O.36 Absorption spectrum calculations using cumulant expansion in electron-phonon interactions

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I implemented the cumulant expansion of the electron phonon interaction in the eph driver of abinit. After the calculation of the Migdal self-energy and the creation of SIGEPH.nc file, one can set the variable tolcum to activate the calculation. This is a post-processing step which reads the SIGEPH.nc file and outputs a CUMULANT.nc file containing the electronic absorption spectrum within the cumulant expansion. The implemented equations can be found in Ref. 1, more specifically eqs. (18-22). With help of Matteo Giantomassi, MPI-parallelism (over k, q, and bands) can be used to speed up the calculations. The spectral function can then also be used to determine electronic mobilities using the Kubo formalism, eq. (3) of Ref. 2, which is being implemented.

Why the implementation of the cumulant expansion? The effect of the phonons on the electronic properties can be very strong, not only at 0K in the renormalization of the band gap [4], but also at higher temperatures e.g. in limiting electronic mobilities [2]. In these cases it is essential to go beyond the description of electron-phonon interactions determined by Dyson-Migdal theory [3], which is currently implemented in abinit. This means that we need to include higher order electron-phonon interactions and to do that we use the cumulant expansion approach originally studied by Kubo [5]. Several successful results for binding energies of polarons [1], number of satellites [6] and electronic mobilities [2] have appeared in the recent literature using the cumulant expansion.

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[1] J. P. Nery, P. B. Allen, G. Antonius, A. Miglio, X. Gonze, Physical Review B 97, 115145 (2018)

[2] J.-J. Zhou, M. Bernardi, Physical Review Research 1, 033138 (2019)

[3] A.B. Migdal, Soviet Physics JETP 34, 996 (1958)

[4] S. Poncé; Y. Giillet, J. Laflamme Janssens, A. Marini, M. Verstraete, X. Gonze, The Journal of Chemical Physics 143, 102813 (2015)

[5] R. Kubo, Journal of the Physical Society of Japan 17, 1100 (1962)

[6] C. Verdi, F. Caruso, F. Giustino, Nature Communications 8, 15769 (2017)