Computational implementation of the Kubo formula for the static conductance: application to two-dimensional quantum dots

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Kubo formula is used to get the d.c conductance of a statistical ensemble of two-dimensional clusters of the square lattice in the presence of standard diagonal disorder, a uniform magnetic field and random magnetic fluxes. Working within a one-band tight-binding approach the calculation is quite general. The shape of the cluster is rectangular with ideal leads attached to opposite corners. Both geometrical characteristics and physical parameters can be easily selected. The output is just the conductance of a system of given parameters or a statistical ensemble of conductances measured for different disorder realizations.

Section 7.9 of the Program Library Index

PROGRAM SUMMARY

Title of program: KUBO
Catalogue identifier:
Distribution format: Uuencoded gzipped tar file
Computer for which the program is designed and others on which it has been tested: Alphaserver 1200, DECstation 3000 Model 400
Computers:
Installations:
Operating systems or monitors under which the program has been tested: Digital Unix 4.0D
Programming language used: Fortran
Memory required to execute with typical data: 7.04 Mwords
Number of bits in a word: 64
Number of processors used: 1
Has the code been vectorized or parallelized?: Vectorised version of inversion LAPACK subroutines are available on the computer (DXML library)
Number of bytes in distributed program, including test data, etc.: 7305
Keywords: Conductance, Kubo formula, one-band two-dimensional tight-binding Hamiltonian, magnetic field, random fluxes, diagonal disorder.

Nature of the physical problem
Conductance evaluation plays a central role in the study of the physical properties of quantum dots [1]. The finite mesoscopic system under study is connected to infinite leads defining an infinitesimal voltage drop. Kubo formula is used for the conductance calculation once the Green function of the whole system is known. Dependence of the conductance on the number of conducting modes in the leads, size and shape of the dot, Fermi energy, presence
of conventional diagonal disorder or random magnetic fluxes through the plaquettes and a uniform magnetic field through the sample can be considered as needed.

Method of solution
The calculation of the Green function of the system formed by the quantum dots and the leads is the main concern of the program [2]. Firstly, the selfenergy due to a semiinfinite ideal lead is calculated. Secondly, this selfenergy is used as the starting value for an iteration through the sample that takes into account its shape and local disorder and magnetic fluxes. Thirdly, the final selfenergy is matched via a two-slab Green function calculation with the selfenergy coming from the opposite sample side. Finally, Kubo formula is used for obtaining the system conductance from the current traversing the dot.

Restrictions on the complexity of the program
The more important restriction is the use of just a one-band tight-binding Hamiltonian. Other program characteristics, like the rectangular shape of the sample, the position of the leads near opposite sample corners, etc. can be easily changed.

Typical running time
The calculation of the conductance at a fixed Fermi energy for ten random realizations of $100 \times 100$ disordered samples takes 225 seconds on a DECstation 3000 Model 400.

References
[1] For reviews of mesoscopic physics see C.W.J. Beenakker and H. van Houten, in Solid State Physics, edited by H. Ehrenreich and D. Turnbull (Academic Press, New York, 1991), Vol. 44, pp. 1–228; Mesoscopic Phenomena in Solids, edited by B.L. Altshuler, P.A. Lee, and R.A Webb (North–Holland, New York, 1991).
[2] The following book by Datta gives a good account of both the basic concepts and the practical things that should be solved to get the conductance of a mesoscopic system, S. Datta, Electronic Transport in Mesoscopic Systems, (Cambridge University Press, Cambridge, 1995).

LONG WRITE-UP

I. INTRODUCTION

This paper deals with the numerical calculation of the conductance of a two-dimensional system via Kubo formula which is the standard microscopic approach to the problem. It has been proved that it is equivalent to the more intuitive point of view of expressing the conductance as a sum of transmission coefficients over channels. Actually, a transmittance calculation for a disordered square lattice has been implemented as an example of the use of the block recursion method.

Both measurement and calculation of the conductance of mesoscopic systems is an important issue in the study of their physical properties. The calculation is as realistic as it is possible within present computer facilities. Actually, the main limitation of the program is just the consideration of a one-band tight-binding Hamiltonian. In principle, this one-orbital per site basis can be enlarged within the present scheme. The necessary effort makes only sense when simulating a particular physical system. On the other hand, the one-band tight-binding basis can also be seen as the first approach to free electrons moving in two-dimensions. Certainly, the lower part of the band shows a quadratic dispersion relation.

Following well-known formalisms, the system includes both a transversal uniform magnetic field and a random component giving variable fluxes through the plaquettes. Conventional diagonal disorder is also considered for completeness. Further possibilities like other kinds of non-diagonal disorder are absent but would be easily incorporated if necessary. Also size of the sample, shape, number of modes transported by the leads can be tuned at convenience. Again further complications like the inclusion of more leads of different widths or going to a tunneling regime in the contacts between sample and leads only imply minor changes in the computer code. In order to keep the program understandable, I have left such kind of modifications for the readers. Another interesting generalization is the calculation of three-dimensional conductances. This has been actually done in the study of manganites.
II. LATTICE MODEL

The system is composed by a left ideal lead allowing up to \( m \) modes, an \( L \times M \) cluster and a right ideal lead similar to the left one. Leads are semiinfinite and are connected to opposite corners of the rectangular dot by ideal contacts. Sites form a subspace of the whole square lattice. The Hamiltonian describing the quantum system is:

\[
\hat{H}_0 = \sum_{i \geq 1} \sum_{j=1}^{M_i} \epsilon_{i,j} \hat{c}_{i,j}^\dagger \hat{c}_{i,j} - t \sum_{i \geq 1} \sum_{j=1}^{M_i-1} \left( e^{2\pi i \phi_{i,j+1,j}} \hat{c}_{i,j}^\dagger \hat{c}_{i+1,j} + e^{-2\pi i \phi_{i,j+1,j}} \hat{c}_{i,j+1}^\dagger \hat{c}_{i,j} \right) ,
\]

where \( \hat{c}_{i,j}^\dagger \) creates an electron on site \((i, j)\), \( \epsilon_{i,j} \) are random diagonal energies chosen with equal probability from the interval \([-W/2, W/2]\), and \(-t\) is the hopping energy. Sums in \( j \) depend on the local width \( M_i \) which is \( m \) for the leads and \( M \) for the dot. The flux through the lattice loop which left lower corner is \((i, j)\) is given by \( \Phi_{i,j} = \phi_{i,j+1} - \phi_{i+1,j} \) measured in units of flux quantum \( \Phi_0 = \hbar c/e \). Uncorrelated fluxes are randomly selected with equal probability from the interval \([-\phi_{\text{max}}/(2\pi), \phi_{\text{max}}/(2\pi)\]). A transversal uniform magnetic field \( h_\perp \) is easily incorporated adding to all \( \Phi_{i,j} \) within the sample the number of quantum fluxes traversing any plaquette of the dot \( (h_\perp a^2/\Phi_0, a \) being the lattice constant). With this gauge choice, when the system is solved layer by layer, the matrix giving intralayer hopping is constant while the interlayer coupling includes all effects due to the magnetic field. Both disorder and magnetic fluxes are restricted to the dot, that is, have non-zero values for \( 1 \leq i \leq L \). It is also implicitly assumed that the number of modes (width) of the leads \( m \) is smaller than or equal to the dot width \( M \). Nevertheless, a constriction (i.e., the \( m > M \) case) can be similarly handled.

III. D.C. CONDUCTANCE VIA KUBO FORMULA

In order to study the linear electric response of the system, an electric potential profile should be assumed. The simplest possibility is just a stepwise potential: all dot and right lead sites \((i < 1)\) remain at 0. This choice defines a position operator:

\[
\hat{x} = \sum_{i \geq 1} \sum_{j=1}^{M_i} \hat{c}_{i,j}^\dagger \hat{c}_{i,j}
\]

and the corresponding perturbing Hamiltonian:

\[
\hat{H}_1 = -eV \cos(\omega t) \hat{x}
\]

where a simple cosine time dependence is included. \( \hat{H}_1 \) produces transitions among the stationary eigenstates of the system and a time dependent current develops. If the charge at the right part of the system is defined by:

\[
\hat{Q} = -e \sum_{i \geq 1} \sum_{j=1}^{M_i} \hat{c}_{i,j}^\dagger \hat{c}_{i,j} = -e\hat{x}
\]

the charge traversing the sample per unit time, i.e., the current through the system is given by operator \( \hat{I} \) that obeys the following equation of motion:

\[
i\hbar \hat{I} = \left[ \hat{H}, \hat{Q} \right] = -e \left[ \hat{H}, \hat{x} \right] = -e\hbar \hat{v}_x
\]

Therefore, the current operator is the velocity operator apart from a constant: \( \hat{I} = -e \hat{v}_x \). Using the total Hamiltonian of the system \( \hat{H} = \hat{H}_0 + \hat{H}_1 \) and the equation of motion for \( \hat{x} \), the first important result is obtained:

\[
i\hbar \hat{v}_x = -t \sum_{j=1}^{m} \left( \hat{c}_{0,j}^\dagger \hat{c}_{1,j} + \hat{c}_{1,j}^\dagger \hat{c}_{0,j} \right)
\]

This equation shows that the knowledge of the charge flux in the contact between the left lead and the sample is enough to evaluate the total current through the system. Of course, the result comes from the flux conservation along the whole system.
Now, first order time-dependent perturbation theory is used to get the time evolution of the stationary eigenfunctions. The mean value of the current is:

\[
<\dot{I}> = \sum_\alpha f_\alpha <\Psi_\alpha |\dot{\hat{I}}|\Psi_\alpha>,
\]

where \(\Psi_\alpha\) are the perturbed eigenfunctions and \(f_\alpha\) their occupation. A straightforward but tedious calculation gives the linear electric response of the system:

\[
G = \lim_{\omega \to 0} \frac{<\dot{I}>}{V} = -e^2 \hbar \pi \lim_{\omega \to 0} \sum_{\alpha,\beta} |<\alpha|\hat{\nu}_x|\beta>|^2 \frac{f_\alpha - f_\beta}{\epsilon_\alpha - \epsilon_\beta} \delta(\epsilon_\beta - \epsilon_\alpha - \hbar \omega),
\]

being \(G\) the system conductance. To arrive at this formula, the basic relation between the matrix elements of position and velocity operators implied by the equation of motion has been used:

\[
i\hbar <\alpha|\hat{\nu}_x|\beta> = (\epsilon_\alpha - \epsilon_\beta) <\alpha|\hat{x}|\beta>.
\]

Former conductivity calculations based on Kubo formalism used Eq. 8 to calculate the static conductivity. Nevertheless, direct use of Eq. 8 leads to a lot of numerical troubles since eigenvalues are discrete for isolated samples and the conductance is obtained as a sum of delta functions. This fact forces the use of some averaging procedure over finite \(\omega\) values that distorts the final static (\(\omega = 0\)) value.

When Green functions are used instead of eigenfunctions to express the conductance, a more convenient form of the Kubo formula at \(T = 0\) is obtained:

\[
G = 2 \left(\frac{e^2}{\hbar}\right) \text{Tr} \left[(i\hbar \hat{\nu}_x) \text{Im} \hat{G}(E)(i\hbar \hat{\nu}_x) \text{Im} \hat{G}(E)\right],
\]

where \(\text{Im} \hat{G}(E)\) is obtained from the advanced and retarded Green functions:

\[
\text{Im} \hat{G}(E) = \frac{1}{2i} \left[\hat{G}^R(E) - \hat{G}^A(E)\right],
\]

and the energy \(E\) is the Fermi energy of the system. Traditionally, the static electrical conductivity \(\sigma_{xx}\) was calculated. It coincides with \(G\) in a two-dimensional system. Conductance is given in units of \(e^2/\hbar\) which is the quantum conductance unit. The trace in Eq. 10 is dimensionless since the energy dimension of \(i\hbar \hat{\nu}_x\) is cancelled by the inverse energy dimension of the imaginary part of the Green function. Eq. 10 shows that Green functions are the last ingredient needed for the calculation of the conductance. Actually, only Green function matrix elements at slabs \(i = 0\) and \(i = 1\) are necessary owing to the simple form of \(\hat{\nu}_x\) (see Eq. 1) and the presence of the trace. This feature dictates the method for choice in the Green function calculation. Starting from the right end, the selfenergy of the ideal right lead is obtained, then iterated through the sample layer by layer, and finally, connected to the selfenergy coming from the left ideal lead (which in fact coincides with the right lead selfenergy). The equation defining the iteration is obtained from Dyson equation for the Green function and has the following form:

\[
\Sigma_{i-1} = \mathbf{V}_{i-1,i}(E \mathbf{I} - \mathbf{V}_{i,i} - \Sigma_i)^{-1}\mathbf{V}_{i,i-1}.
\]

This allows the calculation of \(\Sigma_{i-1}\) once the former selfenergy matrix and the intralayer \(\mathbf{V}_{i,i}\) and interlayer \(\mathbf{V}_{i-1,i} \quad \text{(} \mathbf{V}_{i,i-1} = \mathbf{V}_{i,i-1}^\dagger \text{)}\) matrices are known. After iterating the right side from \(+\infty\) to 1 and the left side from \(-\infty\) to 0, the needed Green function matrix elements are given by:

\[
[E\mathbf{I} - \mathbf{H} - \Sigma_i(E) - \Sigma_{i}(E)]\hat{G}(E) = \mathbf{I},
\]

where \(\mathbf{H}\) is the matrix representing the layer 0 plus layer 1 system Hamiltonian and \(\Sigma_{i}(E)\) stand for the left (right) selfenergy matrices.

Alternatively, instead of iterating the ordered ideal leads, one can analytically solve the problem in the basis of the transversal modes. Later on, a basis transformation provides the desired selfenergy matrices. Specifically, the retarded selfenergy due to the mode of wavevector \(k_y\) at energy \(E\) is given by:

\[
\Sigma(k_y) = \frac{1}{2} \left( E - \varepsilon(k_y) - i\sqrt{4t^2 - (E - \varepsilon(k_y))^2} \right),
\]
within its band \(|E - \varepsilon(k_y)| \leq 2|t|\) and by:

\[
\Sigma(k_y) = \frac{1}{2} \left( E - \varepsilon(k_y) \mp \sqrt{(E - \varepsilon(k_y))^2 - 4t^2} \right),
\]

(15)

outside the band (minus sign for \(E > \varepsilon(k_y) + 2|t|\) and plus sign for \(E < \varepsilon(k_y) - 2|t|\)), where \(\varepsilon(k_y) = 2t\cos(k_ya)\) is the eigenenergy of the \(k_y\) mode which is quantized:

\[
k_y = \frac{i_y \pi}{(m + 1)a},
\]

\(i_y\) being an integer from 1 to \(m\). The transformation from normal modes to the local tight-binding basis is obtained from the amplitudes of the normal modes:

\[
<n_y|k_y> = \sqrt{\frac{2}{m + 1}} \sin(k_y n_y a),
\]

(16)

where \(n_y\) is the tight-binding orbital position. The elements of the retarded selfenergy matrix are thus:

\[
<n_{y1}\Sigma(E)n_{y2}> = \sum_{k_y} <n_{y1}|k_y> \Sigma(k_y) <n_{y2}|k_y>
\]

(17)

Advanced Green function matrix elements are obtained as the transposed complex conjugate elements of the retarded Green function matrix elements.

Kubo formula (Eq.10) shows that since \(\hat{x}\) operator is chosen dimensionless, the hopping integral \(t\) appears twice in the numerator and also twice in the denominator of the trace. Consequently, its value is irrelevant in the conductance evaluation and can be set equal to 1 within the computer code for simplicity. Apart from the iterative calculation of lead selfenergy and a bit more restrictive geometrical set-up, the paper by Lee and Fisher seems to be the first application of the formalism presented in the last two sections.

IV. PROGRAM STRUCTURE

The structure of the program is extremely simple. Subroutines are not necessary. Hard work is done by state of the art inversion subroutines. An enumeration of the main program steps followed by a simple explanation is enough for its understanding.

After reading the input and logging it for further reference, both the intralayer matrix interaction \(V_{i,i}\) (which does not depend on \(i\) owing to the gauge choice) and the lead eigenvectors (Eq. 16) are initialized. For a given Fermi energy \(E\), selfenergies are calculated in the eigenvectors basis using Eqs. 14 or 15 and transformed to the tight-binding basis using Eq. 17. The resulting selfenergy matrix is called \(tt\) within the program. Here, we arrived at the main part of the calculation: selfenergy matrix is iterated from right to left through a randomly generated sample that incorporates the desired disorder. Once the selfenergy is known at the left side of the sample, it is matched to the lead selfenergy coming from the left by Eq. 13. This allows the evaluation of the imaginary part of the Green function via Eq. 11 and the use of Kubo formula for the obtaining of the conductance (see Eq. 10) that is the only program output (Conductance is written in units of the quantum unit \(e^2/h\)). Notice that the multiplication by the matrix representing the velocity operator in the local tight-binding basis (Eq. 6) is done without building explicitly the very sparse matrix. The calculation of the conductance is repeated the number of times that are necessary for the knowledge of the statistical behavior of the conductance due to disorder. Of course, the step is not repeated when disorder is absent.

The heavy part of the computational work is just the inversion of a large number of matrices of moderate size. It is achieved by external calls to LAPACK subroutines that are conveniently adapted to the hardware configuration. If not belonging to the machine software, they are available via Internet (http://www.netlib.org).

A portable simple version of a generator of pseudo-random numbers is included within the distributed source. This allows to check the distributed sample results. Nevertheless, a better generator should be used in the working version of the program. Notice that the generator included within the source code has a maximum period of 259200 which is really insufficient when a good disorder statistics of large samples should be obtained. In any case, let me remind that the seed of the generator should be smaller than \(im\), i.e., smaller than 259200.
V. INPUT AND OUTPUT

Input parameters have all a simple physical meaning. They are given in Table I. Output is just the conductance as a function of the parameters (Fermi energy, for example) that are varied within the external do loops of the program. Conductance is given in units of its quantum $e^2/h$.

VI. TEST RUN

Input and output files corresponding to three typical calculations are included in the distribution. The first one gives the conductance of a small cluster in the presence of a uniform magnetic field. It is obtained as a function of the Fermi energy. This run does not use the pseudo-random numbers generator. The second one studies the effect of disorder. One hundred samples are randomly generated and their conductance calculated. The third one shows the effect of geometric parameters. While the two previous runs deal with a highly symmetric system ($32 \times 32$ cluster attached to leads of the same width), this case gives the conductance for a less symmetric dot.

One additional test is also possible. Conductance is an integer when disorder is absent and leads perfectly match opposite rectangle sides. It gives just the number of open (conducting) channels (modes) in the leads.

The same fortran code has been compiled and run on a Pentium II in a Linux environment using g77 and local inversion subroutines. Results do not differ from the given output samples.

ACKNOWLEDGMENTS

I acknowledge Luis Martín-Moreno who helped me checking the computer code used in this work running his own program based on a different implementation of the transfer matrix technique. I also thank Rafael Ramírez for checking the code on a PC running under Linux. This work has been partially supported by Spanish Comisión Interministerial de Ciencia y Tecnología (grant PB96-0088).

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A. Input 1

032 width
032 length
032 modes
0.0d0 phimax
0.101341699d0 hmag
1751 loteria
1 ntimes
0.0d0 0.0d0 1.0d0 W1,W2,W3
-4.0d0 -3.0d0 0.01d0 energy1,energy2,energy3

B. Input 2

032 width
032 length
032 modes
3.14159265d0 phimax
0.0d0 hmag
1751 loteria
100 ntimes
0.1d0 0.1d0 1.0d0 W1,W2,W3
0.1751d0 1.0d0 1.0d0 energy1,energy2,energy3

C. Input 3

028 width
038 length
006 modes
0.0d0 phimax
0.0d0 hmag
1751 loteria
1 ntimes
0.0d0 0.0d0 1.0d0 W1,W2,W3
-4.0d0 -3.0d0 0.01d0 energy1,energy2,energy3

TEST RUN OUTPUT

D. Output 1

| sample disorder_width | Fermi_level | conductance     |
|-----------------------|-------------|-----------------|
| 1                     | 0.0000      | -4.000000 0.52279883E-30 |
| 1                     | 0.0000      | -3.990000 0.37576695E-15 |
| 1                     | 0.0000      | -3.980000 0.10174681E-13 |
| 1                     | 0.0000      | -3.970000 0.35160914E-13 |
| 1                     | 0.0000      | -3.960000 0.13971441E-11 |
| 1                     | 0.0000      | -3.950000 0.90081246E-11 |
| 1                     | 0.0000      | -3.940000 0.19577031E-10 |
| 1                     | 0.0000      | -3.930000 0.26700263E-09 |
| 1                     | 0.0000      | -3.920000 0.73710663E-09 |
| 1                     | 0.0000      | -3.910000 0.58263154E-07 |
| 1                     | 0.0000      | -3.900000 0.15099144E-02 |
|   |         |         |               |
|---|---------|---------|---------------|
| 1 | 0.0000  | -3.890000 | 0.99895187E+00 |
| 1 | 0.0000  | -3.880000 | 0.99605711E+00 |
| 1 | 0.0000  | -3.870000 | 0.98332107E+00 |
| 1 | 0.0000  | -3.860000 | 0.99814562E+00 |
| 1 | 0.0000  | -3.850000 | 0.99428901E+00 |
| 1 | 0.0000  | -3.840000 | 0.99899589E+00 |
| 1 | 0.0000  | -3.830000 | 0.99661623E+00 |
| 1 | 0.0000  | -3.820000 | 0.99941302E+00 |
| 1 | 0.0000  | -3.810000 | 0.99773298E+00 |
| 1 | 0.0000  | -3.800000 | 0.99865209E+00 |
| 1 | 0.0000  | -3.790000 | 0.9974332E+00  |
| 1 | 0.0000  | -3.780000 | 0.99753821E+00 |
| 1 | 0.0000  | -3.770000 | 0.99946904E+00 |
| 1 | 0.0000  | -3.760000 | 0.99999165E+00 |
| 1 | 0.0000  | -3.750000 | 0.99962089E+00 |
| 1 | 0.0000  | -3.740000 | 0.99937579E+00 |
| 1 | 0.0000  | -3.730000 | 0.99952032E+00 |
| 1 | 0.0000  | -3.720000 | 0.99980170E+00 |
| 1 | 0.0000  | -3.710000 | 0.19550936E+01 |
| 1 | 0.0000  | -3.700000 | 0.19914236E+01 |
| 1 | 0.0000  | -3.690000 | 0.19900318E+01 |
| 1 | 0.0000  | -3.680000 | 0.19861029E+01 |
| 1 | 0.0000  | -3.670000 | 0.19941228E+01 |
| 1 | 0.0000  | -3.660000 | 0.19974424E+01 |
| 1 | 0.0000  | -3.650000 | 0.19962072E+01 |
| 1 | 0.0000  | -3.640000 | 0.19979441E+01 |
| 1 | 0.0000  | -3.630000 | 0.19983424E+01 |
| 1 | 0.0000  | -3.620000 | 0.19973790E+01 |
| 1 | 0.0000  | -3.610000 | 0.19977287E+01 |
| 1 | 0.0000  | -3.600000 | 0.19987828E+01 |
| 1 | 0.0000  | -3.590000 | 0.19972511E+01 |
| 1 | 0.0000  | -3.580000 | 0.19933848E+01 |
| 1 | 0.0000  | -3.570000 | 0.19989170E+01 |
| 1 | 0.0000  | -3.560000 | 0.19995162E+01 |
| 1 | 0.0000  | -3.550000 | 0.19988242E+01 |
| 1 | 0.0000  | -3.540000 | 0.19985759E+01 |
| 1 | 0.0000  | -3.530000 | 0.19989692E+01 |
| 1 | 0.0000  | -3.520000 | 0.20108456E+01 |
| 1 | 0.0000  | -3.510000 | 0.29588509E+01 |
| 1 | 0.0000  | -3.500000 | 0.29880224E+01 |
| 1 | 0.0000  | -3.490000 | 0.29890605E+01 |
| 1 | 0.0000  | -3.480000 | 0.29934051E+01 |
| 1 | 0.0000  | -3.470000 | 0.29829712E+01 |
| 1 | 0.0000  | -3.460000 | 0.29908045E+01 |
| 1 | 0.0000  | -3.450000 | 0.29939537E+01 |
| 1 | 0.0000  | -3.440000 | 0.29913380E+01 |
| 1 | 0.0000  | -3.430000 | 0.29956061E+01 |
| 1 | 0.0000  | -3.420000 | 0.29991560E+01 |
| 1 | 0.0000  | -3.410000 | 0.29996230E+01 |
| 1 | 0.0000  | -3.400000 | 0.29985708E+01 |
| 1 | 0.0000  | -3.390000 | 0.29977878E+01 |
| 1 | 0.0000  | -3.380000 | 0.29978828E+01 |
| 1 | 0.0000  | -3.370000 | 0.29985529E+01 |
| 1 | 0.0000  | -3.360000 | 0.29991855E+01 |
| 1 | 0.0000  | -3.350000 | 0.29992141E+01 |
| 1 | 0.0000  | -3.340000 | 0.29981113E+01 |
| 1 | 0.0000  | -3.330000 | 0.29730935E+01 |
E. Output 2

| sample | disorder_width | Fermi_level | conductance |
|--------|----------------|-------------|-------------|
| 1      | 0.1000         | 0.175100    | 0.15757571E+01 |
| 2      | 0.1000         | 0.175100    | 0.90865074E+00 |
| 3      | 0.1000         | 0.175100    | 0.89621507E+00 |
| 4      | 0.1000         | 0.175100    | 0.17411444E+01 |
| 5      | 0.1000         | 0.175100    | 0.17895467E+00 |
| 6      | 0.1000         | 0.175100    | 0.16377963E+01 |
| 7      | 0.1000         | 0.175100    | 0.13946143E+01 |
| 8      | 0.1000         | 0.175100    | 0.17833471E+01 |
| 9      | 0.1000         | 0.175100    | 0.14445051E+01 |
| 10     | 0.1000         | 0.175100    | 0.15230297E+01 |
| 11     | 0.1000         | 0.175100    | 0.14065148E+01 |
| 12     | 0.1000         | 0.175100    | 0.15391601E+01 |
| 13     | 0.1000         | 0.175100    | 0.14052089E+01 |
| 14     | 0.1000         | 0.175100    | 0.13567799E+01 |
| 15     | 0.1000         | 0.175100    | 0.16651201E+01 |
| 16     | 0.1000         | 0.175100    | 0.17878714E+01 |
| 17     | 0.1000         | 0.175100    | 0.11109133E+01 |
|   |      |      |                  |
|---|------|------|------------------|
| 18| 0.1000| 0.175100| 0.89038712E+00  |
| 19| 0.1000| 0.175100| 0.12773366E+01  |
| 20| 0.1000| 0.175100| 0.11877100E+01  |
| 21| 0.1000| 0.175100| 0.79052484E+00  |
| 22| 0.1000| 0.175100| 0.14452282E+01  |
| 23| 0.1000| 0.175100| 0.19539141E+01  |
| 24| 0.1000| 0.175100| 0.14051744E+01  |
| 25| 0.1000| 0.175100| 0.13141107E+01  |
| 26| 0.1000| 0.175100| 0.15579377E+01  |
| 27| 0.1000| 0.175100| 0.17998757E+01  |
| 28| 0.1000| 0.175100| 0.15839267E+01  |
| 29| 0.1000| 0.175100| 0.15788136E+01  |
| 30| 0.1000| 0.175100| 0.18356223E+01  |
| 31| 0.1000| 0.175100| 0.16829076E+01  |
| 32| 0.1000| 0.175100| 0.16927771E+01  |
| 33| 0.1000| 0.175100| 0.14242584E+01  |
| 34| 0.1000| 0.175100| 0.20767889E+01  |
| 35| 0.1000| 0.175100| 0.13799149E+01  |
| 36| 0.1000| 0.175100| 0.13587508E+01  |
| 37| 0.1000| 0.175100| 0.96175170E+00  |
| 38| 0.1000| 0.175100| 0.10228039E+01  |
| 39| 0.1000| 0.175100| 0.12647448E+01  |
| 40| 0.1000| 0.175100| 0.15151721E+01  |
| 41| 0.1000| 0.175100| 0.14502308E+01  |
| 42| 0.1000| 0.175100| 0.15174573E+01  |
| 43| 0.1000| 0.175100| 0.12829172E+01  |
| 44| 0.1000| 0.175100| 0.19077400E+01  |
| 45| 0.1000| 0.175100| 0.18329162E+01  |
| 46| 0.1000| 0.175100| 0.14944505E+01  |
| 47| 0.1000| 0.175100| 0.15520437E+01  |
| 48| 0.1000| 0.175100| 0.15797294E+01  |
| 49| 0.1000| 0.175100| 0.15870156E+01  |
| 50| 0.1000| 0.175100| 0.19959013E+01  |
| 51| 0.1000| 0.175100| 0.19913650E+01  |
| 52| 0.1000| 0.175100| 0.12217520E+01  |
| 53| 0.1000| 0.175100| 0.16039270E+01  |
| 54| 0.1000| 0.175100| 0.17024037E+01  |
| 55| 0.1000| 0.175100| 0.14668939E+01  |
| 56| 0.1000| 0.175100| 0.15284083E+01  |
| 57| 0.1000| 0.175100| 0.12557186E+01  |
| 58| 0.1000| 0.175100| 0.12838046E+01  |
| 59| 0.1000| 0.175100| 0.18537063E+01  |
| 60| 0.1000| 0.175100| 0.16127581E+01  |
| 61| 0.1000| 0.175100| 0.15376409E+01  |
| 62| 0.1000| 0.175100| 0.15619712E+01  |
| 63| 0.1000| 0.175100| 0.17955325E+01  |
| 64| 0.1000| 0.175100| 0.14001172E+01  |
| 65| 0.1000| 0.175100| 0.97460353E+00  |
| 66| 0.1000| 0.175100| 0.11018902E+01  |
| 67| 0.1000| 0.175100| 0.15973680E+01  |
| 68| 0.1000| 0.175100| 0.13172499E+01  |
| 69| 0.1000| 0.175100| 0.89201764E+00  |
| 70| 0.1000| 0.175100| 0.12745779E+01  |
| 71| 0.1000| 0.175100| 0.20770076E+01  |
| 72| 0.1000| 0.175100| 0.12221830E+01  |
| 73| 0.1000| 0.175100| 0.16596201E+01  |
| 74| 0.1000| 0.175100| 0.96965211E+00  |
| 75| 0.1000| 0.175100| 0.13451393E+01  |
| sample disorder_width | Fermi_level  | conductance  |
|-----------------------|--------------|--------------|
| 1                     | 0.0000       | -4.000000    | 0.41985273E-31 |
| 1                     | 0.0000       | -3.990000    | 0.71259408E-32 |
| 1                     | 0.0000       | -3.980000    | 0.13096324E-31 |
| 1                     | 0.0000       | -3.970000    | 0.89940928E-31 |
| 1                     | 0.0000       | -3.960000    | 0.84981659E-32 |
| 1                     | 0.0000       | -3.950000    | 0.74052006E-31 |
| 1                     | 0.0000       | -3.940000    | 0.10438540E-30 |
| 1                     | 0.0000       | -3.930000    | 0.56327809E-32 |
| 1                     | 0.0000       | -3.920000    | 0.86474255E-31 |
| 1                     | 0.0000       | -3.910000    | 0.21088933E-31 |
| 1                     | 0.0000       | -3.900000    | 0.38364524E-30 |
| 1                     | 0.0000       | -3.890000    | -0.20299302E-30 |
| 1                     | 0.0000       | -3.880000    | 0.26000054E-32 |
| 1                     | 0.0000       | -3.870000    | 0.83486242E-31 |
| 1                     | 0.0000       | -3.860000    | 0.30814879E-31 |
| 1                     | 0.0000       | -3.850000    | 0.20360691E-30 |
| 1                     | 0.0000       | -3.840000    | 0.31061398E-29 |
| 1                     | 0.0000       | -3.830000    | 0.44989724E-30 |
| 1                     | 0.0000       | -3.820000    | -0.80580909E-30 |
| 1                     | 0.0000       | -3.810000    | 0.14202891E-29 |
| 1                     | 0.0000       | -3.800000    | 0.12988896E+00 |
| 1                     | 0.0000       | -3.790000    | 0.43092998E-01 |
| 1                     | 0.0000       | -3.780000    | 0.19481001E+00 |
| 1                     | 0.0000       | -3.770000    | 0.22292412E+00 |
| Value | 0.0000 | -3.760000 | 0.77581649E+00 |
|-------|--------|-----------|----------------|
| Value | 0.0000 | -3.750000 | 0.77562524E+00 |
| Value | 0.0000 | -3.740000 | 0.66989858E+00 |
| Value | 0.0000 | -3.730000 | 0.28693757E-01 |
| Value | 0.0000 | -3.720000 | 0.67556799E+00 |
| Value | 0.0000 | -3.710000 | 0.98570186E+00 |
| Value | 0.0000 | -3.700000 | 0.97495692E+00 |
| Value | 0.0000 | -3.690000 | 0.99581430E+00 |
| Value | 0.0000 | -3.680000 | 0.97023908E-01 |
| Value | 0.0000 | -3.670000 | 0.82385509E+00 |
| Value | 0.0000 | -3.660000 | 0.91641977E-02 |
| Value | 0.0000 | -3.650000 | 0.48033012E-01 |
| Value | 0.0000 | -3.640000 | 0.88955232E+00 |
| Value | 0.0000 | -3.630000 | 0.85081542E+00 |
| Value | 0.0000 | -3.620000 | 0.66479842E+00 |
| Value | 0.0000 | -3.610000 | 0.64385114E+00 |
| Value | 0.0000 | -3.600000 | 0.99855320E+00 |
| Value | 0.0000 | -3.590000 | 0.28084687E+00 |
| Value | 0.0000 | -3.580000 | 0.38374067E+00 |
| Value | 0.0000 | -3.570000 | 0.10191610E+00 |
| Value | 0.0000 | -3.560000 | 0.57763375E+00 |
| Value | 0.0000 | -3.550000 | 0.96053453E+00 |
| Value | 0.0000 | -3.540000 | 0.97642322E+00 |
| Value | 0.0000 | -3.530000 | 0.98907542E+00 |
| Value | 0.0000 | -3.520000 | 0.99980992E+00 |
| Value | 0.0000 | -3.510000 | 0.99966610E+00 |
| Value | 0.0000 | -3.500000 | 0.44537039E+00 |
| Value | 0.0000 | -3.490000 | 0.16269503E+00 |
| Value | 0.0000 | -3.480000 | 0.25320153E+00 |
| Value | 0.0000 | -3.470000 | 0.33512914E+00 |
| Value | 0.0000 | -3.460000 | 0.43581456E-01 |
| Value | 0.0000 | -3.450000 | 0.86944911E+00 |
| Value | 0.0000 | -3.440000 | 0.97491430E+00 |
| Value | 0.0000 | -3.430000 | 0.77663803E+00 |
| Value | 0.0000 | -3.420000 | 0.86652483E+00 |
| Value | 0.0000 | -3.410000 | 0.17048486E+00 |
| Value | 0.0000 | -3.400000 | 0.52572889E+00 |
| Value | 0.0000 | -3.390000 | 0.99697782E+00 |
| Value | 0.0000 | -3.380000 | 0.97017401E+00 |
| Value | 0.0000 | -3.370000 | 0.76690068E-01 |
| Value | 0.0000 | -3.360000 | 0.65180288E+00 |
| Value | 0.0000 | -3.350000 | 0.91149142E-01 |
| Value | 0.0000 | -3.340000 | 0.55435669E+00 |
| Value | 0.0000 | -3.330000 | 0.78091884E+00 |
| Value | 0.0000 | -3.320000 | 0.82541535E+00 |
| Value | 0.0000 | -3.310000 | 0.79649338E+00 |
| Value | 0.0000 | -3.300000 | 0.72273498E+00 |
| Value | 0.0000 | -3.290000 | 0.80582563E+00 |
| Value | 0.0000 | -3.280000 | 0.99113612E+00 |
| Value | 0.0000 | -3.270000 | 0.99944946E+00 |
| Value | 0.0000 | -3.260000 | 0.98089019E+00 |
| Value | 0.0000 | -3.250000 | 0.34866254E+00 |
| Value | 0.0000 | -3.240000 | 0.80427201E+00 |
| Value | 0.0000 | -3.230000 | 0.10280973E+01 |
| Value | 0.0000 | -3.220000 | 0.10774430E+01 |
| Value | 0.0000 | -3.210000 | 0.99631329E+00 |
| Value | 0.0000 | -3.200000 | 0.11419407E+01 |
| Value | 0.0000 | -3.190000 | 0.78964694E+00 |
| X   | Y   | Value         |
|-----|-----|---------------|
| 0.0000 | -3.180000 | 0.77838727E+00 |
| 0.0000 | -3.170000 | 0.12652009E+01 |
| 0.0000 | -3.160000 | 0.10966078E+01 |
| 0.0000 | -3.150000 | 0.12197723E+01 |
| 0.0000 | -3.140000 | 0.12790068E+01 |
| 0.0000 | -3.130000 | 0.99891612E+00 |
| 0.0000 | -3.120000 | 0.12284234E+01 |
| 0.0000 | -3.110000 | 0.10230287E+01 |
| 0.0000 | -3.100000 | 0.10131873E+01 |
| 0.0000 | -3.090000 | 0.14859354E+01 |
| 0.0000 | -3.080000 | 0.11383726E+01 |
| 0.0000 | -3.070000 | 0.10832137E+01 |
| 0.0000 | -3.060000 | 0.70474129E+00 |
| 0.0000 | -3.050000 | 0.83114497E+00 |
| 0.0000 | -3.040000 | 0.12279884E+01 |
| 0.0000 | -3.030000 | 0.11348148E+01 |
| 0.0000 | -3.020000 | 0.18572412E+01 |
| 0.0000 | -3.010000 | 0.15447665E+01 |
| 0.0000 | -3.000000 | 0.11718278E+01 |
**TABLE I. Physical meaning of the program parameters that are read on unit 5**

| Parameter   | Description                                                                 |
|-------------|-----------------------------------------------------------------------------|
| width       | width of the sample, $M$ (integer*4)                                        |
| length      | length of the sample, $L$ (integer*4)                                       |
| modes       | number of modes in the leads, $m$ (integer*4)                               |
| phimax      | half the width of the random flux distribution, $\phi_{max}$ (real*8)       |
| hmag        | uniform magnetic field in the sample, $h_{\perp}$ (real*8)                 |
| loteria     | seed for the pseudorandom number generator (integer*4)                      |
| ntimes      | number of samples in the statistical ensemble (integer*4)                   |
| W1          | initial width ($W$) of diagonal disorder distribution (real*8)              |
| W2          | final width ($W$) of diagonal disorder distribution (real*8)                |
| W3          | step in the disorder analysis (real*8)                                      |
| energy1     | initial Fermi energy ($E$) (real*8)                                         |
| energy2     | final Fermi energy ($E$) (real*8)                                           |
| energy3     | step in the Fermi energy analysis (real*8)                                  |