

| | Shankar's (lindbladInit) | Mine (lindbladInit_for-DMD-4.4) |
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| Output data files (required by later real-time dynamics) | A single file ldbd.dat | Multi files in the folder ./ldbd_data, each storing one kind of quantity (additionally ImSigma_ePh and eigenvectors for electron-impurity and electron-electron scatterings) |
| Output electron- phonon quantities | $G^- = g^- \sqrt{\delta}$ stored in sparse form | <p>E-ph-related matrices for both Lindblad and conventional equation. For Lindblad,</p> $P_{1234}^I = \sum_{\pm\lambda} G_{13}^{\pm} G_{24}^{\pm,*} n^{\pm}$ $P_{1234}^{II} = \sum_{\pm\lambda} G_{31}^{\pm} G_{42}^{\pm,*} n^{\mp}$ <p>For conventional,</p> $P_{1234}^I = \sum_{\pm\lambda} g_{13}^{\pm} g_{24}^{\pm,*} n^{\pm}$ $P_{1234}^{II} = \sum_{\pm\lambda} g_{31}^{\pm} g_{42}^{\pm,*} n^{\mp}$ $G = g\delta$ <p>of a k pair (ik,jk) with ik <= jk ($P^{I,kk'} = P^{II,k'k,*}$ and $P^{II,kk'} = P^{I,k'k,*}$) in dense form.</p> <p>Due to the difference of output e-ph quantities, energy conservation for k pair selection is not the same</p> |
| Information in std::out | | Spin-relaxation time calculated using P? matrices and G matrices with different kind of smearings (constant or ImSigma_ePh) |
| Energy ranges | Two – one for probe ; one for pump and e-ph for both conduction and valance bands | Three – for probe ; for pump ; for e-ph, if ePhOnlyElec (ePhOnlyHole) = 1, only e-ph of conduction (valence) bands will be written down; Parameter nkBT is added to control energy range, default 7, 7 is enough for real-time but may not be for rate formula |
| Energy conservation range | nEphDelta = 5 | nEphDelta is an input parameter. This is important for (i) electron-electron scattering (ii) spin lifetime computations inside the code, since different smearings (e.g., max of ImSigm_ePh can be much larger than ePhDelta) will be used |

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| VBM & CBM determination | | In case VBM is not zero (metal, Fermi smearing or finite electric field), parameter band_skipped , starting band index of wannier relative to DFT, can be used to determine VBM and CBM correctly |
| k-point selection | | In 3D cases, there can be too many k points. To speed up eLoop, we need temporally turn off spin and velocity matrices computations. This is achieved by introducing <code>eEneOnly</code> in FeynWann (see <code>if (eEneOnly) return;</code> in <code>setState</code> in FeynWann.cpp) |
| Parallel for e-ph | K points | K pairs |
| E-ph matrix elements computation | Use ePhLoop with mask (whether satisfying energy conservation) | <p>Firstly, run eCalc at all selected k points in parallel (and use bcastState_inEphLoop to collect them) and store electronic states in <code>std::vector<FeynWann::StateE> state_elec;</code></p> <p>Secondly, use <code>ePhCalc</code> for each k pair with stored <code>FeynWann::StateE state_elec[ik]</code> and <code>state_elec[jk]</code>.</p> <p>In some cases, compute1 is slow, e.g., GaN, it is very helpful to run eCalc only once and reuse them in e-ph computations. Otherwise, compute1 must be run for each k pair instead of for each k point</p> <p>My code is however not suitable to the cases where most k points are selected (e.g., iron) or there are more than 10,000 k points so that <code>state_elec</code> will take too huge memory</p> |