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Improved Maximum Entropy Method applied to Real-time Time-Dependent Density Functional Theory

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Abstract content
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Time-dependent density functional theory (TDDFT) is a powerful tool for analyzing optical properties of medium-to-large sized molecule. We employ a real-time and real-space technique to solve the time-dependent Kohn-Sham equations. In our procedure to calculate optical properties, we use the time-series data, namely the dynamic dipole moment, from whose Fourier transform (FT) optical properties are calculated in a usual technique. The spectral resolution depends on the length of the dipole moment. To obtain the good resolution, the computational cost is quite expensive.

To solve this difficulty, we apply Maximum entropy method (MEM) to the spectral analysis of time-dependent dipole moments of molecules. As a new improved MEM, we proposed to use the concatenated data set made from several-times repeated raw data together with the phase to avoid the side effect of the artificial periodicity. With this improvement, we have successively obtained the much better spectral resolution of the target peak. In the analysis of optical properties, we are interested in the lower energy peak, corresponding to the band gap area. Basically, to obtain the high resolution of spectrum, MEM requires less number of time steps compared to that of FT, and it is widely used for the analysis of the natural phenomenon of the long period such as seismic waves and solar cycles, obtaining a fairly good resolution and accuracy even with a short time series data. Thus, this improvement will make a further advantage of MEM.

We applied this technique to the spectral analysis of the TDDFT dipole moment of typical some molecules such as oligo-fluorene, benzene and other materials. The results show the higher resolution and the emphasized peak near the band gap without being affected by the artificial periodicity. The characteristic features of this technique will be presented including the further possibilities of improvements.

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