ChiQ: Momentum-dependent susceptibilities in dynamical mean-field theory

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In the 2017 project supported by the Project for Advancement of Software Usability in Materials Science (PASUMS), we developed an open-source software, `DCore`, which implements the dynamical mean-field theory (DMFT) [1, 2]. DMFT accounts for dynamical correlations arising from strong electron-electron repulsion. Combined with density functional theory (DFT), DMFT yields the electronic structure of strongly correlated materials, which can be compared with angle-resolved photoemission spectroscopy (ARPES) experiments. `DCore` accepts inputs from DFT programs via the Wannier90 format and offers interfaces to various advanced quantum impurity solvers, including quantum Monte Carlo and exact diagonalization methods.

In the subsequent 2024 project, we developed additional features to enhance the applicability of `DCore`, notably the momentum-dependent dynamical susceptibility $\chi(\boldsymbol{q}, i\omega)$. Its dynamical component, $\omega \neq 0$, describes spin excitations that are comparable with inelastic neutron scattering (INS) experiments, while its static component, $\omega = 0$, reflects the tendency toward phase transitions involving magnetic, charge, and orbital ordering. We released an open-source software, `ChiQ` [3], which functions as a post-processing tool for `DCore`.

`ChiQ` provides the following four calculation modes:

- **BSE**: Bethe-Salpeter equation,
- **RPA**: Random phase approximation,
- **RRPA**: Renormalized random phase approximation, and
- **SCL**: Strong-coupling-limit formula.

BSE is the standard approach for calculating the dynamical susceptibility within the DMFT. It requires the computation of the two-particle vertex functions and is therefore computationally costly. The SCL formula, an approximation to BSE, does not require vertex calculations [4, 5] and yields reasonable results in the strong-correlation regime. In the following, we present several examples, which are described in greater detail in the online documentation [6].

Figure 1 shows the static susceptibilities $\chi(\boldsymbol{q}, 0)$ obtained from `ChiQ`. The spin susceptibility exhibits enhancement at the M point, $\boldsymbol{q} = (\pi, \pi) \equiv \boldsymbol{Q}$, indicating the antiferromagnetic fluctuations. Figure 2 shows the temperature dependence of the inverse antiferromagnetic susceptibility, $\chi_{\mathrm{AF}} \equiv \chi(\boldsymbol{Q}, 0)$. The value $1/\chi_{\mathrm{AF}}$ vanishes at $T_{\mathrm{N}} \approx 0.467$, indicating the divergence of χ_{AF}. This allows us to identify the second-order phase transition to an antiferromagnetic state.

It is also possible to estimate the intersite exchange interactions $I(\boldsymbol{r}_{ij})$ in an effective Heisenberg model. $I(\boldsymbol{r}_{ij})$ is evaluated from $\chi(\boldsymbol{q}, 0)$ in the BSE mode, while it is directly computed from the DMFT results in the SCL

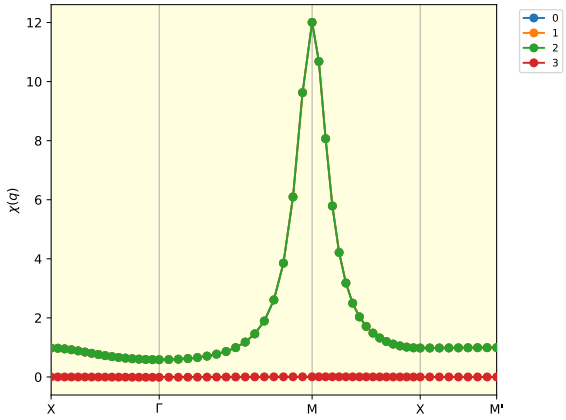

Figure 1: Static susceptibilities $\chi(\boldsymbol{q}, 0)$ for the square-lattice Hubbard model at half filling, calculated using `ChiQ` with the BSE mode. Parameters are $U = 8$ and $T = 0.5$, in units where the nearest-neighbor hopping $t = 1$. The first three modes (labels 0–2) represent spin fluctuations, while the last mode (label 3) represents a charge fluctuation.

mode. Figure 3 presents $I(\boldsymbol{r}_{ij})$ as a function of the distance $\boldsymbol{r}_{ij}$ between two sites, calculated in the BSE mode. The large negative value at $|\boldsymbol{r}_{ij}| = 1$ indicates a strong antiferromagnetic interaction between nearest-neighbor sites. This result converges to the well-known value $-J/2$ with $J = 4t^2/U$ in the strong-coupling limit.

In summary, the open-source software `ChiQ` computes the momentum-dependent susceptibilities $\chi(\boldsymbol{q}, i\omega)$ and the effective interactions $I(\boldsymbol{r}_{ij})$ within the DFT+DMFT framework. The combination `DCore` + `ChiQ` enables the calculation of two-particle responses in realistic materials.

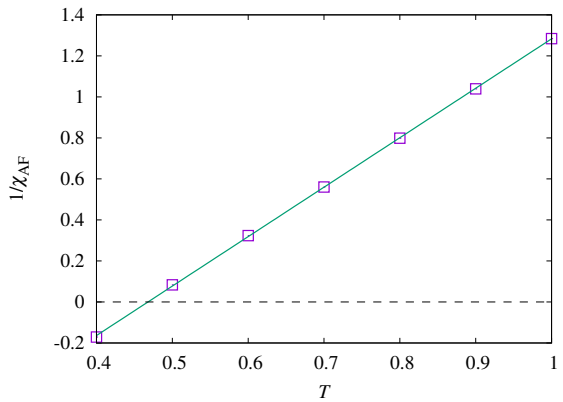

Figure 2: Temperature dependence of the inverse antiferromagnetic susceptibility, $1/\chi_{\mathrm{AF}}$.

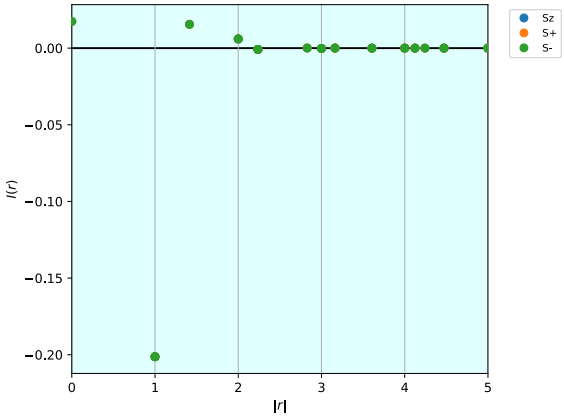

Figure 3: Intersite exchange interactions $I(\boldsymbol{r}_{ij})$ as a function of the distance $\boldsymbol{r}_{ij}$ between two sites. Positive (negative) values indicate ferromagnetic (antiferromagnetic) interactions. The parameters are the same as in Fig. 1. The lattice constant is set to $a = 1$.

References

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[2] `https://github.com/issp-center-dev/DCore`

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