{U}{U_c}$$

$$p = 2|\epsilon_0|N(0) \simeq 1$$

$$F_0^a = p[-1 + \frac{1}{(1+\overline{U})^2}]$$

$$F_0^s = p[\frac{1}{(1-\overline{U})^2} - 1],$$

$$F_0^a(U) = F_0^s(-U)$$

DV (1984)

Gutzwiller approximation and Fermi liquid theory

Fermi liquid relations

Spin susceptibility $$\chi_s = \chi_s^0 \frac{m^*/m}{1+F_0^a}$$

Compressibility $$\kappa = \kappa^0 \frac{m^*/m}{1+F_0^s}$$

Gutzwiller approximation $$F_0^a = p[-1 + \frac{1}{(1+\overline{U})^2}]$$

DV (1984)

$$\bar{U} = \frac{U}{U_c}$$

$$p = 2|\epsilon_0|N(0) \simeq 1$$

$$\Rightarrow F_0^a \xrightarrow{U \to U_c} -\frac{3}{4}p \simeq -\frac{3}{4} = \text{const}$$

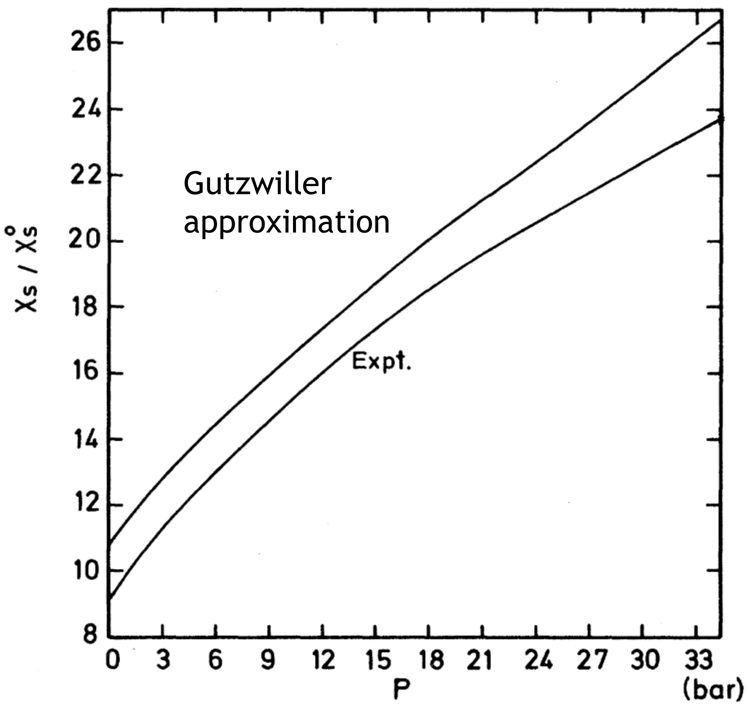
Wilson ratio $$\frac{\chi_s/\chi_s^0}{m^*/m} = \frac{1}{1+F_0^a} \xrightarrow{U \to U_c} \simeq 4 = \text{const}$$

No divergence!

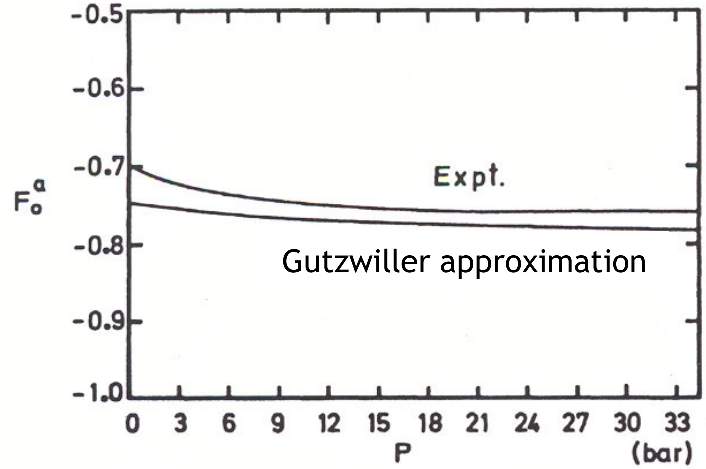
Gutzwiller approximation and Fermi liquid theory

$$\chi_s = \chi_s^0 \, \frac{m^*/m}{1+F_0^a}$$

DV (1984)



Spin susceptibility



$\leftarrow -\frac{3}{4}$

Conclusion:

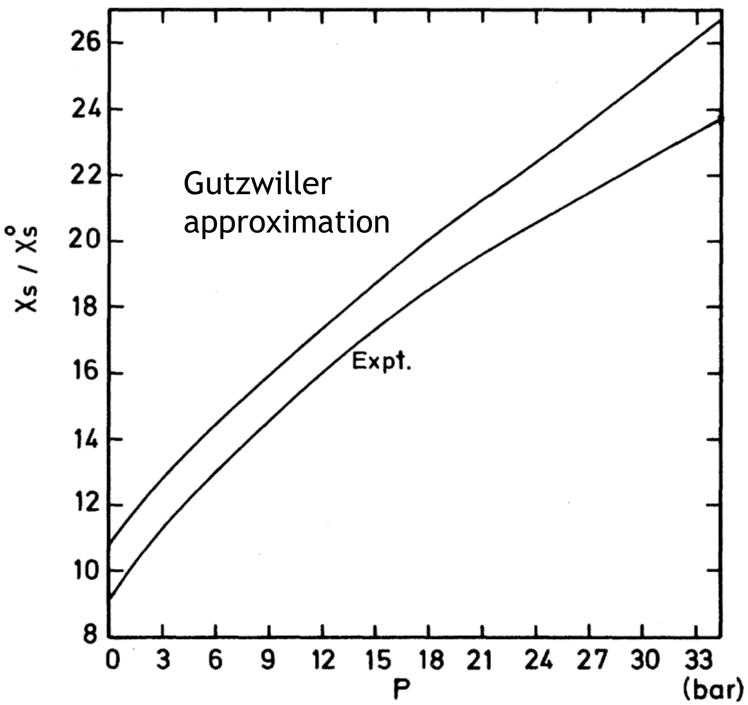
- no magnetic instability
- χ_s becomes large because m^*/m becomes large!

Liquid ^{3}He: "almost localized Fermi liquid" (close to Mott transition at U_c)

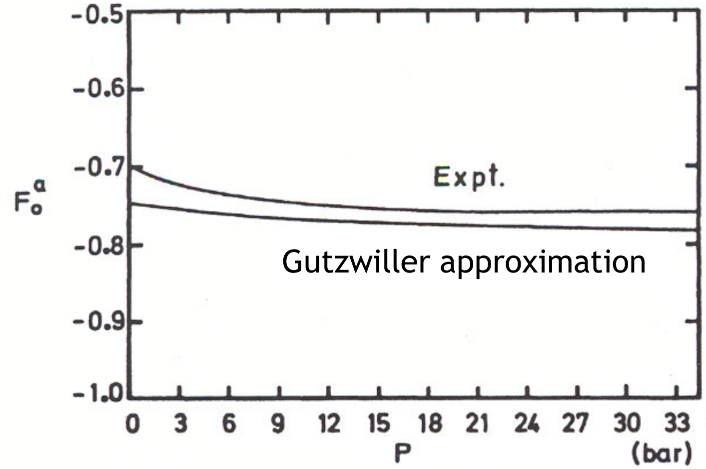
Gutzwiller approximation and Fermi liquid theory

$$\chi_s = \chi_s^0 \frac{m^*/m}{1+F_0^a}$$

DV (1984)



Spin susceptibility



$\leftarrow -\frac{3}{4}$

Conclusion:

- no magnetic instability
- χ_s becomes large because m^*/m becomes large!

Reviews of Modern Physics, Vol. 56, No. 1, January 1984 99

Normal ^{3}He: an almost localized Fermi liquid

Dieter Vollhardt

Max-Planck-Institut für Physik und Astrophysik, Werner Heisenberg-Institut für Physik, D-8000 München 40, Federal Republic of Germany

Gutzwiller approximation:

1) Quasi-classical, non-perturbative approximation scheme for correlated fermions

2) Describes a:
   - correlated Fermi liquid with a
   - Mott metal-insulator transition for n=1 at a critical U_c

3) Shows mean-field behavior

Open question:

Systematic derivation by more conventional methods of quantum many-body theory?

Slave-boson mean-field theory

→ Lecture G. Kotliar

VOLUME 57, NUMBER 11 PHYSICAL REVIEW LETTERS 15 SEPTEMBER 1986

New Functional Integral Approach to Strongly Correlated Fermi Systems: The Gutzwiller Approximation as a Saddle Point

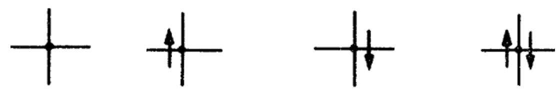
Gabriel Kotliar[(1)] and Andrei E. Ruckenstein[(2)]

[(1)] *Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
[(2)] *Department of Physics, University of California at San Diego, La Jolla, California 92093*

(Received 21 April 1986)

Hubbard model $$H=\sum_{ij,\sigma} t_{ij} f_{i\sigma}^{\dagger} f_{j\sigma} + U\sum_{i} f_{i\sigma}^{\dagger} f_{i\sigma} f_{i-\sigma}^{\dagger} f_{i-\sigma}$$

Introduce local Bose fields



e_i $p_{i\uparrow}$ $p_{i\downarrow}$ d_i

Local constraints
$$\sum_{\sigma} p_{i\sigma}^{\dagger} p_{i\sigma} + e_i^{\dagger} e_i + d_i^{\dagger} d_i = 1,$$
$$f_{i\sigma}^{\dagger} f_{i\sigma} = p_{i\sigma}^{\dagger} p_{i\sigma} + d_i^{\dagger} d_i, \quad \sigma \pm 1$$

→ $$\boxed{\tilde{H}=\sum_{ij,\sigma} t_{ij} f_{i\sigma}^{\dagger} f_{j\sigma} \tilde{z}_{i\sigma}^{\dagger} \tilde{z}_{j\sigma} + U\sum_{i} d_i^{\dagger} d_i}$$

$\tilde{z}_{i\sigma}$: renormalization factors (operators)

Saddle point approximation → results of Gutzwiller approximation

Gutzwiller wave function

Diagrammatic evaluation of $E_G = \dfrac{\langle \psi_G | \hat{H} | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$

Metzner, DV (1987, 1988)

$$|\Psi_G\rangle = g^{\hat{D}}|\mathrm{FG}\rangle \;,\; 0 \le g \le 1$$

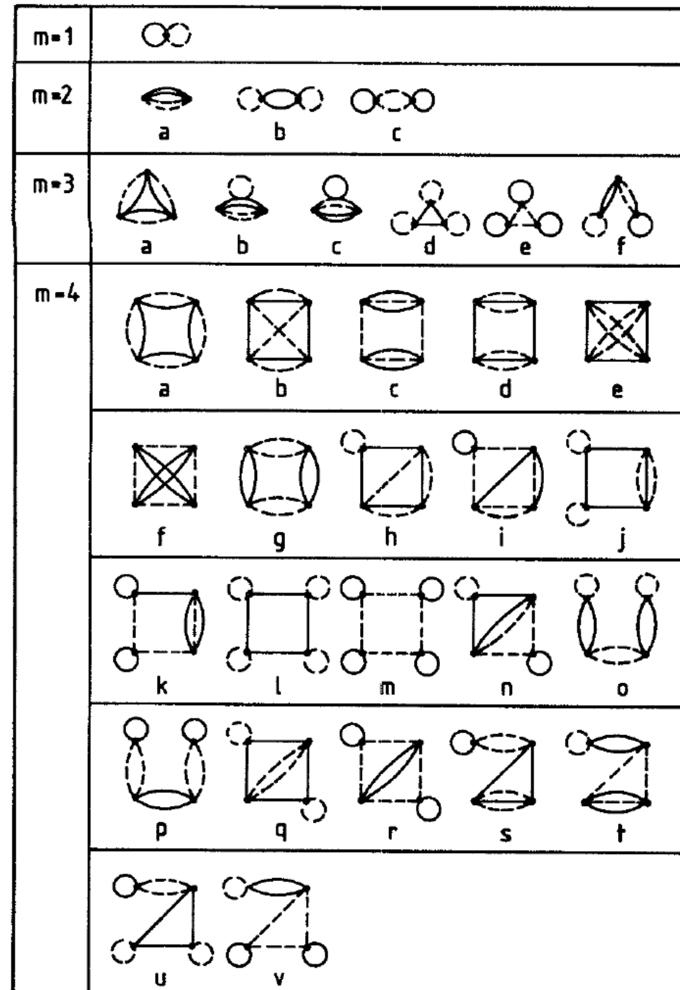
$$= \prod_i \; [1-(1-g)\hat{D}_i]|\mathrm{FG}\rangle$$

1) $\left\langle \hat{H}_{\mathrm{int}} \right\rangle_G = U \left\langle \hat{D} \right\rangle_G = LU d(g,n)$

$$= LUg^2 \sum_{m=1}^{\infty} (g^2-1)^{m-1} c_m(n)$$

Diagrammatic representation of $c_m(n)$

$c_m(n)$



Diagrams for the Hubbard interaction (φ^4 theory)

Lines correspond to $g^0_{ij,\sigma} = \left\langle c^\dagger_{i\sigma} c_{j\sigma} \right\rangle_0 \overset{FT}{\longleftrightarrow} n^0_{\mathbf{k}\sigma}$

(probability amplitude/ momentum distribution)

$$\boxed{g^0_{ij,\sigma} = \lim_{t\to 0^-} G^0_{ij,\sigma}(t)}$$

Gutzwiller wave function

Diagrammatic evaluation of $E_G = \dfrac{\langle \psi_G | \hat{H} | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$

Metzner, DV (1987, 1988)

$$|\Psi_G\rangle = g^{\hat{D}}|\mathrm{FG}\rangle \ , \ 0 \le g \le 1$$

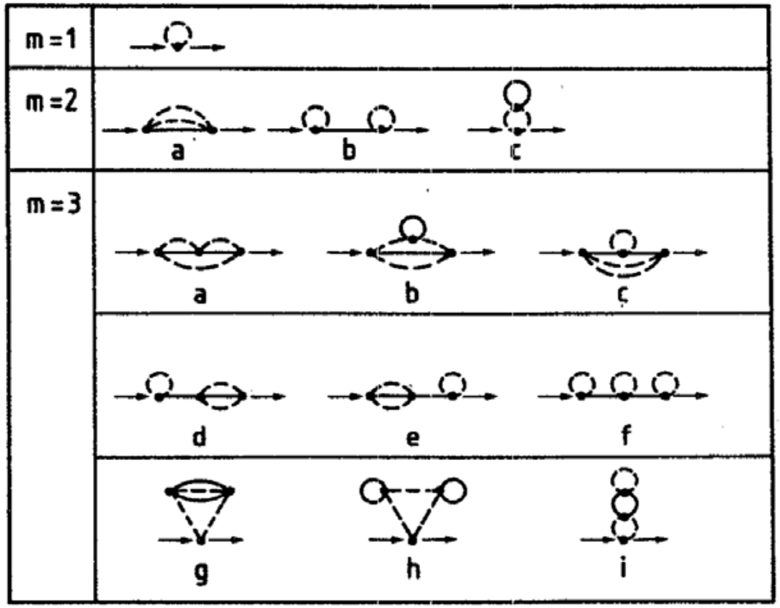
$$= \prod_i [1-(1-g)\hat{D}_i]|\mathrm{FG}\rangle$$

2) $$\left\langle \hat{H}_{\mathrm{kin}} \right\rangle_G = \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k}) \underbrace{\left\langle \hat{n}_{\mathbf{k}\sigma} \right\rangle_G}_{n_{\mathbf{k}\sigma}}$$

$$n_{\mathbf{k}\sigma}(g,n) = \ \dots \ + \ \dots \sum_{m=2}^{\infty} (g^2-1)^m f_{m\sigma}(\mathbf{k})$$

Diagrammatic representation of $f_{m\sigma}(\mathbf{k})$

$f_{m\sigma}(\mathbf{k})$



Diagrams for the kinetic energy

Lines correspond to $g^0_{ij,\sigma} = \left\langle c^\dagger_{i\sigma} c_{j\sigma} \right\rangle_0 \overset{FT}{\longleftrightarrow} n^0_{\mathbf{k}\sigma}$

(probability amplitude/
momentum distribution)

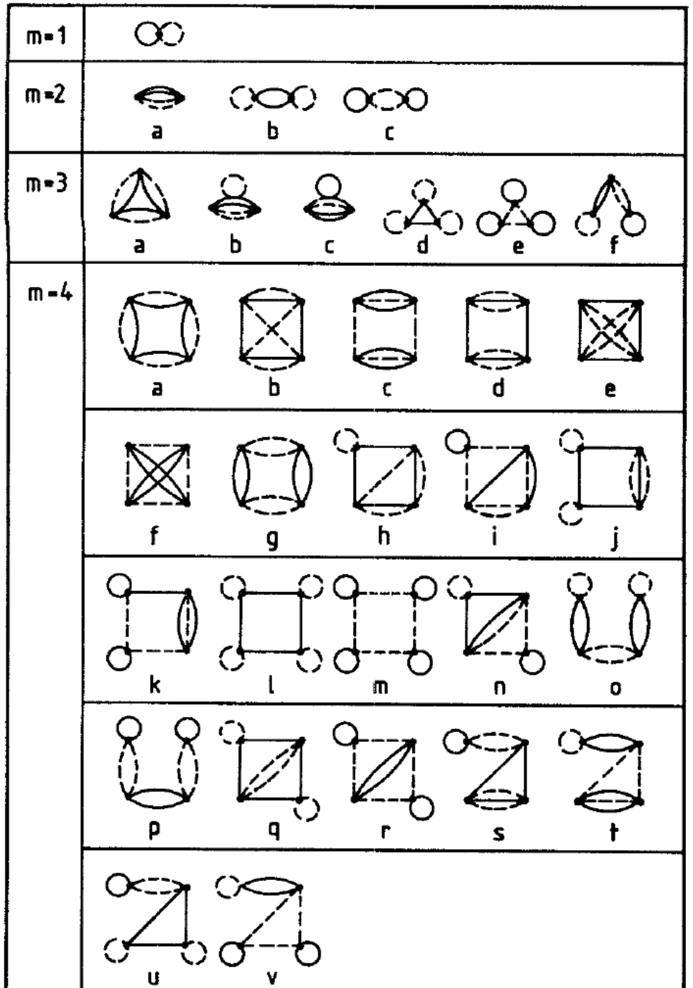
$$\boxed{g^0_{ij,\sigma} = \lim_{t\to 0^-} G^0_{ij,\sigma}(t)}$$

Gutzwiller wave function

Diagrammatic evaluation of $E_G = \frac{\langle \psi_G | \hat{H} | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$

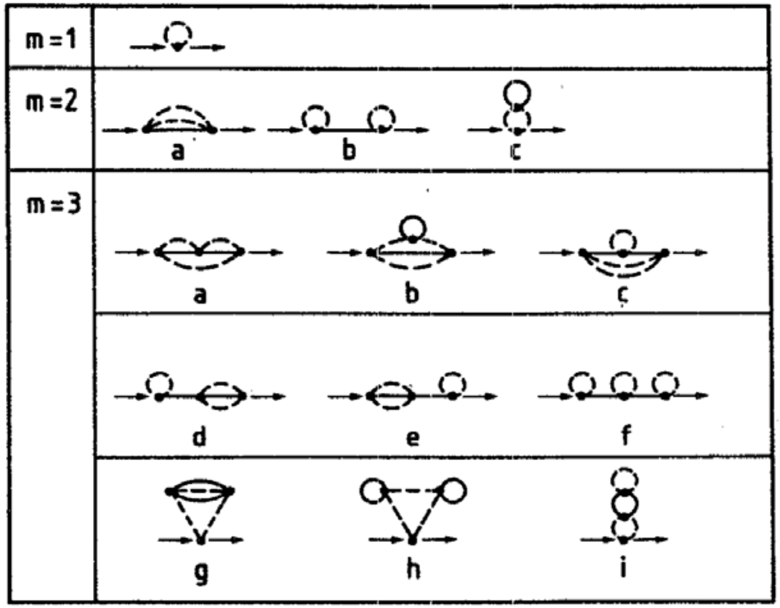
Metzner, DV (1987, 1988)

$c_m(n)$



Diagrams for the Hubbard interaction

$f_{m\sigma}(\mathbf{k})$



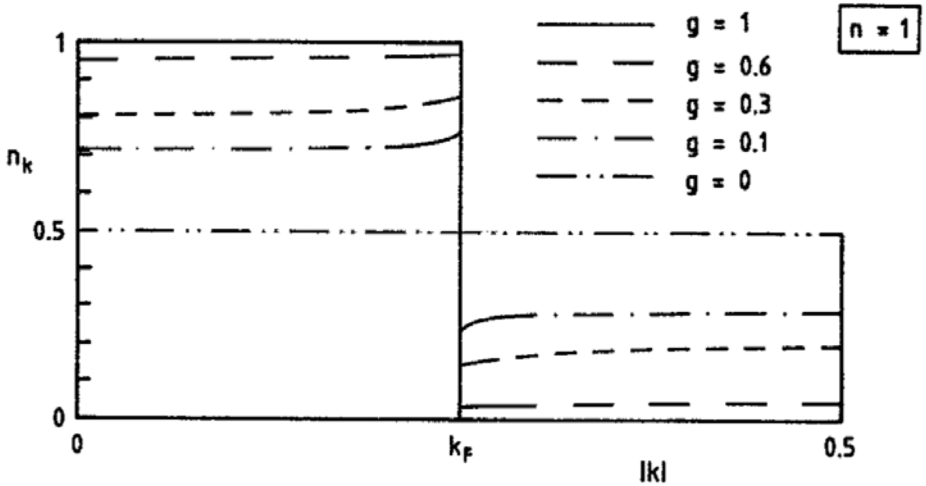
Diagrams for the kinetic energy

d=1: analytic calculation of all diagrams possible

1) $\left\langle \hat{H}_{\text{int}} \right\rangle_G = U \left\langle \hat{D} \right\rangle_G = LU d(g,n)$ density of doubly occupied sites

$$d(g,n) = \frac{g^2}{2(1-g^2)^2}\{-\ln[1-(1-g^2)n]-(1-g^2)n\}$$

2) $\left\langle \hat{H}_{\text{kin}} \right\rangle_G = \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k}) \underbrace{\left\langle \hat{n}_{\mathbf{k}\sigma} \right\rangle_G}_{n_{\mathbf{k}\sigma}}$ momentum distribution



$$\boxed{\Rightarrow \left\langle \hat{H}_{\text{kin}} \right\rangle_G + \left\langle \hat{H}_{\text{int}} \right\rangle_G \equiv E_G}$$

Minimization of $E_G(g,d(g),n,U)$:

$$\boxed{U \gg |\varepsilon_0|: \quad E_G = -\left(\frac{4}{\pi}\right)^2 \frac{t^2}{U} \frac{1}{\ln(U/|\varepsilon_0|)}}$$

Correlation functions

Gebhard, DV (1987, 1988)

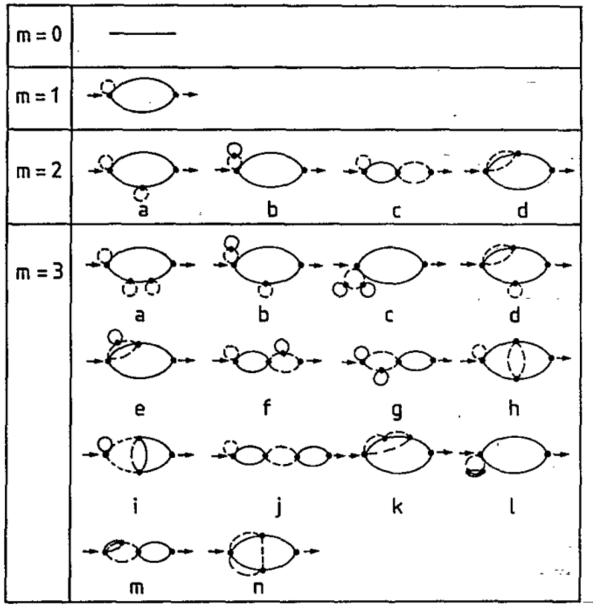
Spin, density, empty sites, doubly occupied sites, local Cooper pairs

d=1: analytic calculation of all diagrams possible

E. g., spin-spin correlations:

$$C^{SS}_{j>0} \overset{U=\infty}{\underset{n=1}{=}} (-1)^j \frac{Si(\pi j)}{\pi j} \overset{j\to\infty}{\sim} \frac{(-1)^j}{2j}$$

Excellent agreement with exact result
for antiferromagnetic Heisenberg chain ($j=1,2$)



One of 4 sets of diagrams

Exact result for S=1/2 antiferromagnetic Heisenberg chain
with exchange coupling $J_{ij} \sim 1/(|i-j|)^2$ Haldane(1988), Shastry (1988)

→ Gutzwiller wave function = Anderson's RVB state in 1D

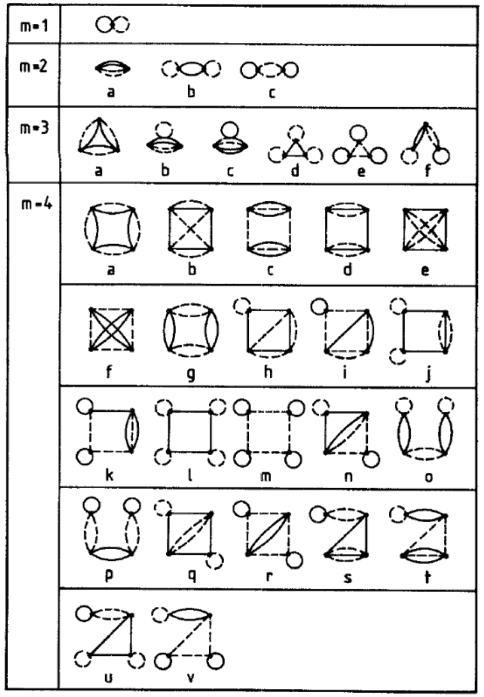
Very interesting wave function! d=2,3?

Gutzwiller wave function

Diagrammatic evaluation of $E_G = \frac{\langle \psi_G | \hat{H} | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$

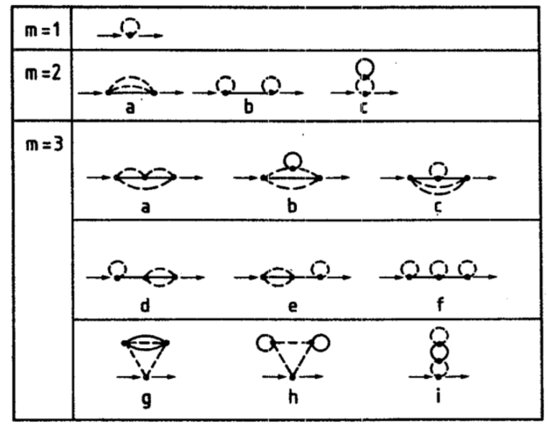
Metzner, DV (1988)

$c_m(n)$



Diagrams for the
Hubbard interaction

$f_{m\sigma}(\mathbf{k})$



Diagrams for the
kinetic energy

Analytic evaluation of all diagrams not possible in d=2,3

Gutzwiller wave function

Diagrammatic evaluation of $E_G = \dfrac{\langle \psi_G | \hat{H} | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$

Metzner, DV (1988)

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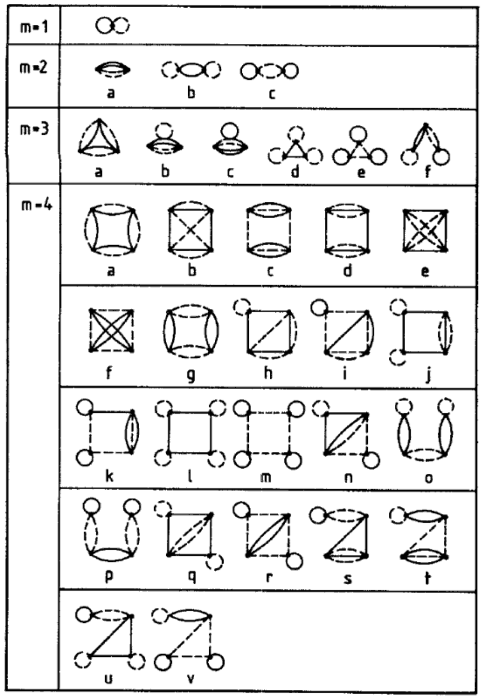
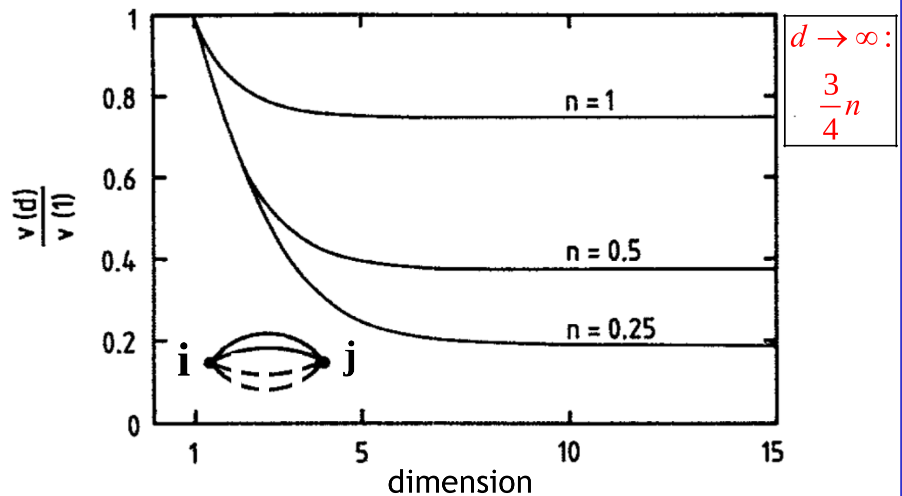


Diagrams for the Hubbard interaction

Calculation of individual diagrams:

Numerical check by Monte-Carlo integration



Each diagram takes simple value $\overset{n_\uparrow = n_\downarrow}{=} \left(\dfrac{n}{2}\right)^{\#\text{ lines}}$

Example:

$$= \begin{cases} \dfrac{2}{3}\left(\dfrac{n}{2}\right)^3, & d = 1 \\ \left(\dfrac{n}{2}\right)^4, & d = \infty \end{cases}$$

Great simplifications for $d \to \infty$:
internal momenta become independent

Gutzwiller wave function

Diagrammatic evaluation of $E_G = \dfrac{\langle \psi_G | \hat{H} | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}$

Metzner, DV (1988)

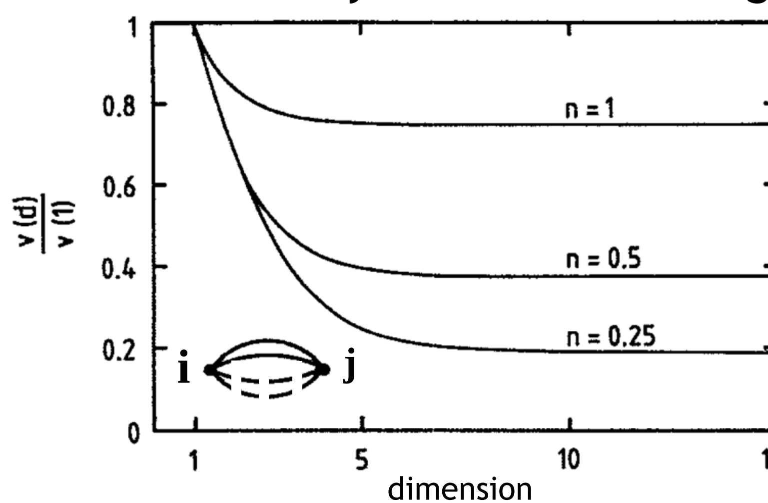
Calculation of individual diagrams:

$d \to \infty$:

$$\frac{\langle \hat{D} \rangle}{L} = \frac{1+n(g^2-1)-[1+(2n-n^2)(g^2-1)]^{1/2}}{2(g^2-1)}$$

Conclusion:
Gutzwiller approximation gives the exact result for expectation values calculated with the Gutzwiller wave function in $d \to \infty$

Numerical check by Monte-Carlo integration



$d \to \infty$: $\frac{3}{4}n$

→ Diagrammatic derivation of Gutzwiller approximation

Optimal form of Gutzwiller wave functions in $d=\infty$

$$|\Psi_G\rangle = g^{\hat{D}} \underbrace{|\Psi_0\rangle}_{\substack{\text{arbitrary}\\ \text{one-particle}\\ \text{wave function}}}$$

In spite of diagrammatic collapse:
Remaining diagrams have to be calculated with $|\Psi_0\rangle$ → difficult

Re-write by gauge transformation

Gebhard (1990)

$$|\Psi_0\rangle = \underbrace{g^{-\sum_{i\sigma}\mu_{i\sigma}\hat{n}_{i\sigma}}}_{\substack{\text{chose local chemical potentials}\\ \text{such that all Hartree bubbles}\\ \text{disappear in } d=\infty}} |\tilde{\Psi}_0\rangle$$

For arbitrary $|\tilde{\Psi}_0\rangle$:

$$\boxed{\langle \hat{H}\rangle_G \overset{d=\infty}{=} -t\sum_{ij,\sigma}\sqrt{q_{i\sigma}}\sqrt{q_{j\sigma}}\,g^0_{ij,\sigma} + U\sum_i \bar{d}_i}$$

renormalization factors $q(\bar{d}_i, n_\sigma \to \tilde{n}_\sigma)$, $\tilde{n}_\sigma = \langle\tilde{\Psi}_0|\hat{n}_\sigma|\tilde{\Psi}_0\rangle$

→ Diagrammatic derivation in $d=\infty$ of the Kotliar-Ruckenstein slave boson saddle point solution

$d \to \infty$ limit for lattice fermions

VOLUME 62, NUMBER 3 PHYSICAL REVIEW LETTERS 16 JANUARY 1989

Correlated Lattice Fermions in $d = \infty$ Dimensions

Walter Metzner and Dieter Vollhardt
Institut für Theoretische Physik C, Technische Hochschule Aachen, Sommerfeldstrasse 26/28, D-5100 Aachen, Federal Republic of Germany
(Received 28 September 1988)

$$\left\langle \hat{H}_{\text{kin}} \right\rangle_0 = -t \sum_{\mathbf{i},\sigma} \underbrace{\sum_{\mathbf{j}(NN\ \mathbf{i})}}_{Z} \underbrace{\left\langle \hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} \right\rangle_0}_{g^0_{ij,\sigma}}$$

Probability amplitude for hopping $\mathbf{j}$ → NN $\mathbf{i}$

$\left|\text{Amplitude for hopping } \mathbf{j} \rightarrow \text{NN } \mathbf{i}\right|^2$ = ***Probability*** for hopping $\mathbf{j}$ → NN $\mathbf{i} \propto \dfrac{1}{Z}$

$$\boxed{\Rightarrow \left|\text{Amplitude for hopping } \mathbf{j} \rightarrow \text{NN } \mathbf{i}\right| = g^0_{ij,\sigma} \propto \frac{1}{\sqrt{Z}} \text{ or } \frac{1}{\sqrt{d}}}$$

In general: $\boxed{g^0_{ij,\sigma} \sim \mathcal{O}\left(1/d^{\|\boldsymbol{R}_i - \boldsymbol{R}_j\|/2}\right)}$ $\quad \| \boldsymbol{R} \| = \sum_{n=1}^{d} |R_n|$

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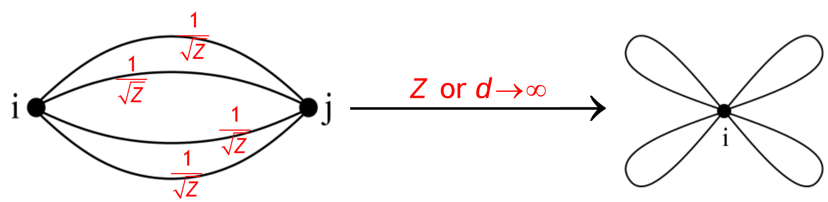
$\xrightarrow{Z \text{ or } d \to \infty}$ Collapse of all connected, irreducible diagrams in position space

Example:



δ_{ij}

Metzner (1989)

→ Great simplification of many-body perturbation theory, e.g., self-energy diagram purely local

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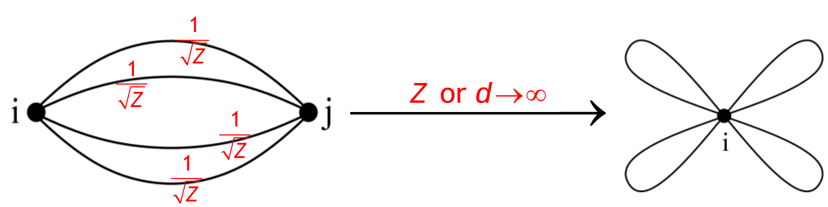

δ_{ij}

Valid for probability amplitude/momentum distribution and the full, time-dependent propagator, since

$$g^0_{ij,\sigma} = \left\langle c^{\dagger}_{i\sigma} c_{j\sigma} \right\rangle_0 \overset{FT}{\leftrightarrow} n^0_{\mathbf{k}\sigma}$$

$$\boxed{g^0_{ij,\sigma} = \lim_{t \to 0^-} G^0_{ij,\sigma}(t)}$$

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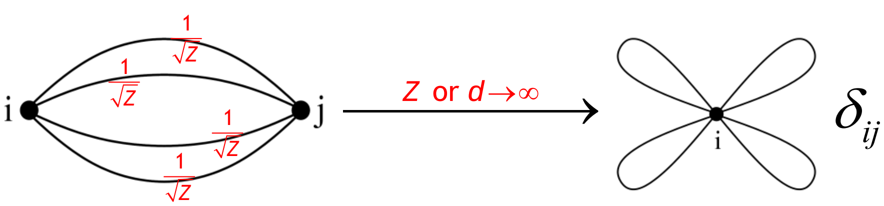
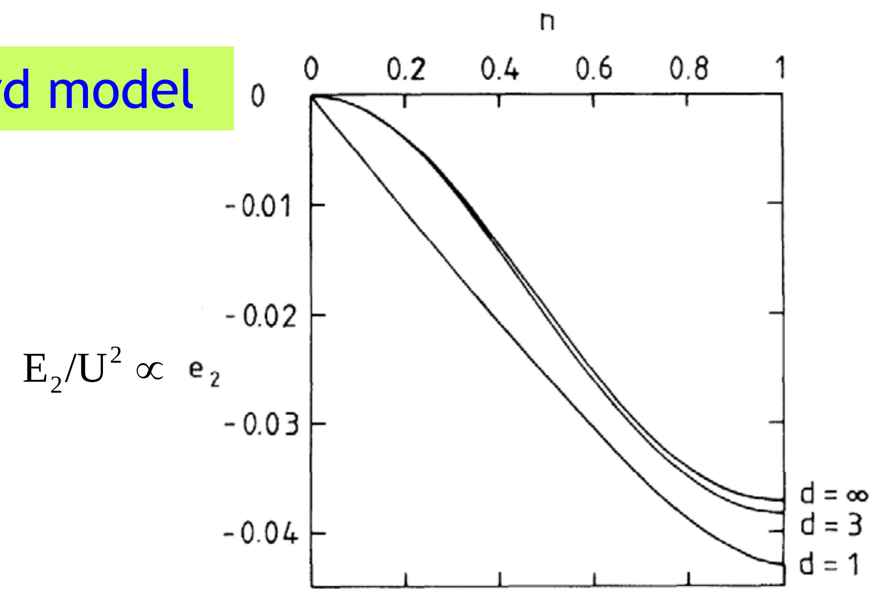
$\xrightarrow{Z \text{ or } d \to \infty}$ Collapse of all connected, irreducible diagrams in position space

Example: correlation energy of Hubbard model





Excellent approximation for d=3

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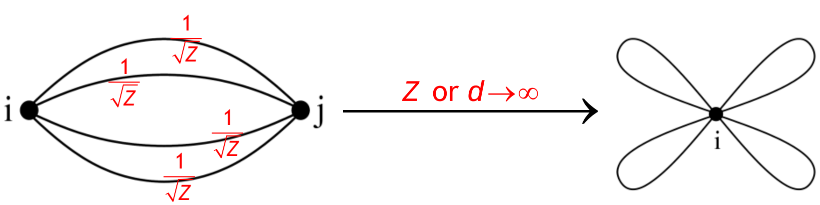
$$\left\langle \hat{H}_{\mathrm{kin}} \right\rangle_0 = \boxed{\underbrace{-t}_{\propto \frac{1}{\sqrt{Z}}}} \sum_{\mathbf{i},\sigma} \underbrace{\sum_{\mathbf{j}(NN\ \mathbf{i})}}_{Z} \underbrace{\left\langle \hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} \right\rangle_0}_{\propto \frac{1}{\sqrt{Z}}}$$

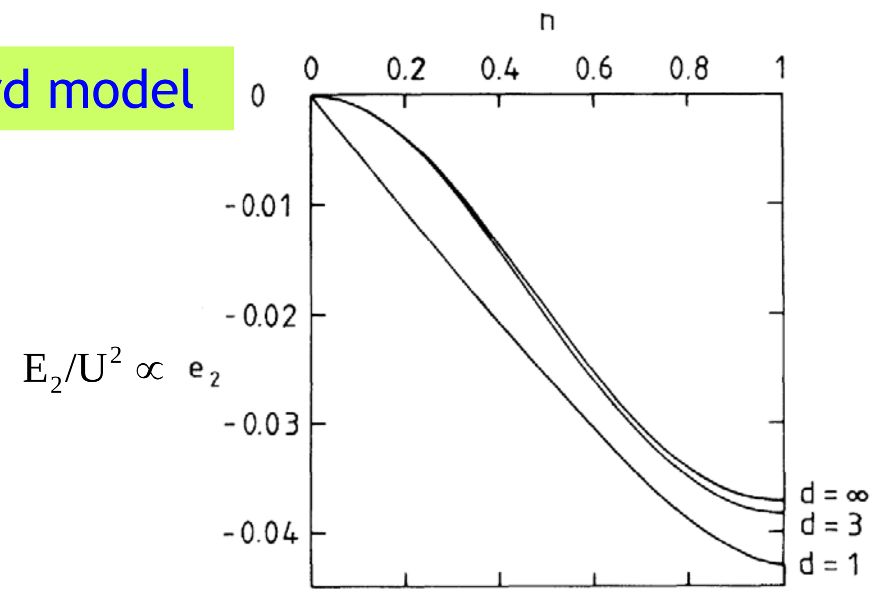
Z or $d \to \infty$

Quantum scaling $t = \dfrac{t^*}{\sqrt{Z}}$

Example: correlation energy of Hubbard model



δ_{ij}



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Z. Phys. B – Condensed Matter 74, 507–512 (1989)

Condensed Matter
Zeitschrift für Physik B

Correlated fermions on a lattice in high dimensions

E. Müller-Hartmann
Institut für Theoretische Physik, Universität zu Köln, Federal Republic of Germany

Received October 12, 1988

- $\Sigma(\cancel{\mathbf{k}}, \omega) \Rightarrow$ Fermi liquid
- Only Hubbard interaction remains dynamical

Z. Phys. B – Condensed Matter 75, 365–370 (1989)

Condensed Matter
Zeitschrift für Physik B

Thermodynamics and correlation functions of the Falicov-Kimball model in large dimensions

U. Brandt and C. Mielsch
Institut für Physik, Universität Dortmund, Federal Republic of Germany

Received December 21, 1988

Solution of the Hubbard model in $d \to \infty$: Towards dynamical mean-field theory

Z. Phys. B – Condensed Matter 83, 227–235 (1991)

Condensed Matter
Zeitschrift für Physik B

A new construction of thermodynamic mean-field theories of itinerant fermions: application to the Falicov-Kimball model*

V. Janiš**

Institut für Physik der Universität, Postfach 500 500, W-4600 Dortmund 50, Federal Republic of Germany

Received October 11, 1990; revised version December 21, 1990

We present a general scheme for a construction of mean-field-like theories of itinerant lattice fermions based on solutions to the exact $d=\infty$ grand canonical potential.

Generalization of coherent potential approximation (CPA) to interacting lattice fermions

Self-consistent DMFT equations:

$$\boxed{\frac{\delta\Omega}{\delta\Sigma_{\alpha\sigma}(n)}=0 \Rightarrow G_{\alpha\sigma}(n)=\frac{1}{N}\sum_{\mathbf{k}} G_{\sigma}^{\alpha\alpha}(i\omega_n+\mu-\Sigma_{\sigma}(n),\mathbf{k})}$$

$$\boxed{\frac{\delta\Omega}{\delta G_{\alpha\sigma}(n)}=0 \Rightarrow G_{\alpha\sigma}(n)=\frac{1}{Z_{\alpha}}\int \mathscr{D}\psi_{\alpha}\,\mathscr{D}\psi_{\alpha}^{*}\,\psi_{\alpha\sigma}(n)\,\psi_{\alpha\sigma}^{*}(n)\,\exp\{\mathscr{A}_{\alpha}[\psi_{\alpha}^{*},\psi_{\alpha}]\}}$$

$$\mathscr{A}_{\alpha}(\psi_{\alpha}^{*},\psi_{\alpha})=\sum_{n=-\infty}^{\infty}\sum_{\sigma}\psi_{\alpha\sigma}^{*}(n)\,[G_{\alpha\sigma}^{-1}(n)+\Sigma_{\alpha\sigma}(n)]\,\psi_{\alpha\sigma}(n)-U_{\alpha}\int_{0}^{\frac{1}{T}}\mathrm{d}\tau\,\psi_{\alpha\sigma}^{*}(\tau)\,\psi_{\alpha\sigma}(\tau)\,\psi_{\alpha-\sigma}^{*}(\tau)\,\psi_{\alpha-\sigma}(\tau)$$

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Condensed Matter
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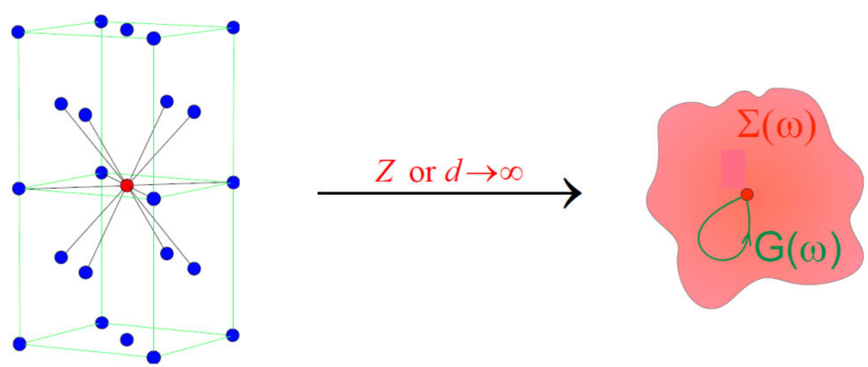


$$G(\omega) = \int d\varepsilon \frac{N^0(\varepsilon)}{\omega - \varepsilon + \mu - \Sigma(\omega)} = G^0(\omega - \Sigma(\omega))$$

→ free electrons in a dynamic potential Σ(ω)

Dynamical (single-site) mean-field theory

Numerical solution?

Preprint May 6, 1991

PHYSICAL REVIEW B VOLUME 45, NUMBER 12 15 MARCH 1992-II

Hubbard model in infinite dimensions

Antoine Georges*
Physics Department, Princeton University, Princeton, New Jersey 08544

Gabriel Kotliar
Serin Physics Laboratory, Rutgers University, Piscataway, New Jersey 08854
(Received 23 September 1991)

Solution of the Hubbard model in $d \to \infty$:
= Mapping to a single-impurity Anderson model + self-consistency condition

→ Lecture A. Georges

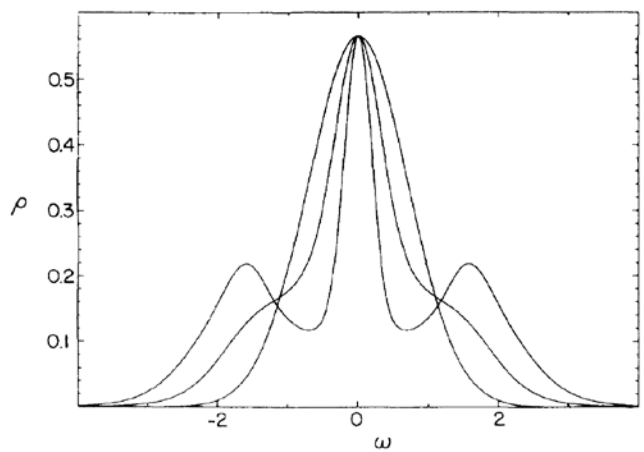


FIG. 2. Local spectral density of the paramagnetic solution at half filling ($n=1$) for $U=0$, $U=1.5$, and $U=2.5$.

Jarrell (1992)

Self-consistent DMFT equations

(i) Effective impurity problem: “local propagator“

$$G = -\frac{1}{Z}\int \mathcal{D}[\psi,\psi^*]\,\psi\psi^*\, e^{\underbrace{\psi^*[G^{-1}+\Sigma]\psi - U\psi^*\psi\psi^*\psi}_{\text{single-site ("impurity") action } A}}$$

(ii) *k*-integrated Dyson equation (“lattice Green function“: lattice enters)

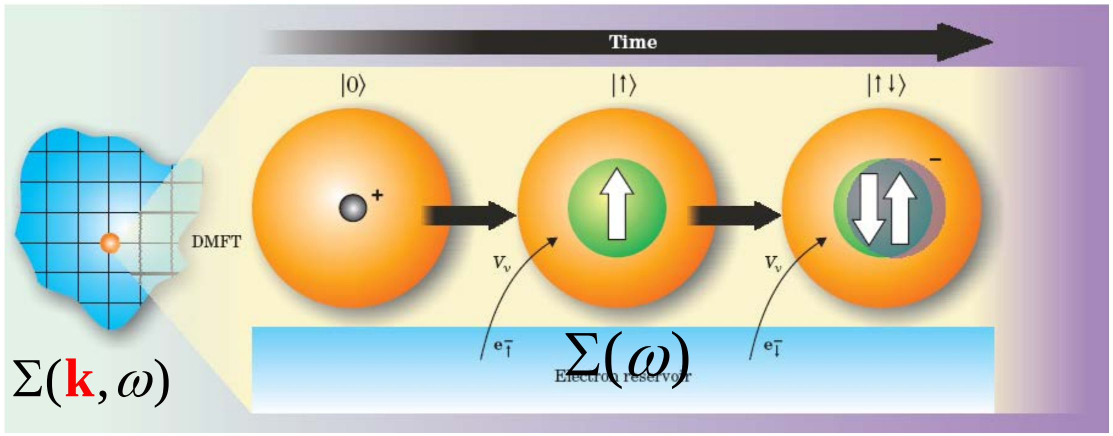
$$G(\omega) = \int d\varepsilon \frac{N^0(\varepsilon)}{\omega - \varepsilon + \mu - \Sigma(\omega)}$$

“Impurity solver“

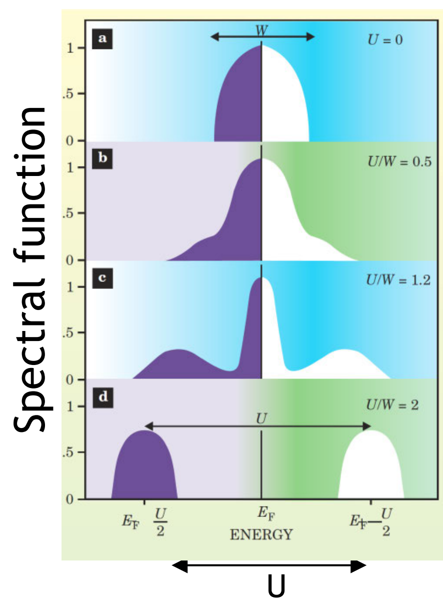
QMC	Hirsch-Fye (1986) → Jarrell (1992)
ED	Caffarel, Krauth (1994), Si *et al.* (1994)
NRG	Bulla (1999)
…	

The solution of the Hubbard model in $d \to \infty$ provides a dynamical mean-field theory (DMFT) of correlated electrons

DMFT: local theory with full many-body dynamics



Kotliar, DV (2004)

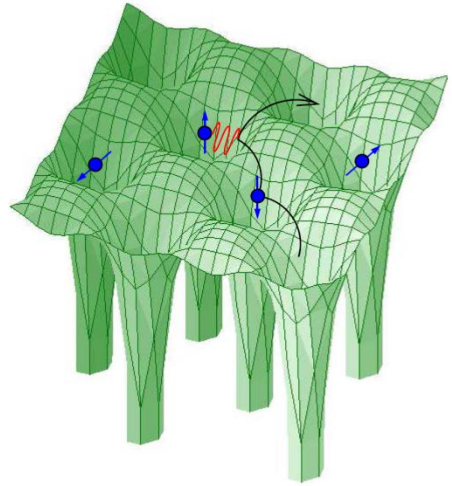


Mott-Hubbard metal-insulator transition

Review: Georges, Kotliar, Krauth, Rozenberg (RMP, 1996)

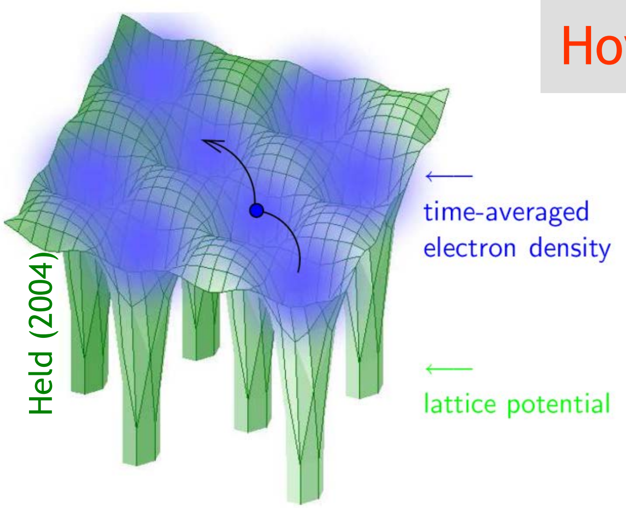
LDA+DMFT for Correlated Electron Materials

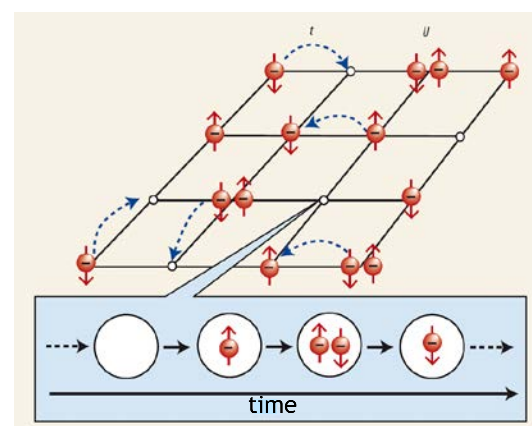
→ Lecture A. Lichtenstein



	DFT/LDA		Model Hamiltonians
+	material specific: "ab initio"	−	input parameters unknown
+	fast code packages	−	computationally expensive
−	fails for strong correlations	+	systematic many-body approach

How to combine?





Computational scheme for correlated electron materials:

Material specific electronic structure
(Density functional theory: **LDA, GGA, ...**) or **GW**

+

Local electronic correlations
(Many-body theory: **DMFT**)

X=LDA, GGA; GW, ...

→ **X+DMFT**

Anisimov, Poteryaev, Korotin, Anokhin, Kotliar(1997)
Lichtenstein, Katsnelson (1998)

Computational scheme for correlated electron materials:

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"LDA+DMFT"

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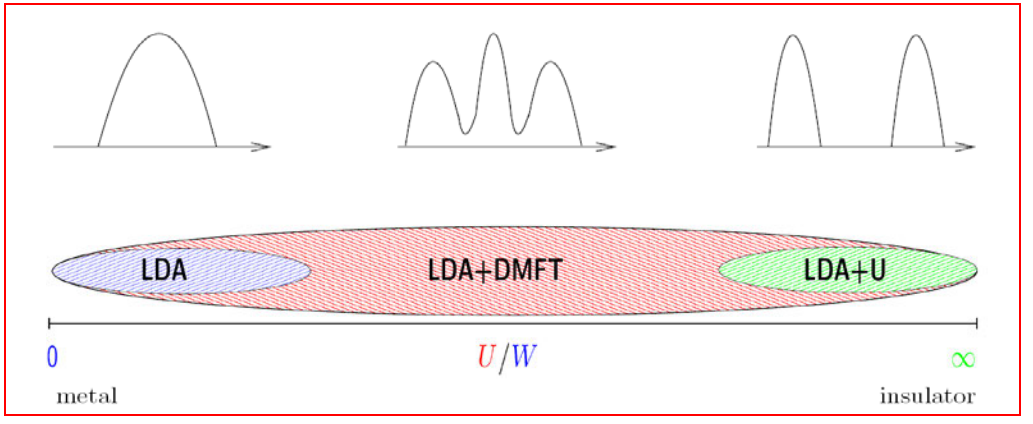

Held, Nekrasov, Keller, Eyert, Blümer, McMahan, Scalettar, Pruschke, Anisimov, DV (Psi-k 2003)

Conclusions and Outlook

- Quantum many-body perturbation theory for lattice fermions greatly simplifies in $d \to \infty$

- Calculations with Gutzwiller wave function in $d \to \infty$ = Gutzwiller approximation

- DMFT: canonical mean-field theory for correlated electrons

- **Goal:** Development of “LDA+DMFT“ into a computational scheme for correlated materials with predictive power