Optical conductivity in the dynamical mean-field theory

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Introduction

Definition and general properties of $\sigma(\omega)$

Current $\vec{j}$, electric induction $\vec{D}$ caused by electric field $\vec{E}$ in linear response (plane waves, $q \to 0$; isotropic case, i.e., cubic symmetry):

$$\vec{j}(\omega) = \sigma(\omega)\vec{E}(\omega), \quad \vec{D}(\omega) = \epsilon(\omega)\vec{E}(\omega),$$

with the dielectic "constant" $\epsilon(\omega)$ related to the optical conductivity $\sigma(\omega)$ by $\epsilon(\omega) = 1 + 4\pi i\sigma(\omega)/\omega$.
Experimentally, the optical conductivity can be inferred from measurements of the reflectivity $r(\omega) = |(1-\kappa^2(\omega))/(1+\kappa^2(\omega))|, \kappa(\omega) = \sqrt{\epsilon(\omega)} = n(\omega) + ik(\omega)$ at a range of frequencies and a Kramers-Kronig analysis of $n(\omega), k(\omega)$.

f-sum rule

$$\boxed{\text{full model: } \int_0^\infty d\omega\sigma(\omega) = \frac{1}{4\pi}\int_0^\infty d\omega\omega Im\epsilon(\omega) = \omega_p^2/8\pi = \frac{ne^2}{2m}}$$

In a model calculation with a finite bandwidth, high-energy excitations are excluded $\longrightarrow$ f-sum rule becomes dependent on hopping, interaction and temperature.

$$\text{Hubbard model:} \quad d\int_0^\infty d\omega\sigma(\omega) = -\pi c\,\langle K\rangle \tag{1}$$

Optical conductivity for the Hubbard model

Hamiltonian of the Hubbard model in d dimensions:

$$\begin{aligned}\hat{H} &= -t\sum_{\langle i,j\rangle,\sigma}(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}) + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \\ &= \sum_i\Big(\sum_{l=1}^d \hat{K}_{i,l} + U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\Big); \hat{K}_{i,l} = -t\sum_\sigma(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + h.c.),\end{aligned}$$

where i, j are lattices sites, $i+l$ symbolizes the nearest neighbor of i in l-direction and $\hat{K}_{i,l}$ is a kinetic energy density on site i in direction l.
The current operator $\hat{\vec{j}}$ can be expressed in k-space for the continuum and a Bravais lattice, or in real space for, e.g., a hypercubic lattice:

$$\begin{aligned}\hat{\vec{j}} &= \sum_{\vec{k},\sigma}\vec{v}_{\vec{k}}\,\hat{n}^\sigma_{\vec{k}}, \quad \vec{v}_{\vec{k}} = \nabla_{\vec{k}}\epsilon_{\vec{k}} \\ &= it\sum_{i,l}\hat{j}_{i,l}\,\vec{e}_l, \quad \hat{j}_{i,l} = it\sum_\sigma(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} - h.c.)\end{aligned}$$

Fluctuation-dissipation theorem (dimension d):

$$\begin{aligned}d\sigma(\omega) &= \frac{1}{i(\omega+i\delta)}\frac{1}{N}\langle\langle\hat{\vec{j}},\hat{\vec{j}}\rangle\rangle(\omega+i\delta) \\ &= \frac{1}{i(\omega+i\delta)}\frac{1}{N}\sum_{\vec{k},\vec{k}',\sigma,\sigma'}\vec{v}_{\vec{k}}\cdot\vec{v}_{\vec{k}'}\,\langle\langle\hat{n}_{\vec{k}\sigma}\hat{n}_{\vec{k}'\sigma'}\rangle\rangle(\omega+i\delta) \quad \text{(Bravais lattice)},\end{aligned}$$

Since $\langle\langle\hat{O},\hat{O}'\rangle\rangle(\omega) = \int_{-\infty}^\infty dte^{-i\omega t}\langle e^{i\hat{H}t}\hat{O}e^{-i\hat{H}t}\hat{O}'\rangle$ it follows that $\sigma(\omega) \propto \delta(\omega)$ when $[\hat{H},\hat{n}_{\vec{k}\sigma}] = 0$. Thus

$$\text{for Bravais lattice:} \quad \sigma(\omega) \xrightarrow{U\to 0} \delta(\omega). \tag{2}$$

Derivations of $\sigma(\omega)$ within the DMFT

$d \to \infty$: Γ becomes local $\Rightarrow$ only particle-hole bubble contributes to $\sigma(\omega)$ [1].
For Bravais lattices (Grassman variables ω_n; Green function G):

$$d\sigma(i\nu) = \frac{1}{\nu N\beta}\sum_{\vec{k}\sigma,\omega_n}\vec{v}^2_{\vec{k}}G_{\vec{k}\sigma}(i\omega_n)\,G_{\vec{k}\sigma}(i\omega_n + i\nu) \tag{3}$$

Since G depends on $\vec{k}$ only via $\epsilon_{\vec{k}}$, the k-integral can be replaced by an energy integral. Continuing to the real axis leads to (constant c, fermi function f, $\tilde{\rho}_0(\epsilon) = \frac{1}{N}\sum_{\vec{k}}\vec{v}^2_{\vec{k}}\delta(\epsilon - \epsilon_k)$, $A_\epsilon(\omega) = -1/\pi ImG(\epsilon,\omega)$)[2]

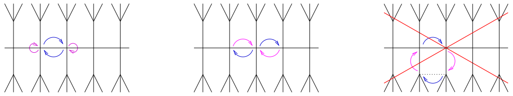
$$d\sigma(\omega) = c\int_{-\infty}^\infty d\epsilon\tilde{\rho}_0(\epsilon)\int_{-\infty}^\infty d\omega' A_\epsilon(\omega')A_\epsilon(\omega'+\omega)\,\frac{f(\omega') - f(\omega'+\omega)}{\omega} \tag{4}$$

Hypercubic lattice

For the hc lattice, $\tilde{\rho}_0(\epsilon) = \langle\vec{v}^2_{\vec{k}}\rangle\rho_0(\epsilon)$ (non-interacting density of states ρ_0). The original proof by Fourier transform and expansion of Bessel functions can be simplified by noting that $\epsilon_{\vec{k}} = \sum_i \epsilon_{k_i} = \epsilon_\parallel + \epsilon_\perp$ for a given direction. In $d \to \infty$, $\epsilon_\parallel \propto 1/d \to 0$, thus $\delta(\epsilon - \epsilon_k)$ can be replaced by $\delta(\epsilon - \epsilon_\perp)$ which leaves the (d-1)-dimensional DOS times $\langle v^2_{k_i}\rangle$ and (in $d = \infty$) reduces to above result.

Bethe lattice

No k-space $\Rightarrow$ real-space picture needed [3]: $\langle\langle\hat{j}_l,\hat{j}_l\rangle\rangle$ ($\hat{j}_l = \sum_i \hat{j}_{i,l}$) consists of terms of the form $\Gamma_{ijkm,\sigma} = \langle\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{k\sigma}\hat{c}^\dagger_{m\sigma}\hat{c}_{j\sigma}\rangle\rangle\delta_{i,k\pm\vec{e}_l}\delta_{m,j\pm\vec{e}_l}$.
Embedding the Bethe lattice locally into a hypercube with same number of nearest neighbors, the current direction can be defined along one row of links which allows to draw diagrams (current operators, connecting propagators):



Concluding that only the left diagram contributes, the conductivity reads:

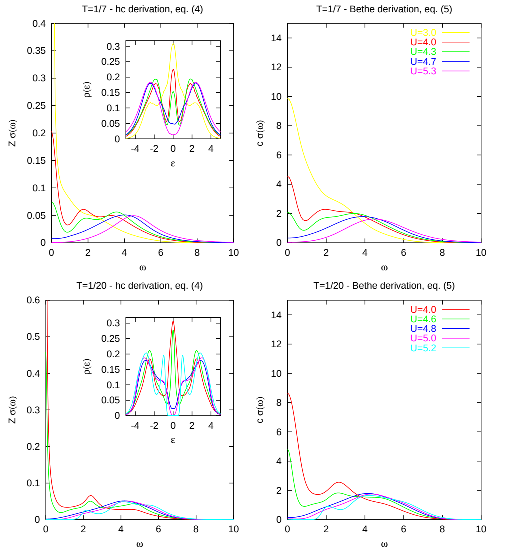
$$\sigma(\omega) = c'\sum_\sigma\int_{-\infty}^\infty d\omega'\rho_A(\omega')\rho_B(\omega'+\omega)\,\frac{f(\omega') - f(\omega'+\omega)}{\omega} \tag{5}$$

Here only interacting DOS enters; equation (2) is not valid. This absence of coherence follows from absence of loops (see right figure).

Generalization to periodically stacked lattices

Within DMFT, adding one more dimension to some given lattice leaves the DOS (and thus all one-particle properties) unchanged, provided that hopping along this new dimension is also scaled as $1/d$. This freedom can be exploited to periodically stack lattices in some current direction c to define a c-axis conductivity.
Connecting all equivalent sites of the stacked planes defines a $k_\parallel$; the c-axis $\sigma(\omega)$ for this case has same form (4) derived for the hc lattice. This justifies using (4) for the Bethe lattice [4].
Connecting the planes only along one perpendicular row leads to eq. (5); the physics is that of an incoherent c-axis conductivity.

Numerical results



Conclusions

- (4) and (5) can be used for arbitrary lattices $\longrightarrow$ (in general) c-axis conductivity (coherent/incoherent).
- (4), applied for other than hc lattice, modifies (1) to $\int\sigma(\omega) \propto \langle K_\parallel\rangle \not\propto \langle K\rangle$.
- Results from (4) and (5) merge at high T, U
- Using (4) with heuristic $\tilde{\rho}$ [5] is unjustified.
- One step towards finite d is using (3) with finite-d $\epsilon_{\vec{k}}$ (cannot include weak localization).

References

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