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Maximum Entropy Method applied to Real-time Time-Dependent Density Functional Theory[1] YASUNARI ZEMPO, MITSUKI TOOGOSHI, SATORU S. KANO, Hosei University — Maximum Entropy Method (MEM) is widely used for the analysis of a time-series data such as an earthquake, which has fairly long-periodicity but short observable data. We have examined MEM to apply to the optical analysis of the time-series data from the real-time TDDFT. In the analysis, usually Fourier Transform (FT) is used, and we have to pay our attention to the lower energy part such as the band gap, which requires the long time evolution. The computational cost naturally becomes quite expensive. Since MEM is based on the autocorrelation of the signal, in which the periodicity can be described as the difference of time-lags, its value in the lower energy naturally gets small compared to that in the higher energy. To improve the difficulty, our MEM has the two features: the raw data is repeated it many times and concatenated, which provides the lower energy resolution in high resolution; together with the repeated data, an appropriate phase for the target frequency is introduced to reduce the side effect of the artificial periodicity. We have compared our improved MEM and FT spectrum using small-to-medium size molecules. We can see the clear spectrum of MEM, compared to that of FT. Our new technique provides higher resolution in fewer steps, compared to that of FT.

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