Density Matrix Dynamics
User Manual

Junqing Xu, Kejun Li, Yuan Ping

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1 Introduction

DMD is a first-principles real time density matrix dynamics code. It uses wannierized ground state electronic structure calculated at the density funcional theory (DFT) level along with various scattering interactions and coherent contributions. Currently, DMD only interfaces with JDFTx, a general purpose DFT code and relies on an intermediate brigding code, FeynWann, for inialization and intermemdiate calculations of the scattering processes.

2 Installation

Create build directory at the same level as `src` directory in the main DMD directory. Change `make.inc` to point to dependencies according to your specific system ennvironment.

1. Make sure intel mpi compiler and command `mpiicpc` or its equivalent exist.
2. GSL and MKL must be installed and ensure `MKLROOT` points to correct location.
3. Modify `GRL_DIR` in `make.inc` and `SRC_DIRS` in `Makefile`, if necessary.
4. If there is no "build" directory, make it.
5. Issue `make` command in the main directory.

3 DMD Input

DMD parses input commands from a simple text file with one command per line, first entry is the command key and the second is command value, if any.

3.1 DMD Commands

Table 1: Parameters in DMD input param.in for task control and algorithms.

parameter	input	meaning
restart	1 (default) or 0	If 1, start from scratch; else if 0, restart.
alg_scatt	lindblad (default) or conventional	It determines the form of the scattering term of the master equation.

alg_eph_sepr_eh, alg_eph_need_elec, alg_eph_need_hole	1 or 0	If alg_eph_sepr_eh = 0, electron and hole will be calculated together. If alg_eph_sepr_eh = 1, electron and hole will be calculated separately. Then, if "ePhOnlyElec 1" is in lindbladInit.in, set alg_eph_need_elec = 1 and alg_eph_need_hole = 0. If "ePhOnlyHole 1" is in lindbladInit.in, set alg_eph_need_elec = 0 and alg_eph_need_hole = 1.
alg_sparseP	1 or 0 (default)	If 1, the code will convert the generalized scattering-rate matrix P to a sparse matrix. If 0, matrix P is kept dense. Search for "ns_tot" in output to see how many elements of P_i matrices are larger than several thresholds (default 1e-40) generally, larger energy range and smaller smearing make P_i more sparse.
alg_phenom_relax	1 or 0 (default)	If 1, phenomenon relaxation $\dot{\rho} = -(\rho - \rho_{\mathrm{eq}})/\tau_{\mathrm{phenom}}$ will be turned on. If 0, it will be turned off.
alg_phenom_recomb	bool (default 0)	If 1, phenomenonlogical recombination to represent spontaneous emission will be turned on.
tau_phenom_recomb	float (default 10^{15} ps)	Phenomenonlogical recombination time in pico seconds.
Bxpert, Bypert, Bzpert	a number, e.g. 0.0 (default)	Magnetic field perturbation, one of the mothods that perturbs a system to generate spin unbalance, in the unit of Tesla. x, y and z are cartesian coordinates consistent to input cell parameters.

pumpMode	coherent or lindblad or perturb	Perturbation by pumping, the other method that is used to perturb a system to generate spin unbalance. The pump pulse is Gaussian. coherent : real-time pump using coherent formula $-i[\mathrm{P}(t), \rho]$. lindblad : real-time pump using lindblad formula. perturb : generate an initial pump perturbation.
pumpA0	a number, e.g. 0.0	Pump amplitude, pump power = (pumpE * pumpA0)^2 / $(8\pi\alpha)$
pumpPoltype	LC or RC or Ex or Ey	Pump polarization type.
pumpE	a number, e.g. 0.1	Pump energy in eV.
pumpTau	a number, e.g. 50	Pump pulse width in the unit of fs. This introduces a weight function $\exp(-t^2/2\tau^2)/\sqrt{\sqrt{\pi} * \tau}$ into pump amplitude
probePoltype1	LC or RC or Ex or Ey	The first probe polarization type.
probePoltype$i$	LC or RC or Ex or Ey	The i-th probe polarization type.
probeEmin, probeEmax	a number	These parameters specify the probe energy range in the unit of eV.
probeDE	a number, e.g. 0.01	Probe energy step in the unit of eV.
probeTau	a number, e.g. 2000	Probe pulse width in unit the unit of fs.
t0	a number, e.g. 0 (default)	The initial time of spin dynamics in the unit of fs.
tend	a number, e.g. 1e6	The end time of spin dynamics for reporting in the unit of fs. This number needs to be larger at lower temperature because spin dynamics is slower at lower temperature. 1e6 is used for T=4K.

tstep	a number, e.g. 1e3	Time step in the unit of fs.
tstep_pump	a float	Time step for reporting during pump (pump time center ±6*pumpTau), in the unit of fs.
freq_measure_ene	a integer	This parameter specifies how often to print energy-resolved observables.
temperature	a number, e.g. 300	Temperature at which calculation is done. Currently, it is actually directly read from the output of the initialization calculation, so that it is not necessary to set temperature.
mu	a number, e.g. 0.5	Chemical potential in the unit of eV, usually relative to VBM, must be in range [dmuMin, dmuMax] in initialization
carrier_density	a number, e.g. 1e18	Carrier density in the unit of cm^{-d}, where d (3,2,1,0) is the dimension of the material. Positive means electron density and negative means hole density. It can be referred to and smaller than the carrier density in the lindblad initialization output lindbladInit.out. When this parameter is used, mu is ignored.
tau_phenom	float	Phenomenon relaxation time in the unit of ps.
scrMode	medium or none (default)	"none" means no screening will be computed. "medium" means the dielectric function = interband dielectric constant * intraband dielectric function. interband one must be provided by epsilon_background. intraband one will be computed by the program.

epsilon_background	a number, e.g. 30	static dielectric constant ε_0.
eeMode	Pee_update or Pee_fixed_at_eq	The electron-electron scattering matrix P depends on the density matrix ρ. There are options of updating the scattering matrix P^{e-e} (Pee_update) and fixing the matrix (Pee_fixed_at_eq) during spin dynamics.
freq_update_ee_model	integer	This parameter controls how often P^{e-e} is updating duing spin dynamics. If <= 0, P^{e-e} is updated every step.
alg_eph_enable	1 (default) or 0	If 1, enable the electron-phonon scattering. If 0, diable electron-phonon scattering.
alg_only_eimp	1 or 0 (default)	If 1, only consider the electron-impurity scattering. If 0, consider the scattering processes other than electron-impurity.
impMode	ab_neutral or model_ionized	Currently, the electron-impurity scattering by neutral defects is computed by supercell method at DFT, and that by charge defects is computed by a charge defect model. If ab_neutral, electron-impurity scattering considers short-range interaction due to neutral defects. If model_ionized, the scattering considers long-range interaction due to charge defects.
impurity_density	a number, e.g. 1e18	Impurity density in the unit of cm^{-d}, where d (3,2,1,0) is the dimension of the material.