3.6 Software Advancement Projects and Workshop Support

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

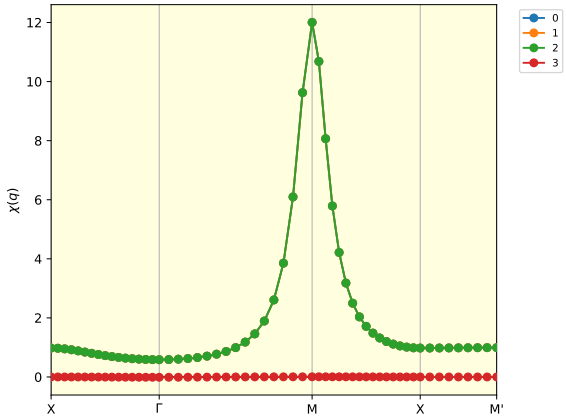

Figure 1: Static susceptibilities $\chi(\boldsymbol{q}, 0)$ for the square-lattice Hubbard model at half filling, calculated using `ChiQ` with the BSE mode. Parameters are $U = 8$ and $T = 0.5$, in units where the nearest-neighbor hopping $t = 1$. The first three modes (labels 0–2) represent spin fluctuations,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

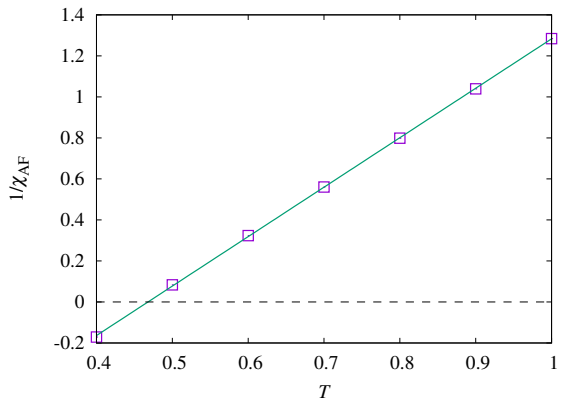

Figure 2: Temperature dependence of the inverse antiferromagnetic susceptibility, $1/\chi_{\mathrm{AF}}$.

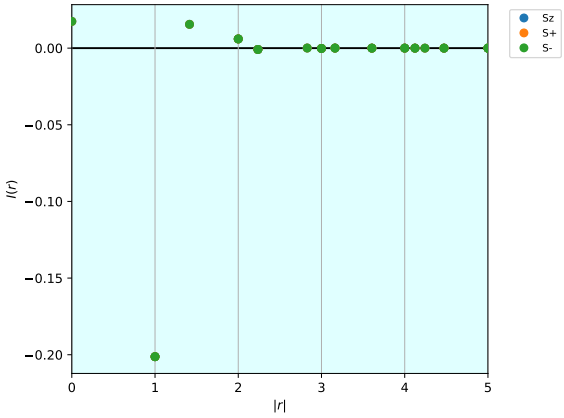

Figure 3: Intersite exchange interactions $I(\boldsymbol{r}_{ij})$ as a function of the distance $\boldsymbol{r}_{ij}$ between two sites. Positive (negative) values indicate ferromagnetic (antiferromagnetic) interactions. The parameters are the same as in Fig. 1. The lattice constant is set to $a = 1$.

References

[1] H. Shinaoka, J. Otsuki, M. Kawamura, N. Takemori, K. Yoshimi, SciPost Phys. **10**, 117 (2021).

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

[3] `https://github.com/issp-center-dev/ChiQ`

[4] J. Otsuki, K. Yoshimi, H. Shinaoka, Y. Nomura, Phys. Rev. B **99**, 165134 (2019).

[5] J. Otsuki, K. Yoshimi, H. Shinaoka, H. O. Jeschke, Phys. Rev. B **110**, 035104 (2024).

[6] `https://issp-center-dev.github.io/ChiQ/`

Report of CCMS hands-on sessions in the 2024 fiscal year

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In the 2024 fiscal year, Center for Computational Materials Science (CCMS) in the Institute for Solid State Physics (ISSP) held 5 hands-on sessions where the ISSP supercomputer was used [1-4]. In this report, we briefly summarize them.

Table 1 shows the list of the hands-on sessions in the 2024 fiscal year. There are 5 hands-on sessions were held. In the last hands-on session, we introduced 5 software related to the *ab initio* downfolding method: Quantum ESPRESSO, RESPACK, H-wave, HΦ and mVMC. Development of the software except for ALAMODE and Quantum ESPRESSO was supported by "Project for advancement of software usability in materials science" (PASUMS) [6].

Features of each software are as follows. ALAMODE is open-source software for calculating phonon properties such as harmonic/anharmonic force constants and lattice thermal conductivity [7]. moller is a tool for generating a job script for performing high-throughput calculations [8]. abICS is open-source software for performing configurational sampling in disordered systems such as alloys [9]. 2DMAT is a software package to search optimal results of given optimization problems by using search algorithms combined with direct-problem solvers [10]. Quantum ESPRESSO is a software package for *ab initio* calculations based on the pseudo potential method using the plane-wave basis [11]. RESPACK is open-source software for the *ab initio* downfolding method [12]. H-wave, HΦ and mVMC are software for analyzing quantum many-body systems using the mean-field approximation, exact diagonalization methods, and the variational Monte Carlo method, respectively [13-15].

Table 1: List of CCMS hands-on sessions where the ISSP supercomputer was used in the 2024 fiscal year.

Date	Lecturer	Software	# of applicants
Aug. 5	T. Tadano et al.	ALAMODE [7]	30
Oct. 18	T. Aoyama et al.	moller[8]	20
Nov. 7	S. Kasamatsu et al.	abICS[9]	14
Dec. 2	T. Hoshi et al.	2DMAT[10]	26
Feb. 6-7	T. Koretsune, T. Misawa et al.	Quantum ESPRESSO [11], RESPACK [12], H-wave [13], HΦ[14], mVMC [15]	28

In all of the hands-on sessions, lecturers explained the basics of each software and gave its tutorial. Materials of some hands-on sessions are available on each official page.

References

[1] https://ccms.issp.u-tokyo.ac.jp/event/6904
[2] https://ccms.issp.u-tokyo.ac.jp/event/6947
[3] https://ccms.issp.u-tokyo.ac.jp/event/6980
[4] https://ccms.issp.u-tokyo.ac.jp/event/7002
[5] https://ccms.issp.u-tokyo.ac.jp/event/7027
[6] https://www.pasums.issp.u-tokyo.ac.jp/en/
[7] http://ttadano.github.io/alamode/
[8] https://www.pasums.issp.u-tokyo.ac.jp/htp-tools/en/
[9] https://www.pasums.issp.u-tokyo.ac.jp/abics/en/
[10] https://www.pasums.issp.u-tokyo.ac.jp/2dmat/en/
[11] https://www.quantum-espresso.org
[12] https://sites.google.com/view/kazuma7k6r
[13] https://www.pasums.issp.u-tokyo.ac.jp/h-wave/en/
[14] https://www.pasums.issp.u-tokyo.ac.jp/hphi/en/
[15] https://www.pasums.issp.u-tokyo.ac.jp/mvmc/en/

Supercomputer course of Computational Materials Design (CMD®) workshop

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The 45th Computational Materials Design (CMD®) workshop (CMD45) was held from September 1st to September 5th, and the 46th CMD® workshop (CMD46) took place from February 17th to February 21st. Both were held online. In this workshop, we offer the supercomputer course to train human resources for advancing research using the System B supercomputer at the Institute for Solid State Physics (ISSP), the University of Tokyo.

In CMD45, three participants took the supercomputer course and followed a tutorial on STATE-Senri developed by Y. Morikawa. After an introductory lecture on large-scale computing and an explanation of how to use the supercomputer of ISSP by M. Geshi, the participants started constructing computational models for their own research subjects with the help of the lecturers. Then they carried out calculations using supercomputers. Specific themes included molecular adsorption and reactions on solid surfaces, atom doping bulk Si, and materials desing using generative models. The participants performed calculations and examined their results.

In CMD46, two participants took the supercomputer course and used the supercomputer of ISSP. They got a tutorial on RSPACE developed by T. Ono. After giving the introductory lecture of large-scale computing by M. Geshi and introducing the calculation method of electronic structures and electron-transport property using RSPACE by T. Ono, Y. Egami, and M. Uemoto, the exercises instructed in the textbook were carried out. Then, electronic structure calculations were carried out for various molecules, and the electronic density distribution was visualized. The attendees also performed massively parallel calculations to confirm the efficiency for parallel computing. Finally, the electronic structures of the bulks and interfaces were investigated using large scale models.