Report on "Kernel Polynomial Method for Linear Spin Wave Theory"

March 20, 2024

Dear Editor,

The authors describe a method of calculating spin wave spectra for Inelastic neutron scattering experiments, especially designed for large systems and unit cells and where explicit diagonalization is not needed. This paper is very well written, clear and well documented. I would definitely recommend its publication. Below are my comments:

- In addition to Ref [21-25], the authors may want to cite SpinWave, a software dedicated to spin wave simulations, S. Petit and F. Damay, Neutron News, Volume 27, Issue 4 (pp 27-28) (2016).

- Eq. 23 is quite complicated as arguments of Heaviside and Dirac functions are matrices (if I understand correctly). This could be pointed out in the text, for the sake of clarity.

- Eq. 25 - 27 are quite confusing, mixing properties of $C_{\omega'}$, with those imposed on $G(\omega, \omega')$. It also seems that the integration over ω' has vanished in obtaining Eq. 26. Why should $\theta(x)$ mask negative values of x since $C(\omega)$ already does ? This part is definitely not very clear to me. Some additional explanations are needed welcome.

- Eq. 29 is also quite complicated, especially because the method needs a proper value of γ, which is, seemingly, obtained from much more complex methods. It is difficult to figure out wheter this part makes the method much more complex or not, for anybody who would like to implement it. Could the authors comment about this ?

- The authors explain that the KPM method becomes more efficient than conventional LSWT for system size above ~ 200 (Figure 6). It seems this corresponds to quite large systems, with very likely complicated magnetic structures. I thus have two questions : given these larges unit cells, does it remain possible to fit the exchanges couplings ? Furthermore, what about the mean field step inherent to SW based methods. Is it reasonable for such sizes ? Does it still converge properly ?