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1 introduction

Study about electron and nuclear flux correlation in LiF excited state molecule.

2 Total flux

2.1 Data

~/calc/LiF/enbranch/accD_sa_6_9_part2/cov_diss_p18
electronic state : CASSCF(6,9)
p=18 at crossing point. r=7 at t=0.0.

2.2 probability

Seeing time dependency of probability, fast probability change occurs at t=60 fs.

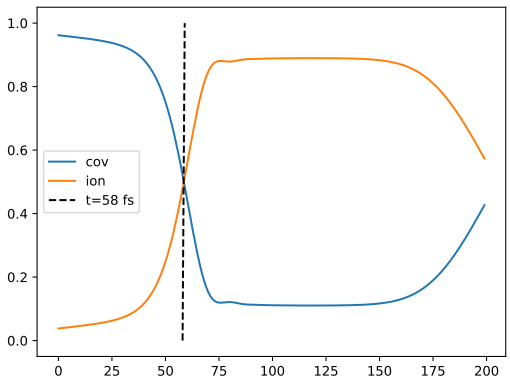
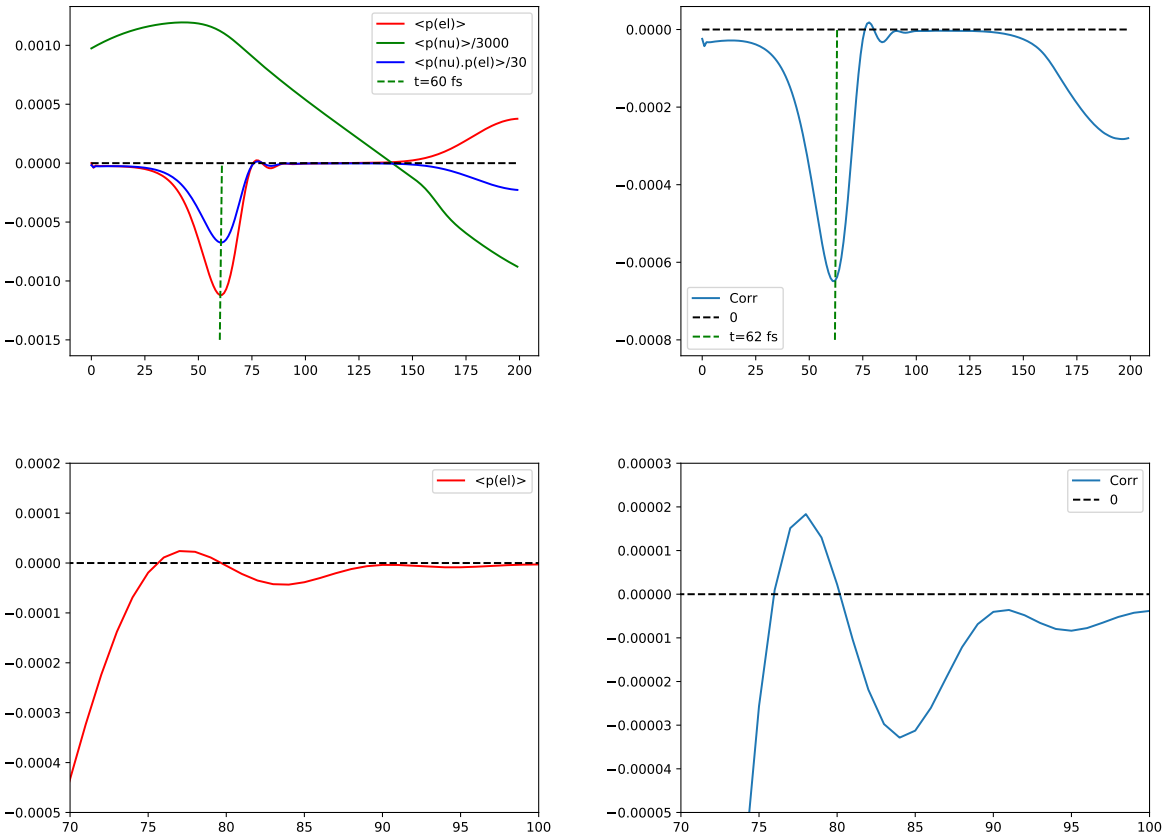


図 1 prob

2.3 electron and nuclear flux

integration of flux density is equal to expectation value of velocity. so, first we consider the momentum expectation value for each time.



Left figure show the expectation value of electron momentum and nuclear momentum. large peak of electron momentum at t=60 fs means charge transfer of LiF$-$ $>$ $Li^{+}F^{-}$. Nuclear momentum have peak at t=50 fs. The accesalation at of nuclear momentum is come from shallow slope of covalent electronic state. Decreasing of nuclear momentum after t=50 fs is come from repulsive potential curve of ionic electronic state.

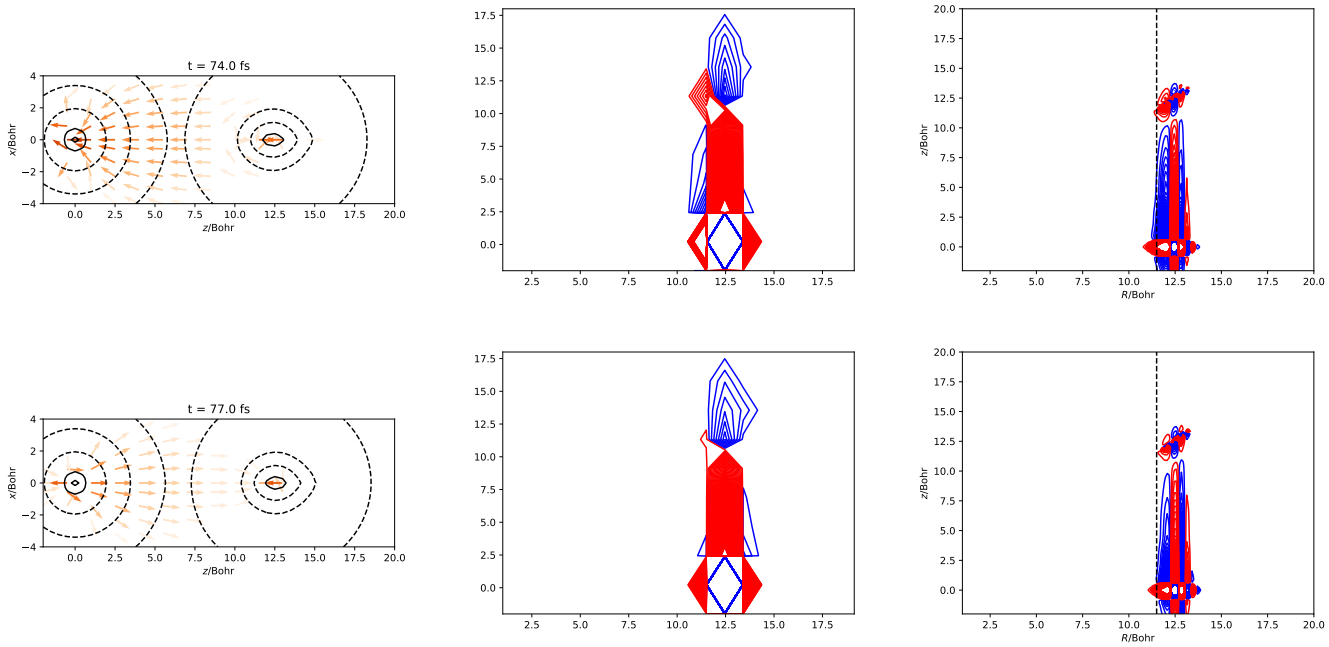
In electronic momentum, there is small oscillation after large peak at t=60 fs. Especially, at t=75 fs momentum expectation value become positive. We do not have proper interpretation for this phenomena now.

Correlation function have also small oscillation after big peak induced by charge transfer. This oscillation is also obserbed at probability.

2.4 total flux-flux correlation

Next, we concentrate on flux-flux density correlation function.

At t=74.0 fs, electron flux is transfered from Li to F. However, at t=77.0 fs, electron flux is directed inverse. Electron flux nuclear flux correlation function does not change significantly in this time interval.



The flux flux correlation function have oscillation structure to R direction. This "interference" like strucure is also obserbed in time-dependent Dyson orbital.

Calcualtion may be incorrect. Electron flux density and electron component of electron nuclear flux density are not matched at all.

There are two questions. 1. why flux-flux correlation function does not change? 2. why flux-flux correlation function have "interference" structure?

2.5 phase of coefficient

`calculate width, center and momentum of nuclear wave packet.`