# LINEAR RESPONSE THEORY VS KUBO–GREENWOOD APPROACHES TO DYNAMICAL CONDUCTIVITY

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Relation between the generalized Linear Response Theory (gLRT) and the Kubo-Greenwood (KG) approaches to complex dynamical conuctivity (CDC) are discussed using the derivation of both with the help of the method of the nonequilibrium statistical operator (NSO) [1–3]. The derivation gives expressions for CDC in terms of complex correlation functions (CCF).

Using Liouville-von Neumann equation with an infinitesimal source for NSO $\hat{\rho}(t)$, it's formal solution in terms of relevant statistical operator $\hat{\rho}_{\rm rel}(t)$, which is is introduced via the principle of maximum information entropy $-{\rm Tr}\{\rho_{\rm rel}(t')\ln(\rho_{\rm rel}(t'))\}$ with the given averages of relevant observables $\hat{P}_n$ expressed in the form of the self-consistency relations,

$$\langle \hat{P}_n \rangle^{t'} \equiv {\rm Tr}\left\{\hat{P}_n \rho(t')\right\} = \langle \hat{P}_n \rangle^{t'}_{\rm rel} \equiv {\rm Tr}\left\{\hat{P}_n \rho_{\rm rel}(t')\right\},$$

the solution for $\rho_{\rm rel}(t)$ in the form of generalized Gibbs ensemble, and the assumption of LRT for small external fields together with different partial integration of CCF and different set of relevant observables, it is shown [4] that both approaches to CDC are formally equivalent one to each other.

The KG expression for CDC is more convenient for numerical calculations and for the separation of intraband and interband contributions to CDC in analytical expressions.

The comparison with the experiments and numerical first-principle simulations have shown that KG approach considering the interband contribution to the dynamical conductivity is necessary to explain the large values of opacities seen in the experiment above the L-edge of the absorption in aluminum.

The gLRT expression for CDC has advantages with respect to the perturbative treatment of interactions when deriving analytic expressions to evaluate CCF and CDC.

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