LEO2D: Draft of Input Documentation

Stephen Carr

October 11, 2017

1 System Settings

These commands define the physical structure of the system, like the number, type, and positions of each 2D layered material. Usually this commands are at the head of the input file, as some commands rely upon these to allocate memory for the input reading.

- **JOB_NAME**: (String, default = "LEO2D_JOB") Sets the name of the job, will be the prefix for most output files
- **MAXSIZE**: (Integer) Determines the maximum grid value for any layer in this calculation. Each layer will run from $\{\text{MINSIZE}, \text{MINSIZE}\}$ to $\{\text{MAXSIZE}, \text{MAXSIZE}\}$, and no unit-cells will be populated past those values.
- **MINSIZE**: (Integer) Determines the minimum grid value for any layer in this calculation. Each layer will run from $\{\text{MINSIZE}, \text{MINSIZE}\}$ to $\{\text{MAXSIZE}, \text{MAXSIZE}\}$, and no unit-cells will be populated past those values.
- **BOUNDARY_CONDITION**: (Integer, default = 0) Can be either 0 (for a finite system) or 1 (for a periodic system). If 1 is chosen, a super-cell needs to be defined in someway.
- **NUM_SHEETS**: (Integer, default = 1) Number of 2D layers in the heterostructure calculation, each one must be defined individually via START_SHEET declarations.

1.1 Defining a 2D layer

- **START_SHEET**: (Integer) Does not use an equal sign, instead one simply writes "START_SHEET X", where X is an integer between 1 and NUM_SHEETS. The program will read the lines between "START_SHEET X" and "END_SHEET X" to define layer X.
- **END_SHEET**: (Integer) Does not use an equal sign, instead one simply writes "END_SHEET X", where X is an integer between 1 and NUM_SHEETS. The program will read the lines between "START_SHEET X" and "END_SHEET X" to define layer X.
- **MATERIAL**: (String) One of the supported material types in the LEO2D Material Database. Can be "Grapehene", "StrainedGraphene", "MoS2", "MoSe2", "WS2", "WSe2"
- **HEIGHT**: (Double) Vertical position in Angstroms from the calculation's origin. For example, if this sheet is supposed to be at 3.4 Angstroms, you would write "HEIGHT = 3.4"
- **ANGLE**: (Double) Angle of this sheet with respect to the x-axis in degrees. The code uses counterclockwise convention, so "ANGLE = 5" would rotate the layer 5° counterclockwise when viewed from the positive z-axis.

1.2 Supercells

- **SUPERCELL_M_N**: (Integer Integer) Makes a twisted bilayer supercell, using the M,N formalism. Takes two integers, the first is M, the second is N
- **SUPERCELL_GRID**: (Integer Integer) Makes a supercell that is equal to X*Y unit-cells, where X is the first integer and Y is the second.

2 Solver Settings

- **NSHIFTS**: (Integer, default = 1) Number of shifts for a configuration sampling solver. This usually creates NSHIFTS*NSHIFTS jobs, but for some solvers it makes only NSHIFTS jobs.
- **ENERGY_RESCALE**: (Double, default = 20.0) A rescaling parameter for the Hamiltonian. Along with ENERGY_SHIFT, use these options to ensure that the Hamiltonian's spectrum lies in [-1, 1] for KPM solvers.
- **ENERGY_SHIFT**: (Double, default = 0.0) A shifting parameter for the Hamiltonian. Along with ENERGY_RESCALE, use these options to ensure that the Hamiltonian's spectrum lies in [-1, 1] for KPM solvers.
- **POLY_ORDER**: (Integer, default = 20) How many terms to use in a KPM polynomial expansion for any solver. Has to be a multiple of 4.
- **USE_B_FIELD**: (Integer, default = 0) Determines if B field is used. Set equal to 0 for no field, and 1 for a field.
- **B_FIELD**: (Double, default = 0.0) Magnitude in Z direction of magnetic field.
- **USE_E_FIELD**: (Integer, default = 0) Determines if E field is used. Set equal to 0 for no field, and 1 for a field.
- **E_FIELD**: (Double, default = 0.0) Magnitude in Z direction of electric field.
- **VACANCY_FILE**: (String) Filename for vacancy data.
- **VACANCY_CHANCE**: (Double) Chance for a random vacancy (I think this is depreciated and currently has no effect on any calculation).
- **NUM_TARGET_SHEETS**: (Integer, default = 1) Number of sheets for which we want to compute the local operator on via the KPM.
- **TARGET_SHEETS**: (List of NUM_TARGET_SHEETS Integers) List of target sheets.
- **NUM_SHIFT_SHEETS**: (Integer, default = 1) Number of sheets for which we want to shift for a configuration-sampling run.
- **SHIFT_SHEETS**: (List of NUM_SHIFT_SHEETS Integers) List of shift sheets.
- **SOLVER_TYPE**: (String, default = "SQ") Can take "SQ" (Square), "LC" (Linecut), "MLMC_VAC" (MLMC Vacancy Defects), "VD_FILE" (Vacancy Defects from File), or "STRAIN" (Custom sampling for strained systems)
- **NUM_LC_POINTS, default = 2**: (Integer) Number of points to include in a linecut (LC) job.
- **LC_POINTS**: (List of NUM_LC_POINTS*2 Doubles, default = 0.0 0.0 1.0 1.0) Linecut points for a linecut job.
- **OBSERVABLE_TYPE**: (String, default = "DOS") Type of Observable to compute. Can be either "DOS" (Density of States) or "COND" (Conductivity).
- **DOS_TRANSFORM**: (Integer, default = 1) Determines if the Density of States computed via the KPM should be converted to energy domain and saved (DOS_TRANSFORM = 1), or if the raw Chebyshev coefficients should be saved (DOS_TRANSFORM = 0).
- **SOLVER_SPACE**: (String, default = "R") Determines space in which the Hamiltonian will be populated. Can take either "REALSPACE" (or any String starting with "R") or "MOMENTUM" (or any String starting with "M").
- **STRAIN_FILE, default = "NONE"**: (String) Input file which contains strain information. The file must exist in the same directory as where the system was called, or in a subdirectory by using e.g. "STRAIN_FILE = subfolder/filename.dat".

- **STRAIN_TYPE**: (String) Determines what kind of strain should be applied to the system, has 5 options:
  - **NONE**: (string starting with "N") No strain type. No strain will be applied to any layer.
  - **SUPERCELL**: (string starting with "S") Supercell strain type. The displacement of each orbital will be determined by its position within the supercell, however that is defined.
  - **CONFIGURATION**: (string starting with "C") Configuration strain type. The displacement of each orbital will be determined by its configuration position relative to the other layer (only implemeneted for bilayer systems!).
  - **REALSPACE**: (string starting with "R") Realspace strain type. The displacement of each orbital will be determined by from only its (x, y, z) position.
  - **FILE**: (string starting with "F") Atomic positions will be directly loaded from a file. The file contains all grid and atom positions (not used very much, might be buggy now!).
- **STRAIN_LAMBDA**: (Double) Sets wavelength of a realspace Strain that is implemented directly (i.e. not from a strain file).

2.1 Debug Options

- **MATRIX_SAVE**: (Integer, default = 0) Set to "1" to save a copy of the Hamiltonian to disk (JOB_NAME_matrix.dat).
- **MATRIX_POS_SAVE**: (Integer, default = 0) Set to "1" to save positions of all orbitals in the calculation to disk.
- **VERBOSE_SAVE**: (Integer, default = 1) Set to "1" to save additional header information for each line in the output file "JOB_NAME.cheb"

2.2 K-point sampling

- **K_SAMPLING**: (Integer, default = 0) Set to "1" to turn on K-point sampling methods for supercells.
- **K_TYPE**: (Integer, default = 0) Set to "0" for a grid sampling (defined by K_GRID), or set to "1" for a linecut sample (hard-coded to go through a few high-symmetry points of the supercell).
- **K_GRID**: (Pair of Integers) Defines the two grid dimensions of the K-sampling grid over the supercell Brillouin zone if K_TYPE = 0.

2.3 Direct Diagonalization

- **DIAGONALIZE**: (Integer, default = 0) Determines if Hamiltonian is diagonalized. Can be either "0" (for non-diagonalization, i.e. KPM, methods) or "1" for direct eigensolver methods.
- **D_WEIGHTS**: (Integer, default = 0) Determines if local weights (on target orbitals) are computed for each eigenvector. Can be either "0" for off or "1" for on.
- **D_VECS**: (Integer, default = 0) Determines if all eigenvectors are computed and saved. Can be either "0" for off or "1" for on.
- **D_COND**: (Integer, default = 0) Determines if the two-point current-current correlation measure is calculated. Can be either "0" for off or "1" for on.
- **CHIRAL_ON**: (Integer, default = 0) Determines if local weights (on target orbitals) are computed for each eigenvector. Can be either "0" for off or "1" for on.

2.4 MLMC Options

- **MLMC**: (Integer, default = 0) Can be "0" for no MLMC jobs, or "1" for a MLMC job. Note that MLMC jobs require additional folder structure (output and temporary folders) and saved results for previous jobs.
- **MLMC_MAX_LEVEL**: (Integer, default = 1) Maximum number of MLMC levels.
- **MLMC_LEVEL**: (Integer, default = 0) Current MLMC level.
- **MLMC_NUM_CLUSTERS**: (Integer, default = 0) Number of clusters from the level above this one.
- **MLMC_CLUSTER_SIZE**: (Integer, default = 4) Number of samples on this level per cluster from the level above this one (Depreciated, the averaging scheme works independent of the number of samples in the cluster!)
- **MLMC_OUT_ROOT**: (String, default = "out") Output directory for final MLMC output files.
- **MLMC_TEMP_ROOT**: (String, default = "temp") Output directory for temporary MLMC files.