Linear Response Functions

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introduction

\[ \chi(q; \omega) \]

response functions
introduction

linear magnetic susceptibility

Kondo problem
(or DMFT impurity problem in certain regime)
scheme of the lecture

- introduction: what is all about
  - theoretical models
  - the many-body problem
  - the LDA+DMFT approach
- basics of linear response theory
  - definitions & properties
  - Kramers-Kronig relations
  - fluctuation-dissipation theorem
- the dynamical susceptibility
  - one-particle Green functions
  - two-particle Green functions
  - generalized susceptibility
- the dynamical susceptibility in LDA+DMFT
  - the bubble term
  - the Bethe-Salpeter equation
  - local-vertex approximation
  - local susceptibility
- example: one-band Hubbard model
theoretical models
theoretical models

what do we mean by *system* or *material*?

what is “gold”?

we have in mind an *idealized* object: thermodynamic limit, ideal crystal,…
what do we want to know about it?

• its *general* properties

• we want to understand *cooperative phenomena*: color, metallicity, … (or superconductivity, ferromagnetism, antiferromagnetism,…)

• identify *elementary entities*

• the latter depend on energy scale (*electron* vs *localized spins*)

• theory describing ideal object: model Hamiltonian

• gold is not iron: material-specific Hamiltonian
At first sight easy, the interactions are all known …

Electronic Hamiltonian (BO first approximation)

\[
\hat{H}_e = -\frac{1}{2} \sum_i \nabla_i^2 + \frac{1}{2} \sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2} \sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}
\]

\[
= \hat{T}_e + \hat{V}_{ee} + \hat{V}_{en} + \hat{V}_{nn}
\]

Lattice Hamiltonian

\[
\hat{H}_n = -\sum_\alpha \frac{1}{2M_\alpha} \nabla_\alpha^2 + \varepsilon(\{\mathbf{R}_\alpha\})
\]

\[
= \hat{T}_n + \hat{U}_n,
\]

If crystal structure known we can concentrate on electrons
material-specific Hamiltonian

interactions are all known ...

we choose a complete one-electron basis

for example choose atomic functions
material-specific Hamiltonian

... and write the Hamiltonian in second quantization
(atomic function: here neglect overlap)

\[
H_{e}^{NR} = - \sum_{ii' \sigma \ mm'} t_{m,m'}^{i,i'} c_{i m \sigma}^{\dagger} c_{i' m' \sigma} + \frac{1}{2} \sum_{ii' \ jj' \ \sigma \ \sigma'} \sum_{mm' \ \tilde{m} \tilde{m}'} \sum_{ii} \sum_{jj} \sum_{\sigma \ \sigma'} \sum_{mm} \sum_{\tilde{m} \tilde{m}} U_{mm' \tilde{m} \tilde{m}'}^{ijij'} c_{i m \sigma}^{\dagger} c_{j m' \sigma'}^{\dagger} c_{j' \tilde{m} ' \sigma'} c_{i' \tilde{m} \sigma}
\]

one-electron terms: hopping integrals + crystal field

\[
t_{m,m'}^{i,i'} = - \int dr \overline{\psi_{im \sigma}(r)} \left[ -\frac{1}{2} \nabla^2 + v_{R}(r) \right] \psi_{i' m' \sigma}(r)
\]

two-electron terms: Coulomb interaction tensor

\[
U_{mm' \tilde{m} \tilde{m}'}^{ijij'} = \int dr_1 \int dr_2 \frac{\overline{\psi_{im \sigma}(r_1) \psi_{jm' \sigma'}(r_2) \psi_{j' \tilde{m} ' \sigma'}(r_2) \psi_{i' \tilde{m} \sigma}(r_1)}}{|r_1 - r_2|}
\]
to make progress we have to solve it
the many-body problem

the problem is known, but no exact solution :(  

\[ H\Psi = E\Psi \]

Do we need it?
classical N-body problem

one body: no interactions

two-body: analytically solvable problem

three-body: chaotic behavior possible
solution very difficult
correlations

many objects with simple two-body interactions can give rise to a very complex system
or papers or learned about at formal presentations. We often don’t know a reference, have no idea who proved that result, how, and when. Usually a colleague mentioned it at a conference dinner, during a coffee-break, or in a friendly discussion in our department. It is striking, it sticks to our mind, and after a while it is part of our mathematical heritage—we just know it. Then we tell it further under similar circumstances, and so the wheel turns on. We will call this component of our knowledge folk-mathematics.

Without denying the positive role folk-mathematics plays in spreading information, we must admit that results gathered through it are sometimes misleading or misunderstood. A typical example is the Cantor set. Everybody knows that the middle-third Cantor set has zero Lebesgue measure, and many believe that the middle-fifth analogue has positive measure. Intuitively this sounds plausible: if we remove each time a smaller segment, the remaining quantity should be larger. Unfortunately, the intuition leads us astray this time. For any

Sundman’s method failed to apply to the $n$-body problem for $n > 3$. It took about 7 decades until the general case was solved. In 1991, a Chinese student, Qidong (Don) Wang, published a beautiful paper [Wa], [D1], in which he provided a convergent power series solution of the $n$-body problem. He omitted only the case of solutions leading to singularities—collisions in particular. (To understand the complications raised by solutions with singularities, see [D2].)

Did this mean the end of the $n$-body problem? Was this old question—unsuccessfully attacked by the greatest mathematicians of the last 3 centuries—merely solved by a student in a moment of rare inspiration? Though he provided a solution as defined in sophomore textbooks, does this imply that we know everything about gravitating bodies, about the motion of planets and stars? Paradoxically, we do not; in fact we know nothing more than before having this solution.

K.F. Sundman $(n=3)$
Q. Wang (generalization)
The following section deals with this apparent paradox.

The Foundations of Mathematics

What Sundman and Wang did is in accord with the way solutions of initial value problems are defined; everything is apparently all right; but there is a problem, a big one: these series solutions, though convergent on the whole real axis, have very slow convergence. One would have to sum up millions of terms to determine the motion of the particles for insignificantly short intervals of time. The round-off errors make these series unusable in numerical work. From the theoretical point of view, these solutions add nothing to what was previously known about the $n$-body problem.

Readers

The fundamentals of differential equations theory, the structure on which a significant part of modern science and technology is based. Do we have an answer to this last challenge?

References


emergent behavior

(from NASA website)
a single iron atom

26 electrons, 78 arguments, $10^{78}$ values
10 X 10 X 10 grid

$\psi_0(r_1, r_2, \ldots, r_{26})$

(from NASA website)
do we need the exact solution?

no.

too many details.

we need answers to interesting questions

• its general properties

• we want to understand cooperative phenomena: color, metallicity, … (or superconductivity, ferromagnetism, antiferromagnetism, …)

• identify elementary entities

• the latter depend on energy scale (electron vs localized spins)

• theory describing ideal object: model Hamiltonian

• gold is not iron: material-specific Hamiltonian
a solid-state example: antiferromagnetism

prediction: Néel (1932) from mean-field theory

experiment: Shull and Smart (1949)

Fig. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.
but the theory was wrong…

Bethe: ground state of linear Heisenberg chain has $S=0$
static mean-field ground state is wrong

Anderson: broken symmetry & quantum fluctuations
after we understood the mechanism everything is simpler…

simple (wrong) method sufficient

static mean-field solution
the standard model
density-functional theory

state-of the art approach; works for a large class of systems

shifts the focus from the wavefunction to the electronic density

\[ \Psi_0(r_1, r_2, \ldots, r_{26}) \rightarrow n(r) \]

exact (T=0) in principle, but only approximate functionals in practice

(LDA, GGA, ...)
density-functional theory

\[ \hat{H} = -\frac{1}{2} \sum_i \nabla_i^2 + \frac{1}{2} \sum_{i \neq i'} \frac{1}{|r_i - r_{i'}|} - \sum_{i, \alpha} \frac{Z_\alpha}{|r_i - R_\alpha|} - \sum_\alpha \frac{1}{2M_\alpha} \nabla_\alpha^2 + \frac{1}{2} \sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|R_\alpha - R_{\alpha'}|} \]

Kohn-Sham Hamiltonian

\[ \hat{h}_e = \sum_i \left[ -\frac{1}{2} \nabla_i^2 + v_R(r_i) \right] = \sum_i \hat{h}_e(r_i) \]

\[ v_R(r) = -\sum_\alpha \frac{Z_\alpha}{|r - R_\alpha|} + \int d\mathbf{r}' \frac{n(r')}{|r - r'|} + \frac{\delta E_{xc}[n]}{\delta n} = v_{en}(r) + v_H(r) + v_{xc}(r) \]

(in practice: LDA, GGA, …)

Walter Kohn

Nobel Prize in Chemistry (1998)

Kohn-Sham equations

understand and predict properties of solids, molecules, biological systems, geological systems…
strongly correlated systems

....those for which DFT (LDA) fails....

....LDA effective potential not enough....

....Coulomb average effects not enough....
strongly correlated systems

how do we recognize them?

anomalous phenomena

Mott insulators
heavy-Fermions
unconventional superconductivity
spin-charge separation
localized electrons

partially filled localized $d$ and $f$ shell; atomic physics plays important role

$$\psi_{nlm}(\rho, \theta, \phi) = R_{nl}(\rho)Y_l^m(\theta, \phi)$$

$$R_{nl}(\rho) = \sqrt{\left(\frac{2Z}{n}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-\rho/n} \left(\frac{2\rho}{n}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2\rho}{n}\right)$$

(hydrogen-like atom: Appendix B)
metal-insulator transition


not explained by mean-field, Hartree-Fock, perturbation theory, Fermi-liquid, DFT, etc....
a Mott insulator

an example: KCuF$_3$

LDA or GGA, or simple functional calculation

in real life: large gap orbitally ordered insulator
magnetic only below 40 K

it not a quantitative failure, but qualitative one
we can start from LDA, however

correlation effects can be seen as correction of DFT (LDA)

we can build one-electron basis from DFT

for example localized Wannier functions

$$
\psi_{in\sigma}(r) = \frac{1}{\sqrt{N}} \sum_k e^{-iR_i \cdot k} \psi_{nk\sigma}(r)
$$
ab-initio Wannier functions

\[ x^2 - y^2 \]

\[ 3z^2 - r^2 \]

\[ xz \]

\[ yz \]

\[ xy \]
realistic models from DFT(LDA)

basis functions

\[ \psi_{in\sigma}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{R}_i \cdot \mathbf{k}} \psi_{nk\sigma}(\mathbf{r}) \]

localized Wannier functions from LDA (GGA, ...)

Hamiltonian

\[ \hat{H}_e = \hat{H}_{\text{LDA}} + \hat{U} - \hat{H}_{\text{DC}} \]

LDA Hamiltonian

\[ \hat{H}_{\text{LDA}} = - \sum_{\sigma} \sum_{in,i'n'} t_{n,n'}^{i,i'} c_{in\sigma}^\dagger c_{i'n'\sigma} \]

\[ t_{n,n'}^{i,i'} = - \int d\mathbf{r} \overline{\psi}_{in\sigma}(\mathbf{r}) \left[ -\frac{1}{2} \nabla^2 + v_R(\mathbf{r}) \right] \psi_{i'n'\sigma}(\mathbf{r}) \]
Coulomb and double counting

\[ \hat{H}_e = \hat{H}^{\text{LDA}} + \hat{U} - \hat{H}_{\text{DC}} \]

\[ \hat{U} = \frac{1}{2} \sum_{ii'jj'\sigma\sigma'} \sum_{nn'pp'} U_{npn'p'}^{iij'j'} c_{in\sigma}^{\dagger} c_{j'p\sigma'}^{\dagger} c_{j'p'\sigma'} c_{i'n'\sigma} \]

bare Coulomb integrals

\[ \hat{U} = \frac{1}{2} U_{npn'p'}^{iij'j'} = \langle in\sigma jp\sigma' | \hat{U} | i'n'\sigma j'p'\sigma' \rangle \]

\[ = \int dr_1 \int dr_2 \overline{\psi}_{in\sigma}(r_1) \overline{\psi}_{jp\sigma'}(r_2) \frac{1}{|r_1 - r_2|} \psi_{j'p'\sigma'}(r_2) \psi_{i'n'\sigma}(r_1) \]

\[ \hat{H}_{\text{DC}} \]

long range Hartree and mean-field exchange-correlation already are well described by LDA (GGA,..)

difference U-H_{\text{DC}} short range!

if it would be long range perhaps \textit{not so strongly correlated}...
light and heavy electrons

electrons

light (weakly correlated): LDA (GGA,..)

heavy (strongly correlated): \( \hat{U} \)

\[
\hat{H}_e = \hat{H}^{LDA} + \hat{U}^l - \hat{H}_D^l
\]

eg. \( l \) shell

short-range correction to LDA

local or almost local

for a \( l \) shell, the local Coulomb interaction is

\[
\hat{U}^l = \frac{1}{2} \sum_i \sum_{\sigma'\sigma} \sum_{m_\alpha m'_\alpha} \sum_{m_\beta m'_\beta} U_{m_\alpha m_\beta m'_\alpha m'_\beta} c_{im_\alpha \sigma}^\dagger c_{im_\beta \sigma'}^\dagger c_{im'_\beta \sigma'} c_{im'_\alpha \sigma}
\]

screening? cRPA, cLDA, .... various approximations to be put to a test
from LDA to minimal models

energy scales

- 10^9 eV: quarks
- 10^7 eV: proton
- 10^5 eV: nucleus
- 10^3 eV: atom
- Crystal

simple low-energy models
typical model

generalized Hubbard model

\[ \hat{H}_e = \hat{H}^{\text{LDA}} + \hat{H}_U^l - \hat{H}_\text{DC}^l \]

\[ \hat{H}^{\text{LDA}} = - \sum_{ii'} \sum_{\sigma} \sum_{m_\alpha m'_\alpha} t_{m_\alpha,m'_\alpha}^{i,i'} c^{\dagger}_{i m_\alpha \sigma} c_{i' m'_\alpha \sigma} = \sum_k \sum_{\sigma} \sum_{m_\alpha m'_\alpha} \left[ \hat{H}^{\text{LDA}}_k \right]_{m_\alpha,m'_\alpha} c^{\dagger}_{k m_\alpha \sigma} c_{k m'_\alpha \sigma} \]

\[ \hat{H}_U^l = \frac{1}{2} \sum_i \sum_{\sigma \sigma'} \sum_{m_\alpha m'_\alpha} \sum_{m_\beta m'_\beta} U_{m_\alpha m_\beta m'_\alpha m'_\beta} c^{\dagger}_{i m_\alpha \sigma} c^{\dagger}_{i m_\beta \sigma'} c_{i m'_\alpha \sigma'} c_{i m'_\beta \sigma'} \]
one-band Hubbard model

\[ \hat{H}_\text{Hubbard} = -\sum_{ii'} \sum_{\sigma} t_{1,1}^{i,i'} c_{i\sigma}^\dagger c_{i'\sigma} + \varepsilon_d \sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

\[ \hat{H}_0 \]

\[ \hat{H}_U \]

\[ \begin{align*}
\varepsilon_d &= -t_{1,1}^{i,i'} \\
t &= t_{1,1}^{(i,i')} \\
U &= U_{1111}
\end{align*} \]

half filling

\( t=0 \): \( N_s \) atoms, insulator

\( U=0 \): half-filled band, metal

model for high-temperature superconducting cuprates
high-$T_c$ superconducting cuprates

$\text{HgBa}_2\text{CuO}_4$

$\text{CuO}_2$ planes
Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_{c\text{ max}}$


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(Received 4 December 2000; published 10 July 2001)

By calculation and analysis of the bare conduction bands in a large number of hole-doped high-temperature superconductors, we have identified the range of the intralayer hopping as the essential, material-dependent parameter. It is controlled by the energy of the axial orbital, a hybrid between Cu 4s, apical-oxygen 2p_z, and farther orbitals. Materials with higher $T_{c\text{ max}}$ have larger hopping ranges and axial orbitals more localized in the CuO_2 layers.
parameters for high-$T_c$ superconductors

Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_c$ max


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we still need a solution method

… should describe at least Mott physics..
… should be flexible, work for all models of Hubbard type..

NB: flexible alone is not enough
e.g.: very flexible: HF, or LDA; however, no Mott transition
DMFT

stat-of-the art approach for Hubbard-like models

\[ G_0^{-1} - G^{-1} = \Sigma(\omega) \]

dynamics captured\tself-energy local\text{exact in infinite dimensions}

Metzner and Vollhardt, PRL 62, 324 (1989); Georges and Kotliar, PRB 45, 6479 (1992)
\( H^{\text{LDA}}_k = \begin{pmatrix} H^{i_c,i_c}_k & H^{i_c,i'_c}_k & \cdots \\ H^{i'_c,i_c}_k & H^{i'_c,i'_c}_k & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \)

\[ G_{i_c m_{\alpha},i'_c m'_{\alpha}}(i\nu_n) = \frac{1}{N_k} \sum_k \left[ \frac{1}{i\nu_n I - H^{\text{LDA}}_k - \Sigma(i\nu_n) + H_{\text{DC}}} \right]_{i_c m_{\alpha},i'_c m'_{\alpha}} \]

\[ G_{m_{\alpha},m'_{\alpha}}(i\nu_n) = G_{i_c m_{\alpha},i'_c m'_{\alpha}}(i\nu_n) \]

\[ G^{-1}(i\nu_n) = G^{-1}(i\nu_n) + \Sigma^{i_c}(i\nu_n) \]

\[ \nu_n \rightarrow \tau \quad G(\tau) \]

\[ G(\tau) \quad \tau \rightarrow \nu_n \]

\[ \Sigma^{i_c}(i\nu_n) = G^{-1}(i\nu_n) - G^{-1}(i\nu_n) \]

\[ \Sigma = \begin{pmatrix} \Sigma^{i_c} & 0 & \cdots \\ 0 & \Sigma^{i'_c} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \]

LDA+DMFT
KCuF$_3$: various types of solutions

- Insulating & AFM
- HF/LDA+U
- LDA
- LDA+DMFT
- Non-magnetic & metallic
- Orbital ordering in paramagnetic phase
early successes: details matter
mechanism of Mott transition in the series explained

Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic 3d$^1$ Perovskites

E. Pavarini, S. Biermann, A. Poteryaev, A. I. Lichtenstein, A. Georges, and O. K. Andersen

\[ t_{2g}^1 \]
\[ \Delta = 200-300 \text{ meV} \]

LDA+DMFT 770 K

a small crystal field plays a key role
Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites

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spectral functions
(one-electron Green function)
what about linear response functions?
Hubbard Model in Infinite Dimensions: A Quantum Monte Carlo Study

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(Received 5 December 1991)

An essentially exact solution of the infinite-dimensional Hubbard model is made possible by a new self-consistent Monte Carlo procedure. Near half filling antiferromagnetism and a pseudogap in the single-particle density of states are found for sufficiently large values of the intrasite Coulomb interaction. At half filling the antiferromagnetic transition temperature obtains its largest value when the intrasite Coulomb interaction $U \approx 3$.

PACS numbers: 75.10.Jm, 71.10.+x, 75.10.Lp, 75.30.Kz
problem:
\[ \mathcal{G}^0(i\omega_n) = \mathcal{G}''(i\omega_n) \]
\[ = \mathcal{G}''(i\omega_n) + \sum_k \mathcal{G}_{ik}^0(i\omega_n) \Sigma_k(i\omega_n) \mathcal{G}_{ki}(i\omega_n), \]  
(2)
where
\[ \Sigma_k(i\omega_n) = \begin{cases} 0, & \text{if } i = k, \\ \Sigma(i\omega_n), & \text{otherwise}. \end{cases} \]
(3)
The prime indicates that the self-energy is set to zero on site \( i \). This spatial dependence of \( \Sigma_k \) is necessary to avoid overcounting of diagrams, since the Green's function \( \mathcal{G} \) is calculated to all orders in \( U \) by the QMC process. The diagrammatic equation shown in Fig. 2 is the same as that needed to solve the Anderson impurity problem. Thus, given \( \mathcal{G}^0 \), I may solve for \( \mathcal{G} \) with the QMC algorithm of Hirsch and Fye [7]. The Green's function calculated in this process may then be inverted to yield a new estimate for \( \Sigma(i\omega_n) \),
\[ \mathcal{G}(i\omega_n)^{-1} = \mathcal{G}^0(i\omega_n)^{-1} - \Sigma(i\omega_n). \]  
(4)
Thus the QMC procedure and Eqs. (2) and (4) constitute a set of self-consistent equations for the lattice self-energy \( \Sigma \) which essentially reduce the problem to a self-consistently embedded Anderson impurity problem [8].

A variety of two-particle properties may also be calculated with this procedure [9], since, using similar arguments applied to the self-energy, one may argue that the irreducible vertex function is also local. For example, the static magnetic susceptibility matrix
\[ \chi_{ij}(i\omega_n,i\omega_m) = \mathcal{G}^0(i\omega_n) \delta_{nm} + T \sum_{p,k} \mathcal{G}_{ik}^0(i\omega_n) \Gamma(i\omega_n,i\omega_p) \]
\[ \times \chi_{kj}(i\omega_p,i\omega_m), \]  
(5)
where \( \omega_n = (2n+1)\pi T \). This is related to the static susceptibilities by
\[ \chi_q = \frac{T}{N} \sum_{n,m,i,j} e^{-i\mathbf{q}\cdot \mathbf{R}_{ij}} \chi_{ij}(i\omega_n,i\omega_m). \]
(6)
The noninteracting part is
\[ \chi_q^0(i\omega_n) = \frac{1}{N} \sum_k \mathcal{G}_k(i\omega_n) \mathcal{G}_{k+q}(i\omega_n), \]  
(7)
where \( \mathcal{G}_k(i\omega_n) = 1/[i\omega_n - \epsilon_k - \Sigma(i\omega_n)] \). Equation (7) may readily be evaluated in the ferromagnetic \([q = (0,0,...)]\) and antiferromagnetic \([q = (\pi,\pi,...)]\) limits, in which it may be reexpressed as an integral over the Gaussian density of states. The function \( \Gamma \) is the local irreducible vertex function which may be calculated in the QMC procedure by solving
\[ \chi_{\|}(i\omega_n,i\omega_m) = \mathcal{G}(i\omega_n)^2 \delta_{nm} - T \sum_p \mathcal{G}(i\omega_n)^2 \Gamma(i\omega_n,i\omega_p) \]
\[ \times \chi_{\|}(i\omega_p,i\omega_m). \]  
(8)
Here \( \chi_{\|} \) is the opposite-spin two-particle Green's function,
\[ \chi_{\|}(i\omega_n,i\omega_m) = -T^2 \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 e^{-i\omega_n(\tau_1-\tau_2)} e^{-i\omega_m(\tau_3-\tau_4)} \langle T_\tau C_\uparrow(\tau_4) C_\downarrow(\tau_3) C_\downarrow(\tau_2) C_\uparrow(\tau_1) \rangle \]  
(9)
non-interacting case

Wick’s theorem holds

\[
\chi_0(q; i\omega_m)_{kL, k'L} = -\beta N_k G_{k\alpha \gamma'}(i\nu_n) G_{k' + q\alpha' \gamma}(i\nu_{n'} + i\omega_m) \delta_{n, n'} \delta_{k, k'}
\]
generalized susceptibility in LDA+DMFT

replace non-interacting $G$ with $G_{\text{DMFT}}$

$G_{\text{DMFT}}$ is the Green function obtained via DMFT

$$[\chi_0(q; \omega_m)]_{L_\alpha, L_\gamma} = -\beta \delta_{nn'} \frac{1}{N_k} \sum_{k} G_{\alpha\gamma'}^{\text{DMFT}}(k; i\nu_n) G_{\alpha'\gamma}^{\text{DMFT}}(k + q; i\nu_n + i\omega_m)$$
Bethe-Salpeter equation

\[
\chi = \chi_0 + \chi_0 \Gamma \chi
\]
[\chi(q; i\omega_m)]_{L_\alpha, L_\gamma} = [\chi_0(q; \omega_m) + \chi_0(q; i\omega_m) \Gamma(i\omega_m) \chi(q; i\omega_m)]_{L_\alpha, L_\gamma}

define local susceptibilities

[\chi_0(i\omega_m)]_{L_{\alpha}^{ic}, L_{\gamma}^{ic}} = \frac{1}{N_q} \sum_q [\chi_0(q; i\omega_m)]_{L_{\alpha}^{ic}, L_{\gamma}^{ic}}, \quad [\chi(i\omega_m)]_{L_{\alpha}^{ic}, L_{\gamma}^{ic}} = \frac{1}{N_q} \sum_q [\chi(q; i\omega_m)]_{L_{\alpha}^{ic}, L_{\gamma}^{ic}}
local-vertex approximation

assume that local BS equation is also valid for the local susceptibility

\[
\left[ \Gamma(i\omega_m) \right]_{L_\alpha, L_\gamma} = \left[ \chi_0^{-1}(i\omega_m) \right]_{L_\alpha, L_\gamma} - \left[ \chi^{-1}(i\omega_m) \right]_{L_\alpha, L_\gamma}
\]

local susceptibility: from quantum impurity solver

insert vertex in BS equation

\[
\left[ \chi(q; i\omega_m) \right]_{L_\alpha, L_\gamma} = \left[ \chi_0(q; \omega_m) + \chi_0(q; i\omega_m) \Gamma(i\omega_m) \chi(q; i\omega_m) \right]_{L_\alpha, L_\gamma}
\]

\(q\)-dependence here from non-interacting part
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![Hirsch-Fye QMC](image)

FIG. 3. Antiferromagnetic susceptibility $\chi_{AF}(T)$ vs temperature $T$ when $U=1.5$ and $\epsilon=0.0$. The logarithmic scaling behavior is shown in the inset. The data close to the transition fit the form $\chi_{AF} \propto |T-T_c|^v$ with $T_c=0.0866\pm 0.0003$ and $v=-0.99\pm 0.05$. The points at $U=0$ reflect exactly known limits.
Li$_2$VOSiO$_4$ vs VOMoO$_4$

poster Amin Kiani
Li$_2$VOSiO$_4$ vs VOMoO$_4$

$q_z = 0$

$\Gamma_{\text{loc}} = 0$

$\Gamma_{\text{loc}} \neq 0$

poster Amin Kiani
In a compact form, the Hamiltonian can include:

- Full self-energy matrix in spin-orbital space
- Full Coulomb matrix
- Spin-orbit

This further reduces the CPU time.


can include:

- Full self-energy matrix in spin-orbital space
- Full Coulomb matrix
- Spin-orbit

Phys. Rev. B 87, 195141

FIG. 3. Ferromagnetic spin polarization as a function of temperature in YTiO₃. The plot shows a transition at the critical temperature $T_c \sim 50$ K, slightly overestimating the experimental value $T_c \sim 30$ K, as one might expect from a mean-field calculation.
linear-response theory
we need some definitions

**a small** space- and time-dependent perturbation $H_1$

\[
\hat{H} \rightarrow \hat{H} + \int dr \, \hat{H}_1(r; t) + \ldots
\]

\[
\hat{H}_1(r; t) = - \sum_\nu \hat{O}_\nu(r; t) h_\nu(r; t),
\]

\[
\hat{O}_\nu(r; t) = e^{i(\hat{H} - \mu \hat{N})t} \hat{O}_\nu(r) e^{-i(\hat{H} - \mu \hat{N})t},
\]

\[
Z = \text{Tr} \, e^{-\beta(\hat{H} - \mu \hat{N})}
\]

partition function

\[
\beta = 1/k_B T
\]

\[
\langle \hat{A} \rangle_0 = \frac{1}{Z} \text{Tr} \left[ e^{-\beta(\hat{H} - \mu \hat{N})} \hat{A} \right]
\]

expectation value

\[
\Delta \hat{A}(r; t) = \hat{A}(r; t) - \langle \hat{A}(r) \rangle_0
\]

difference wrt unperturbed equilibrium case
linear response theory

a small space- and time-dependent perturbation $H_1$

$$\hat{H} \rightarrow \hat{H} + \int dr \, \hat{H}_1(r; t) + \ldots$$

$$\hat{H}_1(r; t) = -\sum_{\nu} \hat{O}_\nu(r; t) h_\nu(r; t),$$

property of the system external field

linear effect on some property $P$

$$\langle \hat{P}_\nu(r; t) \rangle = \langle \hat{P}_\nu(r) \rangle_0 + \langle \delta \hat{P}_\nu(r; t) \rangle_0,$$

$$\langle \delta \hat{P}_\nu(r; t) \rangle_0 = -i \int dr' \int_{-\infty}^{t} dt' \left\langle \left[ \Delta \hat{P}_\nu(r; t), \Delta \hat{H}_1(r'; t') \right] \right\rangle_0.$$
linear response function

replacing $H_1$ with its expression

\[ \langle \delta \hat{P}_\nu(r; t) \rangle_0 = i \sum_{\nu'} \int dr' \int_{-\infty}^{t} dt' \left\langle \left[ \Delta \hat{P}_\nu(r; t), \Delta \hat{O}_{\nu'}(r'; t') \right] \right\rangle_0 h_{\nu'}(r'; t') \]

linear response function

\[ \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(r, r'; t, t') = i \left\langle \left[ \Delta \hat{P}_\nu(r; t), \Delta \hat{O}_{\nu'}(r'; t') \right] \right\rangle_0 \Theta(t - t') \]

\[ \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(r, r'; t, t') \equiv \lim_{h_{\nu'} \to 0} \frac{\partial \langle \hat{P}_\nu(r; t) \rangle}{\partial h_{\nu'}(r'; t')} \]

now recognize the correlation function

\[ S_{\hat{P}_\nu \hat{O}_{\nu'}}(r, r'; t, t') = \langle \Delta \hat{P}_\nu(r; t) \Delta \hat{O}_{\nu'}(r'; t') \rangle_0 \]
..and it is retarded...

a perturbation has only effects after it has been switched on

\[ \chi \hat{P}_\nu \hat{O}_{\nu'}(r, r'; t, t') = i \left\langle \left[ \Delta \hat{P}_\nu(r; t) , \Delta \hat{O}_{\nu'}(r'; t') \right] \right\rangle_0 \Theta(t - t'). \]

effect only after perturbation

\[ \Theta(t - t') = \begin{cases} 
1 & \text{if } t - t' > 0 \\
0 & \text{if } t - t' < 0.
\end{cases} \]
Fourier transform

often it is better to work in Fourier space

for system with time and space translation invariance

\[ \langle \delta \hat{P}_\nu(q; \omega) \rangle_0 = \sum_{\nu'} \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(q; \omega) h_{\nu'}(q; \omega) \]
ideal crystal

rewrite operators in second quantization

\[ \Delta \hat{P}_\nu (r) = \Phi^\dagger (r) \Delta \hat{P}_\nu \Phi (r) \]

\[ \Delta \hat{P}_\nu (r) = \sum_{ii'} \sum_{\alpha \alpha'} \psi_{i\alpha'} (r) \psi_{i'\alpha} (r) \frac{c_{i\alpha'}^\dagger}{\rho_{\alpha'\alpha} (r)} [\Delta \hat{P}_\nu]_{\alpha\alpha'} c_{i'\alpha} = \sum_{ii'} \sum_{\alpha \alpha'} \rho_{\alpha'\alpha} (r) \Delta \hat{P}_{\nu,\alpha\alpha'}^{i,i'} \]

if we use a localized one-electron basis

\[ \Delta \hat{P}_\nu (r) \sim \sum_i \sum_{\alpha \alpha'} \rho_{\alpha'\alpha} (r) \Delta \hat{P}_{\nu,\alpha\alpha'}^i \]
example: magnetic susceptibility

\[ \hat{M}_z(\mathbf{r}) \sim -g\mu_B \sum_i \sum_{m\alpha m'\alpha} \rho_{m\alpha m'\alpha}(\mathbf{r}) \frac{1}{2} \sum_{\sigma \sigma'} c_{im\alpha \sigma}^\dagger [\Delta \hat{M}_z]_{\sigma \sigma'} c_{im'\alpha \sigma'}, \]

\[ [\Delta \hat{M}_z]_{\sigma \sigma'} = \langle \sigma | \hat{\sigma}_z | \sigma' \rangle \]

one-band case, e.g., one-band Hubbard model

\[ \langle \delta \hat{M}_z(\mathbf{q}; \omega) \rangle_0 \sim (g\mu_B)^2 |\rho(\mathbf{q})|^2 \sum_{ii'} e^{-i\mathbf{q} \cdot (T_i - T_i')} \sum_{\sigma \sigma'} \chi^{\sigma \sigma \sigma' \sigma'}_{ii'}(\omega) h_z(\mathbf{q}; \omega) \]

\[ = (g\mu_B)^2 |\rho(\mathbf{q})|^2 \chi_{\hat{S}_z \hat{S}_z}(\mathbf{q}; \omega) h_z(\mathbf{q}; \omega), \]

magnetic field
example: magnetic susceptibility

system with partially filled 3d shells, i.e., localized magnetic moments

\[
\langle \delta \hat{M}_z(q; \omega) \rangle_0 \sim (g \mu_B)^2 |\rho_s(q)|^2 \sum_{ii'} e^{-i\mathbf{q} \cdot (\mathbf{T}_i - \mathbf{T}_{i'})} \sum_{\sigma \sigma'} \chi_{\hat{S}_z \hat{S}_z}(q; \omega) \hat{h}_z(q; \omega)
\]

\[
= (g \mu_B)^2 |\rho_s(q)|^2 \chi_{\hat{S}_z \hat{S}_z}(q; \omega) \hat{h}_z(q; \omega).
\]

question: where do localized magnetic moments come from?

\[
\chi_{\hat{S}_z \hat{S}_z}(q; \omega) = i \int dt \ e^{i\omega t} \left\langle \left[ \hat{S}_z(q; t), \hat{S}_z(-q; 0) \right] \right\rangle_0 \Theta(t).
\]
localized magnetic moments

atomic physics (+ crystal field)

more details: see, e.g., my lecture of last year
many electron atoms

\[ H_{NR}^e = -\frac{1}{2} \sum_i \nabla_i^2 - \sum_i \frac{Z}{r_i} + \sum_{i>j} \frac{1}{|r_i - r_j|} \]

one shell, 2nd quantization

\[ H_{NR}^e = \varepsilon_{nl} \sum_{m\sigma} c_{m\sigma}^{\dagger} c_{m\sigma} + \frac{1}{2} \sum_{\sigma\sigma'} \sum_{mm'm'} U_{mm'm'n}^{l} c_{m\sigma}^{\dagger} c_{m'\sigma'}^{\dagger} c_{m'\sigma'} c_{m\sigma} \]

kinetic+central potential  Coulomb interaction

\[ U_{mm'm'n}^{l} = \int dr_1 \int dr_2 \frac{\overline{\psi_{im\sigma}(r_1)} \psi_{jm'\sigma'}(r_2) \psi_{j'm'\sigma'}(r_2) \psi_{i'm\sigma}(r_1)}{|r_1 - r_2|} \]
many electron atoms

does the atom/ion carry a magnetic moment?

total spin $S$ and total angular momentum $L$

filled shells
$S=L=0$

partially filled shell: magnetic ions

1. Hund’s rule max $S$
origin: Coulomb repulsion

direct term: the same for all N electron states

\[ U_{\text{avg}} = \frac{1}{(2l + 1)^2} \sum_{mm'} U_{mm'mm'}^l \]

exchange term: 1. Hund’s rule

\[ U_{\text{avg}} - J_{\text{avg}} = \frac{1}{2l(2l + 1)} \sum_{mm'} (U_{mm'mm'}^l - U_{mm'm'm'}^l) \]
Coulomb exchange

C atom, p shell

\[ J_{m,m'}^p = U_{mm'm'm}^p \]
\[ = \int dr_1 \int dr_2 \frac{\psi_{im\sigma}(r_1)\psi_{im'\sigma}(r_2)\psi_{im\sigma}(r_2)\psi_{im'\sigma}(r_1)}{|r_1 - r_2|} \]
\[ = \int dr_1 \int dr_2 \frac{\phi_{im\sigma}(r_1)\phi_{im'\sigma}(r_2)}{|r_1 - r_2|} = \frac{1}{V} \sum_k \frac{4\pi}{k^2} |\phi_{im'\sigma}(k)|^2 , \]

positive, hence ferromagnetic

\[ -\frac{1}{2} \sum_{\sigma} \sum_{m \neq m'} J_{m,m'}^p c^\dagger_{m\sigma} c_{m\sigma} c^\dagger_{m'\sigma} c_{m'\sigma} = -\frac{1}{2} \sum_{m \neq m'} 2J_{m,m'}^p \left[ S_z^m S_z^{m'} + \frac{1}{4} n_m n'_m \right] \]
analytic properties of $X(q;\omega)$

$\{\Psi^N_n\}$

$N$: number of electrons

$n$: eigenvalue

\[ P_{\nu}^{nm}(q) = \langle \Psi^N_n | \Delta \hat{P}_\nu(q; 0) | \Psi^N_m \rangle, \]

\[ O_{\nu'}^{mn}(q) = \langle \Psi^N_m | \Delta \hat{O}_{\nu'}(q; 0) | \Psi^N_n \rangle \]

\[ \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(q; \omega) = \frac{1}{Z} \sum_{nm} \frac{e^{-\beta(E^N_n - \mu N)} - e^{-\beta(E^N_m - \mu N)}}{E^N_m - E^N_n - \omega - i\delta} P_{\nu}^{nm}(q) O_{\nu'}^{mn}(-q) \]

$\delta > 0$

analytic in the upper part of the complex plane
Hermitian operators

if the operators are Hermitian

symmetry properties

\[
\begin{align*}
\text{Re} \left[ \chi \hat{P}_\nu \hat{O}_\nu' (q; \omega) \right] &= \text{Re} \left[ \chi \hat{P}_\nu \hat{O}_\nu' (-q; -\omega) \right], & \text{even} \\
\text{Im} \left[ \chi \hat{P}_\nu \hat{O}_\nu' (q; \omega) \right] &= -\text{Im} \left[ \chi \hat{P}_\nu \hat{O}_\nu' (-q; -\omega) \right], & \text{odd}
\end{align*}
\]
Kramers-Kronig relations

analytic function in upper part complex plane + fast decaying

\[ I_c = \oint_C \frac{\chi(q; z)}{z - \omega + i \delta} \, dz = 0 \]

\[ \text{Re} \left[ \chi(q; \omega) \right] - \text{Re} \left[ \chi(q; \infty) \right] = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} \frac{\text{Im} \left[ \chi(q; \omega') \right]}{\omega' - \omega} \, d\omega', \]

\[ \text{Im} \left[ \chi(q; \omega) \right] = -\frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} \frac{\text{Re} \left[ \chi(q; \omega') \right] - \text{Re} \left[ \chi(q; \infty) \right]}{\omega' - \omega} \, d\omega'. \]
thermodynamic sum-rule

let us take the static ($\omega=0$) limit

$$\text{Re} \left[ \chi(q; \omega = 0) \right] - \text{Re} \left[ \chi(q; \infty) \right] = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} \frac{\text{Im} \left[ \chi(q; \omega') \right]}{\omega'} d\omega'$$

let us take in addition the uniform ($q=0$) limit

$$\chi_{\nu \nu'}(0; 0) = \lim_{h_{\nu', \rightarrow 0}} \frac{\partial \langle P_{\nu} \rangle}{\partial h_{\nu'}}$$

response to a uniform and static perturbation
Thomas-Reich-Kuhn sum-rule

\[ \text{if } O \propto P^+ \]

\[ \frac{2}{\pi} \int_{0}^{\infty} \omega \, \text{Im} \left[ \chi_{\hat{P}_\nu} \hat{O}_\nu'(q; \omega) \right] \, d\omega = \left\langle \left[ \hat{P}_\nu, \hat{H} \right], \hat{O}_{\nu'} \right\rangle_0 \]

to proof it use a complete basis of eigenvectors + invariance of trace under cyclic permutations

also known as \( f \)-sum rule
detailed-balance

\[ S_{\hat{P}_\nu \hat{O}_{\nu'}}(q; t) = \left\langle \Delta \hat{P}_\nu(q; t) \Delta \hat{O}_{\nu'}(-q) \right\rangle_0 \]

\[ S_{\hat{P}_\nu \hat{O}_{\nu'}}(q; \omega) = \int_{-\infty}^{\infty} dt \, e^{i\omega t} \left\langle \Delta \hat{P}_\nu(q; t) \Delta \hat{O}_{\nu'}(-q; 0) \right\rangle_0 \]

\[ = \frac{1}{Z} \sum_{nm} \int_{-\infty}^{\infty} dt \, e^{i(\omega + E_n^N - E_m^N)t} e^{-\beta(E_n^N - \mu N)} P_{\nu}^{nm}(q) O_{\nu'}^{mn}(-q) \]

\[ = \frac{2\pi}{Z} \sum_{nm} e^{-\beta(E_n^N - \mu N)} P_{\nu}^{nm}(q) O_{\nu'}^{mn}(-q) \delta(\omega - E_m^N + E_n^N) \]

if \( O \propto P^+ \)

Fermi’s golden rule

\[ P_{\nu}^{nm}(q) = \langle \Psi_m^N | \Delta \hat{P}_\nu(q; 0) | \Psi_m^N \rangle, \]

\[ O_{\nu'}^{mn}(q) = \langle \Psi_m^N | \Delta \hat{O}_{\nu'}(q; 0) | \Psi_n^N \rangle \]
The relation above can be understood as follows. If \( \omega > 0 \), the correlation function \( S_{\hat{O}_\nu, \hat{P}_\nu} (q; \omega) \) describes the probability \( P_{n \to m} \propto n(E_n) [1 - n(E_m)] \) that the system is excited from an initial state with energy \( E_n \) to a final state with higher energy \( E_m = E_n + \omega \). Instead, \( S_{\hat{P}_\nu, \hat{O}_\nu} (-q; -\omega) \), describes the probability \( P_{m \to n} \propto n(E_m) [1 - n(E_n)] \) that the system goes from the initial state with energy \( E_m \) to a final state with lower energy \( E_n = E_m - \omega \). The probability \( P_{m \to n} \) is lower than \( P_{n \to m} \) by the factor \( e^{-\beta \omega} \).
fluctuation-dissipation theorem

if $O \propto P^+$

$$S_{\hat{P}_\nu \hat{O}_\nu}(q; \omega) = 2(1 + n_B) \text{Im} [\chi_{\hat{P}_\nu \hat{O}_\nu}(q; \omega)],$$

$$n_B(\omega) = \frac{1}{e^{\beta \omega} - 1}$$

correlation function

imaginary part of the linear response function

Bose-Einstein dispersion

large temperature limit

$$\text{Re} [\chi_{\hat{P}_\nu \hat{O}_\nu}(q; \omega = 0)] - \text{Re} [\chi_{\hat{P}_\nu \hat{O}_\nu}(q; \infty)] \sim \frac{1}{k_B T} S_{\hat{P}_\nu \hat{O}_\nu}(q; t = 0)$$
Green functions
single-particle Green functions
temperature Green function

for a consistent perturbation theory at finite temperature

\[
G_{\alpha \alpha'}(\tau) = -\langle \mathcal{T} c_{\alpha}(\tau_1) c_{\alpha'}^\dagger(\tau_2) \rangle_0 = -\frac{1}{Z} \text{Tr} \left[ e^{-\beta(\hat{H} - \mu \hat{N})} \mathcal{T} c_{\alpha}(\tau_1) c_{\alpha'}^\dagger(\tau_2) \right]
\]

\[0 < \tau_i < \beta\]

\[o(\tau) = e^{\tau(\hat{H} - \mu \hat{N})} o e^{-\tau(\hat{H} - \mu \hat{N})}\]

invariance of trance under \textbf{cyclic} permutations of operators

\[
G_{\alpha \alpha'}(\tau) = G_{\alpha \alpha'}(\tau_1 - \tau_2)
\]

only one independent imaginary time variable
temperature Green function

\[ G_{\alpha\alpha'}(\tau) = \frac{1}{Z} \sum_{Nnm} \langle \psi_n^N | c_\alpha | \psi_m^N + 1 \rangle \langle \psi_m^{N+1} | c_{\alpha'}^\dagger | \psi_n^N \rangle e^{-\beta(E_n^N - \mu N)} \]

\[
\begin{cases}
-e(E_n^N - E_{m+1}^N + \mu)\tau & \tau > 0 \\
-e((E_n^N - E_{m+1}^N + \mu)(-\beta - \tau) & \tau < 0
\end{cases}
\]

only well defined in the interval

\[-\beta < \tau < \beta\]

and how does it look like?
we can define it everywhere as

\[ \tilde{G}_{\alpha \alpha'}(\tau_1 \pm n_1 \beta, \tau_2 \pm n_2 \beta) \equiv (-1)^{n_1+n_2} G_{\alpha \alpha'}(\tau_1, \tau_2) \]
temperature Green function

let us make it periodic with period $2\beta$

Fourier transform

$$G_{\alpha\alpha'}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} e^{-i\nu_n \tau} G_{\alpha\alpha'}(i\nu_n),$$

$\nu_n$ are fermionic Matsubara frequencies, i.e., the poles of the Fermi distribution function

$$\nu_n = \pi(2n + 1)/\beta$$

Fourier coefficients

$$G_{\alpha\alpha'}(i\nu_n) = \frac{1}{2} \int_{-\beta}^{\beta} d\tau e^{i\nu_n \tau} G_{\alpha\alpha'}(\tau) = \frac{1}{2} (1 - e^{-i\nu_n \beta}) \int_{0}^{\beta} d\tau e^{i\nu_n \tau} G_{\alpha\alpha'}(\tau) = \int_{0}^{\beta} d\tau e^{i\nu_n \tau} G_{\alpha\alpha'}(\tau)$$
sums over Matsubara frequencies

often we have to calculate Matsubara sums

\[ \sum_n f(i\nu_n) \]

how do we do this?
If $F$ decays fast enough, using Cauchy integral theorem

$$
I_C = \frac{1}{2\pi i} \oint_C \mathcal{F}_{k\sigma}(z)n_\sigma(z)e^{z\tau} \, dz
$$

$$
\frac{1}{\beta} \sum_n e^{i\nu_n \tau} \mathcal{F}_{k\sigma}(i\nu_n) = \sum_{z_p} \text{Res} \left[ \mathcal{F}_{k\sigma}(z_p) \right] n_\sigma(z_p)e^{z_p \tau}
$$
\[ \frac{1}{\beta} \sum_n e^{-i\nu_n \nu} G_{k\sigma}(i\nu_n) = G_{k\sigma}(0^-) = n_\sigma(\varepsilon_k), \]

\[ \frac{1}{\beta} \sum_n e^{-i\nu_n \nu} G_{k\sigma}(i\nu_n) = G_{k\sigma}(0^+) = n_\sigma(\varepsilon_k) - 1. \]
Table 1: Some of the most common Matsubara Fourier transforms (fermionic case). The function $n_\sigma(x)$ is the Fermi-Dirac distribution function $n_\sigma(x) = 1/(1 + e^{x/\beta})$. The parameters $x$ and $y$ are real numbers. For $\tau$ we consider the interval $(0, \beta)$.
two-particle Green-functions
two-particle Green-functions

\[ \chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau) = \langle T \Delta \hat{P}_{\alpha\alpha'}(\tau_1, \tau_2) \Delta \hat{O}_{\gamma\gamma'}(\tau_3, \tau_4) \rangle \]

\[ \Delta \hat{P}_{\alpha\alpha'}(\tau_1, \tau_2) = c_{\alpha'}^\dagger(\tau_2) c_\alpha(\tau_1) - \langle T c_{\alpha'}^\dagger(\tau_2) c_\alpha(\tau_1) \rangle, \]
\[ \Delta \hat{O}_{\gamma\gamma'}(\tau_3, \tau_4) = c_{\gamma'}^\dagger(\tau_4) c_\gamma(\tau_3) - \langle T c_{\gamma'}^\dagger(\tau_4) c_\gamma(\tau_3) \rangle. \]

three independent variables

\[ \chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau) = \chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{14}, \tau_{24}, \tau_{34}, 0) \]

(we can also choose \( \tau_{12} \tau_{34} \tau_{23} \))

anti-periodicity

\[ \chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{14} + \beta, \tau_{24}, \tau_{34}, 0) = -\chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau_{14}, \tau_{24}, \tau_{34}, 0), \]
non-interacting example

Wick’s theorem

$$\chi(\tau_{12}, 0^+; \tau_{23}) = -G_{\alpha\alpha}(\tau_{12} + \tau_{23} + 0^+)G_{\alpha\alpha}(-\tau_{23})$$
Matsubara Fourier transform

\[ \chi_{\gamma\gamma'}^{\alpha\alpha'}(\nu) = \frac{1}{16} \int \int \int \int d\tau \ e^{i\nu \cdot \tau} \chi_{\gamma\gamma'}^{\alpha\alpha'}(\tau) \]

\[ \nu = (\nu_1, \nu_2, \nu_3, \nu_4) \]

energy conservation

\[ \nu = (\nu_n, -\nu_n - \omega_m, \nu_n + \omega_m, -\nu_n') \]

\[ \omega_m \quad \text{Bosonic frequency} \]
\[ \chi_{n,n'}^{\alpha\alpha'}(i\omega_m) = \chi_{n',n}^{\gamma'\gamma\alpha'}(i\omega_m) \]

\[ \left| \chi_{n,n'}^{\alpha\alpha'}(i\omega_m) \right| = \left| \chi_{n',n}^{\alpha\alpha'}(i\omega_m) \right|. \]

\textbf{symmetry lines}

\textbf{non-interacting case}

\[ \chi_{\gamma'\gamma}(\tau) = -G_{\gamma'\gamma}(\tau_{14})G_{\gamma\alpha'}(-\tau_{23}) \]
from the two-particle Green-function to the susceptibility
generalized susceptibility

\[ \chi_{\hat{P}^i_{\nu}} \hat{\mathcal{O}}_{\nu'}^i (\tau) = \langle \mathcal{T} \Delta \hat{P}^i_{\nu} (\tau_1, \tau_2) \Delta \hat{\mathcal{O}}_{\nu'}^i (\tau_3, \tau_4) \rangle_0, \]

\[ \hat{P}^i_{\nu} (\tau_1, \tau_2) = \sum_\alpha p^\nu_\alpha c^\dagger_{i\alpha'} (\tau_2) c_{i\alpha} (\tau_1), \]

\[ \hat{\mathcal{O}}_{\nu'}^i (\tau_3, \tau_4) = \sum_\gamma o'^\nu_{\gamma'} c^\dagger_{i'\gamma'} (\tau_4) c_{i'\gamma} (\tau_3). \]

\[ v_{\alpha\gamma} = p^\nu_\alpha o'^\nu_{\gamma'} \]

two-particle Green function tensor

\[ \chi_{\hat{P}^i_{\nu}} \hat{\mathcal{O}}_{\nu'}^i (\tau) = \sum_{\alpha\gamma} v_{\alpha\gamma} \chi_{\gamma i'_{\nu}}^\alpha (\tau), \]
generalized susceptibility

\[ \chi(q; \nu) = \sum_{\alpha \gamma} v_{\alpha \gamma} \sum_{ii'} e^{i(T_i - T_{i'})} \cdot q \chi_{\alpha i}^{\gamma i'}(\nu) = \sum_{\alpha \gamma} v_{\alpha \gamma} \frac{1}{N^2_k} \sum_{kk'} \chi_{\alpha k}^{\gamma k'}(\nu) \]

\[ \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(q; i\omega_m) = \sum_{\alpha \gamma} v_{\alpha \gamma} \frac{1}{\beta^2} \sum_{nn'} [\chi(q; \omega_m)]_{L_{\alpha}, L_{\gamma}} \]

matrix \(L \times L\) \(\quad L_a = n \times \alpha\)

\(n\): fermionic Matsubara frequencies
\(\alpha\): flavors
magnetic susceptibility

\[ \chi_{\hat{P}_\nu \hat{O}_{\nu'}}(q; i\omega_m) = \sum_{\alpha\gamma} v_{\alpha\gamma} \frac{1}{\beta^2} \sum_{nn'} [\chi(q; \omega_m)]_{L\alpha, L\gamma}. \]

\[ v_{\alpha\gamma} = p_{\nu}^\nu o_{\nu'}^\nu \]

\[ o_{\alpha}^{\hat{z}} = -g\mu_B \langle \sigma | \hat{\sigma}_z | \sigma \rangle, \quad p_{\alpha}^{\hat{z}} = -g\mu_B \langle \sigma' | \hat{\sigma}_z | \sigma' \rangle, \]

the prefactor determines the type of response
non-interacting case

Wick’s theorem holds

\[\chi_0(q; i\omega_m)\]_{kL_{\alpha},k'_{\gamma}} = -\beta N_k G_{k\alpha\gamma'}(i\nu_n) G_{k'+q\alpha'\gamma}(i\nu_{n'} + i\omega_m) \delta_{n,n'} \delta_{k,k'}
Bethe-Salpeter equation

\[ \chi_{\nu_{n}+\omega_{m}}^{k+q} \chi_{\nu_{n}+\omega_{m}}^{k'+q} = \chi \]

\[ \chi_{\nu_{n}}^{k+q} \chi_{\nu_{n}}^{k'} = \chi_{\nu_{n}+\omega_{m}}^{k+q} \chi_{\nu_{n}+\omega_{m}}^{k'+q} \]

\[ \chi_{\nu_{n}}^{k+q} \chi_{\nu_{n}+\omega_{m}}^{k'+q} = \chi_{\nu_{n}}^{k+q} \chi_{\nu_{n}+\omega_{m}}^{k'+q} \]

\[ \chi_{\nu_{n}}^{k+q} \chi_{\nu_{n}+\omega_{m}}^{k'+q} = \chi_{\nu_{n}+\omega_{m}}^{k+q} \chi_{\nu_{n}+\omega_{m}}^{k'+q} \]
one-band Hubbard model
magnetic response
the one-band Hubbard model

\[ \hat{H}_{\text{Hubbard}} = -\sum_{ii'} \sum_{\sigma} t^{i,i'}_{1,1} c_{i\sigma}^\dagger c_{i'\sigma} + \varepsilon_d \sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

\[ \begin{align*}
\hat{H}_0 & = -\sum_{ii'} \sum_{\sigma} t^{i,i'}_{1,1} c_{i\sigma}^\dagger c_{i'\sigma} \\
\hat{H}_U & = \sum_{i\sigma} \varepsilon_d n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}
\end{align*} \]

\[
\begin{cases}
\varepsilon_d &= -t_{1,1}^i \\
t &= t_{1,1}^{i,i'} \\
U &= U_{1111}^{iii}
\end{cases}
\]

half filling

- \( t=0 \): \( N_s \) atoms, insulator
- \( U=0 \): half-filled band, metal
the $U=0$ limit
the $U=0$ limit

\[ H_d + H_T = \sum_\mathbf{k} \sum_\sigma [\varepsilon_d + \varepsilon_\mathbf{k}] c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \]

hypercubic lattice

\[ \varepsilon_\mathbf{k} = -2t \sum_{\nu=1}^{d} \cos(k_{r,\nu} a) \]
Pauli paramagnetism

\[ \varepsilon_k \rightarrow \varepsilon_{k\sigma} = \varepsilon_k + \frac{1}{2} \sigma g \mu_B h_z \]
Pauli paramagnetism

\[ M_z = -\frac{1}{2} (g\mu_B) \frac{1}{N_k} \sum_k \left[ n_{k\uparrow} - n_{k\downarrow} \right] \sim \frac{1}{4} (g\mu_B)^2 \rho(\varepsilon_F) h_z \]

zero temperature

\[ \chi^P(0) = \frac{1}{4} (g\mu_B)^2 \rho(\varepsilon_F) \]

finite temperature

\[ \chi^P(T) = \frac{1}{4} (g\mu_B)^2 \int d\varepsilon \rho(\varepsilon) \left( -\frac{dn(\varepsilon)}{d\varepsilon} \right) \]
finite temperature

-2 0 2
energy (eV)

DOS

-2 0 2
T (K)

χₐ

2000 4000

T (K)

d=1
d=2
d=3
temperature Green function

U=0 limit

\[ G_{k\sigma}(\tau) = - \left\langle T \left[ c_{k\sigma}(\tau)c_{k\sigma}^{\dagger}(0) \right] \right\rangle_0 
= - \left[ \Theta(\tau)(1 - n_{\sigma}(\varepsilon_k)) - \Theta(-\tau)n_{\sigma}(\varepsilon_k) \right] e^{-(\varepsilon_k - \mu)\tau} \]

\[ G_{k\sigma}(i\nu_n) = \frac{1}{i\nu_n - \varepsilon_k + \mu} \]
magnetic susceptibility

paramagnetic region

\[ \chi_{zz}(q; i\omega_m) = (g\mu_B)^2 \frac{1}{4} \frac{1}{\beta^2} \sum_{nn'} \sum_{\sigma} \chi_{n,n'}^{\sigma\sigma}(i\omega_m) \]

**U=0 limit**

\[ \sum_{\sigma} \chi_{n,n'}^{\sigma\sigma}(i\omega_m) = -\beta \frac{1}{N_k} \sum_{k} \sum_{\sigma} G_{k\sigma}(i\nu_n) G_{k+q\sigma}(i\nu_n + i\omega_m) \delta_{n,n'} \]

**static case** \((\omega_m=0)\)

<table>
<thead>
<tr>
<th>(g_\alpha(\nu_n; x, y))</th>
<th>(g_\alpha(\tau; x, y) = \frac{1}{\beta} \sum_n e^{-i\nu_n \tau} g_\alpha(\nu_n; x, y))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(g_a(\nu_n; x, y) = [i\nu_n - x]^{-1})</td>
<td>([n_\sigma(x) - 1]e^{-x\tau})</td>
</tr>
<tr>
<td>(g_b(\nu_n; x, y) = [i\nu_n - x]^{-2})</td>
<td>(n_\sigma(x)(\tau - \beta n_\sigma(x))e^{-x(\tau - \beta)})</td>
</tr>
<tr>
<td>(g_c(\nu_n; x, y) = [i\nu_n - x]^{-1} [i\nu_n - y]^{-1})</td>
<td>(-[e^{-x(\tau - \beta)} n_\sigma(x) - e^{-y(\tau - \beta)} n_\sigma(y)] [x - y]^{-1})</td>
</tr>
<tr>
<td>(g_d(\nu_n; x, y) = [i\nu_n - x]^{-1} [i\nu_n + x]^{-1})</td>
<td>([g_a(\tau; x, y) - g_a(\tau; -x, y)]/2x)</td>
</tr>
</tbody>
</table>
\[ \chi_{zz}(0;0) = \frac{1}{4} (g\mu_B)^2 \rho(\varepsilon_F), \]

\[ \rho(\varepsilon_F) = -\sum_{\sigma} \frac{1}{N_k} \sum_{\mathbf{k}} \frac{dn_\sigma(\varepsilon_k)}{d\varepsilon_k} \bigg|_{T=0}. \]
magnetic susceptibility

\[ \varepsilon_k = -2t\left[ \cos(k_x a) + \cos(k_y a) + \cos(k_z a) \right] \]

finite temperature \( \sim 350 \text{ K} \)

\[ \chi_0(q;0) \]

2-dimensional case: M point!

weakly temperature dependent
the $t=0$ limit
atomic limit \((t=0)\) & half filling

| \(|N, S, S_z\rangle\) | \(N\) | \(S\) | \(E(N)\) |
|---------------------|------|------|--------|
| \(|0,0,0\rangle\)   | 0    | 0    | 0      |
| \(|1,\frac{1}{2},\uparrow\rangle\) = \(c_{i\uparrow}^\dagger|0\rangle\) | 1    | \(\frac{1}{2}\) | \(\varepsilon_d\) |
| \(|1,\frac{1}{2},\downarrow\rangle\) = \(c_{i\downarrow}^\dagger|0\rangle\) | 1    | \(\frac{1}{2}\) | \(\varepsilon_d\) |
| \(|2,0,0\rangle\) = \(c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger|0\rangle\) | 2    | 0    | \(2\varepsilon_d + U\) |

\[
H_d + H_U = \varepsilon_d \sum_i n_i + U \sum_i \left[- (S_z^i)^2 + \frac{n_i^2}{4}\right]
\]

emergence of the spin!

half filling: highly degenerate states, \(2^{N_s}\) degrees of freedom

insulating behavior
magnetization

non interacting ions

uniform magnetic field $h_z$, Zeeman term

$$M_z = \langle M^i_z \rangle = -g\mu_B \frac{\text{Tr} \left[ e^{-g\mu_B h_z \beta S^i_z S^i_z} \right]}{\text{Tr} \left[ e^{-g\mu_B h_z \beta S^i_z} \right]} = g\mu_B S \tanh (g\mu_B h_z \beta S)$$

derivative with respect to $h_z$

$$\frac{\partial M_z}{\partial h_z} = (g\mu_B S)^2 \frac{1}{k_B T} \left[ 1 - \tanh^2 (g\mu_B h_z \beta S) \right]$$
Curie susceptibility

Curie behavior

\[ \chi_{zz}(0; 0) = (g\mu_B S)^2 \frac{1}{k_BT} = \frac{C_{1/2}}{T} \]

Curie constant

\[ C_{1/2} = \frac{(g\mu_B)^2 S(S+1)}{3k_B} \]
local spin as emergent entity

one-site Hubbard model

\[
\chi_{zz}(0; 0) \sim \frac{(g\mu_B)^2}{k_B T} \left\{ \frac{\text{Tr} \left[ e^{-\beta(H_i - \mu N_i)} \left( S_z^i \right)^2 \right]}{\text{Tr} \left[ e^{-\beta(H_i - \mu N_i)} \right]} - \left[ \frac{\text{Tr} \left[ e^{-\beta(H_i - \mu N_i)} S_z^i \right]}{\text{Tr} \left[ e^{-\beta(H_i - \mu N_i)} \right]} \right]^2 \right\}
\]

\[
= \frac{C_{1/2}}{T} \frac{e^{\beta U/2}}{1 + e^{\beta U/2}}
\]

\[
U = E(N_i + 1) + E(N_i - 1) - 2E(N_i)
\]

infinite U limit: the spin S=1/2

only S=1/2 part of Hilbert space remains
temperature Green function

\[ G_\sigma(\tau) = -\frac{1}{2} \frac{1}{1 + e^{\beta U/2}} \left[ e^{\tau U/2} + e^{(\beta - \tau) U/2} \right] \]

\[ G_\sigma(i\nu_n) = \frac{1}{2} \left[ \frac{1}{i\nu_n + U/2} + \frac{1}{i\nu_n - U/2} \right] \]
magnetic susceptibility

\( \chi_{i\sigma' i\sigma'}(\tau^+) = \frac{1}{2(1 + e^{\beta U/2})} \left( e^{\tau_{12} U/2 + \tau_{34} U/2} + \delta_{\sigma\sigma'} e^{(\beta - \tau_{12}) U/2 - \tau_{34} U/2} \right) \)

\( \chi_{zz}(\tau^+) = (g\mu_B)^2 \frac{1}{4 \beta} \sum_{\sigma\sigma'} \chi_{i\sigma' i\sigma'}(\tau) = \frac{(g\mu_B)^2}{4 \beta} \frac{1}{1 + e^{\beta U/2}} e^{(\beta - \tau_{12} - \tau_{34}) U/2} \)
Fourier transform

\[ [\chi_{zz}]_{nn'} (i\omega_m) = \beta \frac{1}{4} (g\mu_B)^2 \sum_P \text{sign}(P) f_P \]

\[ f_P(i\omega_{P_1}, i\omega_{P_2}, i\omega_{P_3}) = \int_0^\beta d\tau_{14} \int_0^{\tau_{14}} d\tau_{24} \int_0^{\tau_{24}} d\tau_{34} e^{i\omega_{P_1}\tau_{14} + i\omega_{P_2}\tau_{24} + i\omega_{P_3}\tau_{34}} f_P(\tau_{14}, \tau_{24}, \tau_{34}) \]

\[ f_E(\tau_{14}, \tau_{24}, \tau_{34}) = \frac{1}{1 + e^{\beta U/2}} e^{\beta U/2} e^{-(\tau_{12} + \tau_{34})U/2} = \frac{1}{1 + e^{\beta U/2}} g_E(\tau_{14}, \tau_{24}, \tau_{34}) \]
calculating the integral

\[ I_P(x, -x, x; i\omega_{P_1}, i\omega_{P_2}, i\omega_{P_3}) = \int_0^\beta d\tau_{14} \int_0^{\tau_{14}} d\tau_{24} \int_0^{\tau_{24}} d\tau_{34} e^{i\omega_{P_1}\tau_{14} + i\omega_{P_2}\tau_{24} + i\omega_{P_3}\tau_{34}} e^{x(\tau_{14} - \tau_{24} + \tau_{34})} \]

\[ = + \int_0^\beta d\tau_{14} \int_0^{\tau_{14}} d\tau \int_0^{\tau_{14} - \tau} d\tau' e^{i\omega_{P_1} + i\omega_{P_2} + i\omega_{P_3} + x)\tau_{14} - i(\omega_{P_2} + \omega_{P_3})\tau} e^{-(i\omega_{P_3} + x)\tau'} \]

\[ = + \frac{1}{i\omega_{P_3} + x - i\omega_{P_2} + x} \left[ \frac{1}{i\omega_{P_1} + x} \frac{1}{n(x)} + \beta \delta_{\omega_{P_1} + \omega_{P_2}} \right] \]

\[ + \frac{1}{i\omega_{P_3} + x} \frac{1 - \delta_{\omega_{P_2} + \omega_{P_3}}}{i(\omega_{P_2} + \omega_{P_3})} \left[ \frac{1}{i\omega_{P_1} + x} - \frac{1}{i(\omega_{P_1} + \omega_{P_2} + \omega_{P_3}) + x} \right] \frac{1}{n(x)} \]

\[ + \delta_{\omega_{P_2} + \omega_{P_3}} \frac{1}{i\omega_{P_3} + x} \left\{ \left[ \frac{1}{(i\omega_{P_1} + x)} \right]^2 \frac{1}{n(x)} - \beta \left[ \frac{1}{i\omega_{P_1} + x} \right] \frac{1 - n(x)}{n(x)} \right\}. \]
magnetic susceptibility

result after Matsubara sums

\[
\chi_{zz}(q; 0) = \left(g\mu_B\right)^2 \frac{1}{4k_B T} \frac{e^{\beta U/2}}{1 + e^{\beta U/2}}
\]

Curie-like temperature behavior

infinite U limit: emergence of spin
the small $t/U$ limit
perturbation theory

Hubbard model

\[ H = \varepsilon_d \sum_i \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U \]

half filling: \( N=1 \) electrons per site

\( n_D = \) number of doubly occupied sites

idea: divide Hilbert space into \( n_D=0 \) and \( n_D>0 \) sector

next downfold high energy \( n_D>0 \) sector
two sites

\[ N=1 \text{ per site}; \ N_{\text{tot}}=2 \]

- **\( n_D=0 \) sector**
  - site 1
  - site 2

- **\( n_D=1 \) sector**
  - site 1
  - site 2
Hilbert space

$n_D=0$ sector

$n_D>0$ sector

next downfold high energy $n_D>0$ sector
low energy model

eliminate states with a doubly occupied site

virtual hopping

energy gain

\[ \Delta E_{\uparrow\downarrow} \sim -\sum_I \langle \uparrow, \downarrow | H_T | I \rangle \langle I | \frac{1}{E(2) + E(0) - 2E(1)} | I \rangle \langle I | H_T | \uparrow, \downarrow \rangle \sim -\frac{2t^2}{U}. \]

= t

= 1/U

= t
low energy model

energy gain only for antiferromagnetic arrangement

\[
\frac{1}{2} \Gamma \sim (\Delta E_{\uparrow\uparrow} - \Delta E_{\uparrow\downarrow}) = \frac{1}{2} \frac{4t^2}{U}
\]

\[
H_S = \frac{1}{2} \Gamma \sum_{\langle ii' \rangle} \left[ S_i \cdot S_{i'} - \frac{1}{4} n_i n_{i'} \right]
\]
\[
\langle M_z \rangle = -\sigma_m M_0 \cos(q \cdot R_j) = -g\mu_B m \cos(q \cdot R_j)
\]

relation between critical temperature and couplings

\[
k_B T_q = \frac{S(S+1)}{3} \Gamma_q, \quad \Gamma_q = -\sum_{i,j \neq 0} \Gamma_{00,ij} e^{i q \cdot (T_i + R_j)}
\]

\[
\chi_{zz}(q;0) = \frac{C_{1/2}(1 - \sigma_m^2)}{T - (1 - \sigma_m^2)T_q}
\]

divergence at critical temperature

Curie-Weiss susceptibility
$X_0$ term

atomic limit

$$
\chi_{n,n'}(0) = -\beta \delta_{nn'} \delta_{\sigma\sigma'} \frac{1}{4} \left[ \frac{1}{i\nu_n + U/2} + \frac{1}{i\nu_n - U/2} \right] \left[ \frac{1}{i\nu_n + U/2} + \frac{1}{i\nu_n - U/2} \right]
$$

$$
\chi^0_{zz}(0) = \frac{1}{4} (g\mu_B)^2 \sum_{\sigma} \frac{1}{\beta^2} \sum_n \chi_{n,n}(0) = \frac{1}{4} (g\mu_B)^2 \frac{\beta e^{\beta U/2}}{1 + e^{\beta U/2}} \left[ \frac{1}{1 + e^{\beta U/2}} + \frac{1}{U\beta} \left( \frac{1 - e^{-\beta U}}{1 + e^{-\beta U/2}} \right) \right]
$$
\[ \chi_{zz}^0(0) = \frac{1}{4}(g\mu_B)^2 \sum_{\sigma} \frac{1}{\beta^2} \sum_n \chi_{\sigma\sigma}^{n,n}(0) = \frac{1}{4}(g\mu_B)^2 \frac{\beta e^{\beta U/2}}{1 + e^{\beta U/2}} \left[ \frac{1}{1 + e^{\beta U/2}} + \frac{1}{U\beta} \left( \frac{1 - e^{-\beta U}}{1 + e^{-\beta U/2}} \right) \right] \]

large U: weakly temperature dependent

\[ \chi_{zz}^0(0) \sim (g\mu_B)^2 / 4U \]

small \( t/U \) limit?
\( X_0 \) term

in the \( t=0 \) limit

\[
G(i\nu_n) = \frac{1}{i\nu_n + \mu - \Sigma(i\nu_n)}
\]

\[
\Sigma(i\nu_n) = \mu + \frac{U^2}{4} \frac{1}{i\nu_n}
\]

what about the small \( t/U \) limit?

let us consider an approximate form for the self-energy

\[
\Sigma(i\nu_n) = \mu + \frac{r_U U^2}{4} \frac{1}{i\nu_n}
\]
X_0 term

what about the small t/U limit?

\[ \Sigma(i\nu_n) = \mu + \frac{r_U U^2}{4} \frac{1}{i\nu_n} \]

\[ G_k(i\nu_n) = \frac{1}{i\nu_n - \Sigma(i\nu_n) - \varepsilon_k} = \frac{1}{E_k^+ - E_k^-} \left[ \frac{E_k^+}{i\nu_n - E_k^+} - \frac{E_k^-}{i\nu_n - E_k^-} \right] \]
\[ \chi_{zz}^0(q; 0) = (g \mu_B)^2 \frac{1}{4} \sum_{\sigma} \frac{1}{\beta^2} \sum_n \chi_{n,n}(0) \]

\[ = (g \mu_B)^2 \frac{1}{2} \frac{1}{N_k} \sum_{k} \left[ -I_{k,q}^{++} - I_{k,q}^{--} + I_{k,q}^{+-} + I_{k,q}^{-+} \right] \]

“metallic”

“insulating”

\[ I_{k,q}^{\alpha\gamma} = \frac{E_k^\alpha E_{k+q}^\gamma}{(E_k^+ - E_k^-)(E_{k+q}^+ - E_{k+q}^-)} \frac{n(E_k^\alpha) - n(E_{k+q}^\gamma)}{E_k^\alpha - E_{k+q}^\gamma} \]
\[ \chi_0^0(0; 0) \sim (g\mu_B)^2 \frac{1}{4} \frac{1}{N_k} \sum_k \frac{r_U U^2}{[\varepsilon_k^2 + r_U U^2]^{3/2}} \sim (g\mu_B)^2 \frac{1}{4 \sqrt{r_U U}} \left[ 1 - \frac{3}{2} \frac{1}{N_k} \sum_k \frac{\varepsilon_k^2}{r_U U^2} + \ldots \right] \]

at the \( \Gamma \) point

\[ \chi_0(q_C; 0) \sim (g\mu_B)^2 \frac{1}{4 \sqrt{r_U U}} \left[ 1 - \frac{1}{2} \frac{1}{N_k} \sum_k \frac{\varepsilon_k^2}{r_U U^2} \right] \]

at the \( M \) point

in general

\[ \chi_0(q; 0) \sim (g\mu_B)^2 \frac{1}{4 \sqrt{r_U U}} \left[ 1 - \frac{1}{2} \frac{J_0}{\sqrt{r_U U}} - \frac{1}{4} \frac{J_q}{\sqrt{r_U U}} \right] \]

\[ J_q = 2J[\cos q_x + \cos q_y], \quad J \propto t^2 / U \]
**$X_0$ term & the local vertex $\Gamma$**

Use atomic susceptibility as local susceptibility to determine the vertex via the local Bethe-Salpeter equation

\[
\Gamma \sim \left[ \frac{1}{\chi_{zz}^0(0)} - \frac{1}{\chi_{zz}(0)} \right] \sim \frac{1}{(g\mu_B)^2} \left[ 4\sqrt{r_U} U \left( 1 + \frac{1}{2} \frac{J_0}{\sqrt{r_U} U} \right) - 4k_B T \right]
\]

The expected Curie-Weiss behavior

\[
\chi_{zz}(q; 0) = \frac{1}{[\chi_{zz}^0(q; 0)]^{-1} - \Gamma} \sim (g\mu_B)^2 \frac{1}{4k_B T + J_q/4} = \frac{(g\mu_B)^2}{k_B} \frac{1}{4} \frac{1}{T - T_q}
\]
conclusion

strongly-correlated systems: LDA+DMFT method

compare to data: need a response theory

basics of linear-response theory

\[
\chi \tilde{P}_\nu \tilde{O}_\nu' (\mathbf{r}, \mathbf{r}'; t, t') = i \left\langle \Delta \tilde{P}_\nu (\mathbf{r}; t), \Delta \tilde{O}_\nu' (\mathbf{r}'; t') \right\rangle_0 \Theta(t - t').
\]
Bethe-Salpeter equation

\[
\chi_{\alpha\gamma} = \chi_0 \Gamma \chi
\]

local-vertex approximation

local susceptibility: QMC methods

CT-HYB vs HF

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thank you!