Various options and parameters of the **ANT.G** code are user-controlled through the *<job_name>.ini* input file. This file must be in the same directory as that of the GAUSSIAN03 input file (*<job_name>.com*). If there is no parameter file the program will run with the default values, which are given here. The same holds true for an empty file or a file only containing comments and/or blank lines. Remember that <job_name> is specified in the title line of the <job_name>.com file, it does not take it from the command line!!.

Syntax rules:
The order of statements is arbitrary.

Comment lines start with the symbol "!".

Empty lines are ignored.

General syntax for real and integer variable assignment:
KEYWORD = (value)
where *KEYWORD* is always in uppercase. All allowed keywords are listed
below along with the default value assigned to them.

Logical variable syntax:
KEYWORD
If the keyword is specified, the variable is given the value .TRUE. The default
value is .FALSE. Thus the logical variables act as switches turning on a
specific feature. For example, the keyword *MULLIKEN* dumps the
Mulliken population analysis into a file.

Calculation parameters:
ALPHA (real)
Mixing parameter for density matrix (typically 0.01 < *ALPHA* < 0.1).
Default: *ALPHA* = 5.0D-2

NPULAY (integer)
DIIS convergence parameter (typically *1* < *NPULAY* > 10). Every *NPULAY*
normal convergence steps a Pulay extrapolation kicks in.
Default: *NPULAY* = *4*
PACC (real)
Numerical integration maximum accuracy for density matrix.
Default: *PACC* = 1.0D-5

CHARGEACC (real)
Total charge maximum accuracy.

Default: *CHARGEACC* = 1.0D-3

FERMIACC (real)
Fermi level maximum accuracy (in eV).
Default: *FERMIACC* = 1.0D-3
SMALL, SMALLD (real)
Parameters used for the identification of the crystallographic structure of the
electrodes and for determining the Bethe lattice directions. The smaller, the
more stringent on the
atomic structure. Increase their values if your electrodes are slightly
disordered.
Default: *SMALL* = 0.1
Default: *SMALLD* = 0.1 (Angstrom)
FULLACC (logical)
Turns on full accuracy from the first cycle.

ETA (real)
Small imaginary part of the Green's function. When both electrodes are set to
    GHOST this number might need to be no so small.
Default: *ETA* = 1.0D-10

SL (real)
Convergence criterion for when to switch the infinite electrodes (Bethe
    lattice) on. These are connected when the standard GAUSSIAN03/09
    SCF convergence for the density matrix (RMSDP) reaches RMSDP <
    SL, where the overall convergence criterion is set in the
    GAUSSIAN03/09 input file with the SCF option
    "scf(conver=n)". Remark: If *SL* = 0, the leads are only connected
    after the GAUSSIAN03/09 SCF calculation has converged
    (cycle=1000). This is only recommended for quick and dirty
    calculations.
Default: *SL* = 1.0D-2

FERMISTART (real)
Starting value for Fermi level search (in eV). When reinitializing a calculation
    from a P.<job_name>.dat file it is overruled by the existing value in
    P.<job_name>.dat. Default: *FERMISTART* = -5.0D0

TYPE1 and TYPE2 (string)
Type of model for the semiinfinite electrode. When set to BETHE the effective
selfenergy is connected to the electrode. When set to GHOST, nothing is
connected. When both electrodes are set to GHOST the calculation is similar

to the one performed by the original GAUSSIAN03/09 code on the input cluster, but with all the convergence advantages of **ANT.G**.
Default: *TYPE1* = BETHE and *TYPE2* = BETHE

1 *BLPAR1* and *BLPAR2* (string)
2 Parameters sets of the Bethe lattice for the first and second electrode, respectively (see available options in files BLxxx.dat). Default: *BLPAR1* = Papacon and *BLPAR2* = Papacon
3
4 *OVERLAP* (real)
5 Factor by which the overlap parameters of the Bethe lattice (when specified in the parameters set) are multiplied (0.0 =< *OVERLAP* =< 1.0). When set to a negative value, an automatic procedure to include the overlap (even if not specified in the parameters set) is used. This is the safest option although it slows down the calculation. Set it to 0.0 for faster calculations and compare. Otherwise use it with caution. This parameter may need to be smaller than 1.0 to avoid unphysical density of states for the Bethe lattice when the overlap parameters are > 0.2. Default: *OVERLAP* = -1.0
6
7 *GLUE (real)*
8 Factor by which to multiply the selfenergy. Useful to detach in a controled way the system from the Bethe lattice.
9 Default: *GLUE* = 1.0
10
11   *NEMBED1* and *NEMBED2* (integer)
12   Number of atoms to be connected to a Bethe lattice branch. These atoms are not taken into account on computing the charge of the system when *OVERLAP* > 1. 3D Default: *NEMBED1* = All atoms in the outermost plane of first electrode and *NEMBED2* = All atoms in the outermost plane of second electrode (this is typically a good choice). 2D Default: *NEMBED1* = All atoms in the electrode 1 and *NEMBED2* = All atoms in electrode 2 (since you do probably not want this default, you should specify these).
NATOMEL1 and *NATOMEL2* (integer)
Number of atoms in first and second electrode. Only useful when the system is composed of a single element or one wants to select especific regions for analysis.
Default: *NATOMEL1* = Number of atoms in first metallic electrode and *NATOMEL2* = Number of atoms in second metallic electrode.
1

Reinitialization options:

1 When the file *P.<job_name>.dat* is present, the calculation is initialized
from the density matrix stored in *P.<job_name>.dat*. It is advisable to
include the keyword *nodamp* in the SCF options of the GAUSSIAN03
input line "scf=(nodamp)" and **make sure** that the standard
orientation of the system is the same as the one of the density matrix
stored in P.<job_name>.dat. You also need to add "nosymm" to the
input file <job_name>.com as "scf(nodamp,nosymm)" if you want to
start with an educated guess for magnetic systems with an unusual
spin texture or apply a finite bias voltage. The "nosymm" keyword
placed alone on the SCF especifications line (not in the scf brackets) is
useful to prevent GAUSSIAN03/09 from rotating the system and is
usually necessary for optimizations since GAUSSIAN03/09 likes to
change the standard orientation from step to step.

2

3 *PFIX* (logical)

4 When present, part of a previously computed density matrix can be used.

5 Syntax:

6 *PFIX*

7 *'P.<old_job_name>.dat'*

8 where *'P.<old_job_name>.dat'* is the file containing the density matrix you
want to use. This is useful, .e.g., to change the basis set on a
restricted set of atoms while preserving the convergency already
achieved in the rest of the system (see *NFIX*).

9 Default: .false. (no supplementary matrix provided).

10

11   *NFIX* (integer)

12   Number of atoms NOT to be touched when using PFIX.

13   Syntax:

14   *NFIX = N*

15   #atom1, #atom2, ...

16   where the second line indicates the atoms to be preserved.

Bias and gate voltage related parameters:

1 *BIASVOLT* (real)

2 Bias voltage (in eV). It is recommended to perfom first a calculation at zero
bias and then reinitialize from P.<job_name>.dat. Succesive
calculations at different bias voltages can be perfomed starting from a
previous calculation in the same way. You need to add "nosymm" to
the SCF specifications line in the GAUSSIAN03 input file as
"scf(nosymm)". The potential drop profile can be finally read from the
file V.<job_name>.dat where the atom on-site energies (averaged to
all orbitals in the atom) are stored.   Default: *BIASVOLT* = 0.0

3

4 *QEXCESS* (real)

5 The effect of a gate voltage can be simulated through the addition of positive charges in the GAUSSIAN03/09 input file. To compensate and keep overall charge neutrality, an equal number of electrons should be added. This can be acomplished with this keyword. (Of course one is free to violate charge neutrality if physically required.) It overrules the initial charge given to GAUSSIAN03/09 through its input file, but it is recommended these two quantities to be equal for a more efficient calculation. Default: *QEXCESS* = 0.0

Spin related parameters:

1 *SWOFFSPL* (real)

2 Convergence criterion for switching off spin locking in a spin unrestricted calculation (default). Thus in a spin-unrestricted calculation the total spin of the device is kept fixed to the value $(M-1)/2$ given by the multiplicity M in the GAUSSIAN03/09 input file until a certain convergence is reached: RMSDP < *SWOFFSPL*. (See also NSPINLOCK below) Advice: *SWOFFSPL* < *SL*

3 Default: *SWOFFSPL* = 1.0D-3

4

5 *NSPINLOCK* (integer)

6 Number of steps with spin locking on. It supercedes the *SWOFFSPL* criterion when >= 0 (see keyword *SWOFFSPL* above) Default: *NSPINLOCK* = 0.

7

8 *UD, DU, DD* (logical)

9 Magnetization direction of the Bethe lattice electrodes when these are magnetic. U stands for "up" and and D for "down". Useful after editing the density matrix to create an educated guess for a new calculation. Default: .false. (both electrodes "up").

10

11   *MRSTART* (integer)

12   Useful to create an educated guess for a new calculation with an unusual spin texture starting from a precomputed density matrix. In particular, it reverses the magnetization direction for all atoms with numbers >= *MRSTART*. You need to add "nosymm" to the SCF specifications line in the GAUSSIAN03/09 input file as "scf(nosymm)". Default: *MRSTART* = 0 (No effect).

13

14   *SPINEDIT* (logical)

15   Useful to create an educated guess for a new calculation with an unusual spin texture starting from a precomputed density matrix. In particular, it manipulates the magnetization direction (spin) of

individual atoms. You need to add "nosymm" to the SCF specifications line in the GAUSSIAN03/09 input file as "scf(nosymm)". Syntax:

16 *SPINEDIT*
17 #natoms
18 #atom1, #atomspin1, #atom2, #atomspin2, ...
19 where #natoms is the number of atoms where the spin is altered. The list below gives the atom numbers and the atom spins for the atoms to be altered where the atom spin can either be maintained (1), reversed (-1), or erased (0).   Default: .false. (off)
20
21 *SOC* (real)
22 Atomic spin-orbit coupling parameter. When different from zero, the transmission and DOS are computed adding the spin-orbit coupling to the converged solution in the absence of spin-orbit coupling (this is obviously not justified for large values). As expected, in magnetic systems the spatial orientation determines the result.   Default: *SOC* = 0.0
23

Evaluation parameters

1 ESTEP (real)
2 Energy step (in eV) for printing out transmission and DOS.
3 Default: ESTEP = 1.0D-2
4
5 EW1 and EW2 (real)
6 Define an energy window for printing out transmission and DOS.
7 Default: EW1 = -3.0D0 and EW2 = 3.0D0.
8
9 DOSENERGY (real)
10   Energy at which to evaluate the DOS projected on atoms when keyword MULLIKEN on.
11   Default: 0.0 (Fermi Energy).
12
13   LDOS_BEG and LDOS_END (integer)
14   Atoms numbers onto which the local density of states is evaluated.
15   Default: LDOS_BEG = 1 and LDOS_END = 0 (LDOS evaluation off).
16
17   NCHANNELS (integer)
18   Number of eigenchannles to print out in T.<job_name>.dat. If NCHANNELS > 0 then the tranmission matrix (calculated in the non-hermitian or hermitian form, see keyword HTRANSM) is diagonalized and the NCHANNELS largest eigenvalues (i.e. the eigenchannel transmissions) are printed. Default: NCHANNELS = 0 (eigenchannel

calculation off).

19

20 *LEADDOS (logical)*

21 *Prints out the DOS of the Bethe lattice. Output files: Lead1DOS.dat, Lead2DOS.dat Default: .false. (off).*

22

23 *HTRANSM (logical)*

24 *Compute Transmision matrix in hermitian form T = \Gamma_L^{1/2} G^\dagger \Gamma_R G \Gamma_L^{1/2}. The default is the easier non-hermitian form \Gamma_L G^\dagger \Gamma_R G which is considerably faster for large clusters. The diagonalization of both forms yield the same eigenvalues. Default: .false. (transmission matrix in non-hermitian form).*

25

26 *RTM_BEG and RTM_END (integer)*

27 *Perform eigenchannel analysis with reduced transmission matrix [see PRB **73**, 075429 (2006)] on atoms from atom RTM_BEG to atom RTM_END Default: RTM_BEG = 1 and RTM_END = 0 (eigenchannel analysis off).*
    MULLIKEN (logical)

Dumps the Mulliken population analysis in the file Q.<job_name>.dat. The DOS projected on atoms at the Fermi energy (or at the energy selected by DOSENERGY) is also dumped when LDOS_BEG < LDOS_END.
Default: .false. (not print).

ANT1D (logical)
Requests to write all the necessary input files to be used with the [ANT1D transport program](#).

Options for electronic correlations

CORRBLOCKS
This keyword specifies a block of atomic orbitals (usually a d- or f-shell of an atom) for further treatment beyond DFT taking into account local electronic correlations.
Syntax:
<num_corrblocks>
<ao_beg> <ao_end> <U> <J>
...
where <num_corrblocks> is the number of correlated blocks within the device region. For each correlated block a line "<ao_beg> <ao_end> <U>

<J>" has to be specified where <ao_beg> ist the number of the first atomic orbital and <ao_end> is the last atomic orbital of the correlated block. <U> is the direct Coulomb repulsion and <J> Hund's rule coupling for the correlated block.

DFT+U (logical)
Requests a DFT+U calculation where a Hubbard interaction term (U and J) is put onto each correlated block which is treated within Hartree-Fock.

HYBFUNC (logical)
Requests the calculation of the hybridization function for each correlated block which serves as an input for an impurity solver calculation. A mesh file "mesh.dat" needs to be present specifiying the energy points for which to calculate the hybridization function.

PORTHO (logical)
Requests to perform a "projective orthogonalization" prior to calculation of the hybridization function. Thereby the device region is orthogonalized in a Gram-Schmidt like manner that preserves the original correlated subspace composed of all correlated blocks.

DIAGCORRBL (logical)
Prior to calculation of the hybridization function the Hamiltonian of each correlated subspace is diagonalized. This is useful in case of strong crystal-field splitting leading to large off-diagonal elements in the hybridization function. Using this option the crystal-field basis is found, and hence off-diagonal elements of the hybridization function are minimized. This option is also useful in case that the correlated subspace is described by more than one set of orbitals (e.g. double-zeta basis). In this case, the diagonalization yields the low-energy subspace of the correlated shell.