Proyecto

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```
Clear["Global`*"]
```
borra

```
Zigzag = 4.;
Armchair = 4.;

NZigzag = 1. + 2 * Zigzag;
NArmchair = 2 * Armchair;

NEdos = 1 * NZigzag * NArmchair;

t = -1.;
```

```
(*   Notacion {n;...} ={0,...,0,1,0,...,0;...}  *)

Base = Table[ Table[ -0. , {i, 1, 6}] , {j, 1, 1}];
```
tabla tabla

```
Base = Flatten[ Table[   Base   , {i, 1, NZigzag * NArmchair , 1}] , 1];
```
aplana tabla

```
Do[    Do[   Base[[i, 1]] = j   , {i, 1 + 1 * (j - 1), 1 + 1 * (j - 1), 1}]    ,
```
repite repite

```
  {j, 1., NZigzag * NArmchair , 1.}];

Print[  Style["Base ", 18, Bold, Purple]  ]
```
escribe estilo negrita púrpura

```
MatrixForm[ Base ]
```
forma de matriz

Base

1.	0.	0.	0.	0.	0.
2.	0.	0.	0.	0.	0.
3.	0.	0.	0.	0.	0.
4.	0.	0.	0.	0.	0.
5.	0.	0.	0.	0.	0.
6.	0.	0.	0.	0.	0.
7.	0.	0.	0.	0.	0.
8.	0.	0.	0.	0.	0.
9.	0.	0.	0.	0.	0.
10.	0.	0.	0.	0.	0.
11.	0.	0.	0.	0.	0.
12.	0.	0.	0.	0.	0.
13.	0.	0.	0.	0.	0.
14.	0.	0.	0.	0.	0.
15.	0.	0.	0.	0.	0.

```
16.  0.  0.  0.  0.  0.
17.  0.  0.  0.  0.  0.
18.  0.  0.  0.  0.  0.
19.  0.  0.  0.  0.  0.
20.  0.  0.  0.  0.  0.
21.  0.  0.  0.  0.  0.
22.  0.  0.  0.  0.  0.
23.  0.  0.  0.  0.  0.
24.  0.  0.  0.  0.  0.
25.  0.  0.  0.  0.  0.
26.  0.  0.  0.  0.  0.
27.  0.  0.  0.  0.  0.
28.  0.  0.  0.  0.  0.
29.  0.  0.  0.  0.  0.
30.  0.  0.  0.  0.  0.
31.  0.  0.  0.  0.  0.
32.  0.  0.  0.  0.  0.
33.  0.  0.  0.  0.  0.
34.  0.  0.  0.  0.  0.
35.  0.  0.  0.  0.  0.
36.  0.  0.  0.  0.  0.
37.  0.  0.  0.  0.  0.
38.  0.  0.  0.  0.  0.
39.  0.  0.  0.  0.  0.
40.  0.  0.  0.  0.  0.
41.  0.  0.  0.  0.  0.
42.  0.  0.  0.  0.  0.
43.  0.  0.  0.  0.  0.
44.  0.  0.  0.  0.  0.
45.  0.  0.  0.  0.  0.
46.  0.  0.  0.  0.  0.
47.  0.  0.  0.  0.  0.
48.  0.  0.  0.  0.  0.
49.  0.  0.  0.  0.  0.
50.  0.  0.  0.  0.  0.
51.  0.  0.  0.  0.  0.
52.  0.  0.  0.  0.  0.
53.  0.  0.  0.  0.  0.
54.  0.  0.  0.  0.  0.
55.  0.  0.  0.  0.  0.
56.  0.  0.  0.  0.  0.
57.  0.  0.  0.  0.  0.
58.  0.  0.  0.  0.  0.
59.  0.  0.  0.  0.  0.
60.  0.  0.  0.  0.  0.
61.  0.  0.  0.  0.  0.
62.  0.  0.  0.  0.  0.
63.  0.  0.  0.  0.  0.
64.  0.  0.  0.  0.  0.
65.  0.  0.  0.  0.  0.
66.  0.  0.  0.  0.  0.
67.  0.  0.  0.  0.  0.
68.  0.  0.  0.  0.  0.
69.  0.  0.  0.  0.  0.
70.  0.  0.  0.  0.  0.
71.  0.  0.  0.  0.  0.
72.  0.  0.  0.  0.  0.
```

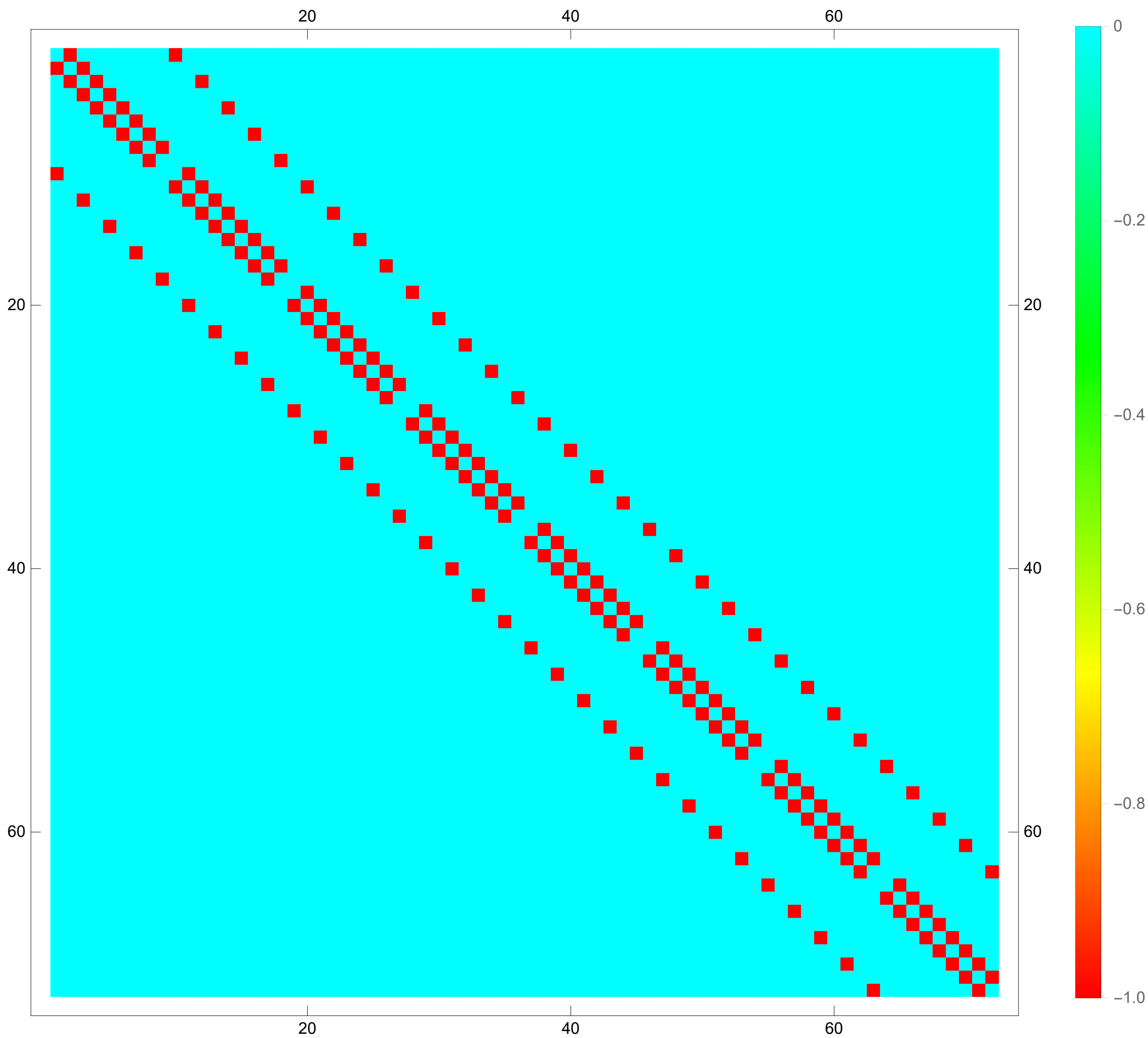
```
(********************** ----- HAMILTONIANO
  en Espacio de Estados ----- **********************)


HEdoBase = Table[Table[ 0. , {i, 1, NEdos, 1}], {j, 1, NEdos, 1}];
           tabla  tabla



(* NO DIAGONAL:  Transicion entre sitios*)

(*Transporte entre sitios*)
Base[[1]];
Base[[1 + 1]];
Base[[1]] + UnitVector[6, 1] ;
            vector unidad
(*   Notacion:  b_{n+1}^† b_n {n;...} = √1 √(0+1) {0,...,0,1-1,0+1,...,0;...} = {n+1;...} *)


Do[ Do[ HEdoBase[[i, i + 1]] = t , {i,   1 + 1 * NZigzag * (j - 1) ,
rep··repite
    1 * (  NZigzag - 1 + (j - 1) * NZigzag  )   , 1}] , {j, 1, NArmchair, 1} ]
(*Para interacciones entre filas  {n;...} y {n+1;...} en direccion zigzag *)


Do[ Do[ HEdoBase[[  i + 1 * (j - 1),  i + 1 * (j - 1 + NZigzag) ]] = t , {i,  1 ,  1  , 1}] ,
rep··repite
 {j, 1,  (NArmchair - 1) * NZigzag  , 2} ]
(*Para interacciones entre filas  {n;...} y {n+1;...} en direccion zigzag *)



HEdoBase  = (HEdoBase + ConjugateTranspose[HEdoBase]);
                        transpuesto conjugado



(* Se ingresa las posiciones atomicas que actuaran de Fuente y Drenante *)
PosicionFuente = Table[  i  , {i, 1, NZigzag, 1}];  (*Table[   i   ,{i,1,NZigzag,1}]*)
                 tabla                                tabla
PosicionDrentante = Table[  NEdos - NZigzag + i  , {i, 1, NZigzag, 1}];
                    tabla

PosicionFuente =  Table  [  Round[{PosicionFuente[[i]] , PosicionFuente[[i]] }]  ,
                  tabla      entero más próximo
```

```
                    tabla       entero más próximo
   {i, 1, Length[PosicionFuente], 1}];
          longitud
(* Genera las posiciones correspondientes a la matriz *)
PosicionDrentante = Table [ Round[{PosicionDrentante[[i]] , PosicionDrentante[[i]] }] ,
                     tabla      entero más próximo
   {i, 1, Length[PosicionDrentante], 1}];
          longitud

(* Matrices de Autoenergías *)
   matrices
SigmaFuente = -i * tF *
   SparseArray[{   PosicionFuente → Table[1. , {i, 1, Length[PosicionFuente], 1} ]   },
   array disperso                    tabla              longitud
    {NEdos, NEdos}];
SigmaDrenante = -i * tD * SparseArray[{   PosicionDrentante →
                          array disperso
      Table[1. , {i, 1, Length[PosicionDrentante], 1} ]   }, {NEdos, NEdos}];
      tabla               longitud



HEdoBase I = HEdoBase - SigmaDrenante;
        número i



HEdoBase // MatrixForm;
           forma de matriz
MatrixPlot[HEdoBase , PlotTheme → "Detailed", ImageSize → Large, ColorFunction → Hue]
representación de matriz   tema de representación   tamaño de i···  grande  función de color  tonalidad


(*  Solución Numerica   *)
{eval, evec} = Eigensystem[HEdoBase,  1, Method → {"Arnoldi", "Criteria" → "RealPart"} ]
               autovalores y autovectores          método

Print[  Style["Energias Numericas ", 18, Bold, Purple]   ]
escribe  estilo                              negrita púrpura
Style[  MatrixForm[ eval ]  , {Medium, Bold, Purple}]
estilo   forma de matriz              tamaño··· negrita púrpura



(*  Solución Exacta:    Usa el mismo hamiltoniano de interacción   *)

t1 * HEdoBase  // MatrixForm;
                  forma de matriz

Print[  Style["Energias Exactas ", 18, Bold, Purple]   ]
escribe  estilo                              negrita púrpura
```

```
escribe     estilo                              negrita púrpura
Quiet[
silencioso
 Solve[ Det[    t1 * HEdoBase - En * IdentityMatrix[ Round[NEdos] ]    ] == 0  , En]    ]
 resuelve  determinante                   matriz identidad      entero más próximo

(*Eigenfunction*)
```

Set: Tag Times in

i {{0., -1., 0., 0., 0., 0., 0., 0., 0., -1., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., ≪22≫}, {-1., 0., -1., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., ≪22≫}, ≪48≫, ≪22≫} is Protected.



{{2.85911},
 {{0.0235754, -0.0298333, 0.0617212, -0.0482713, 0.0762916, -0.0482713, 0.0617212,
   -0.0298333, 0.0235754, -0.0375713, 0.0838451, -0.098363, 0.135664, -0.121583,
   0.135664, -0.098363, 0.0838451, -0.0375713, 0.0588429, -0.103788, 0.154053,
   -0.167932, 0.19042, -0.167932, 0.154053, -0.103788, 0.0588429, -0.0644503, 0.125428,
   -0.168733, 0.202946, -0.208566, 0.202946, -0.168733, 0.125428, -0.0644503,
   0.0644503, -0.125428, 0.168733, -0.202946, 0.208566, -0.202946, 0.168733, -0.125428,
   0.0644503, -0.0588429, 0.103788, -0.154053, 0.167932, -0.19042, 0.167932,
   -0.154053, 0.103788, -0.0588429, 0.0375713, -0.0838451, 0.098363, -0.135664,
   0.121583, -0.135664, 0.098363, -0.0838451, 0.0375713, -0.0235754, 0.0298333,
   -0.0617212, 0.0482713, -0.0762916, 0.0482713, -0.0617212, 0.0298333, -0.0235754}}}

Energias Numericas

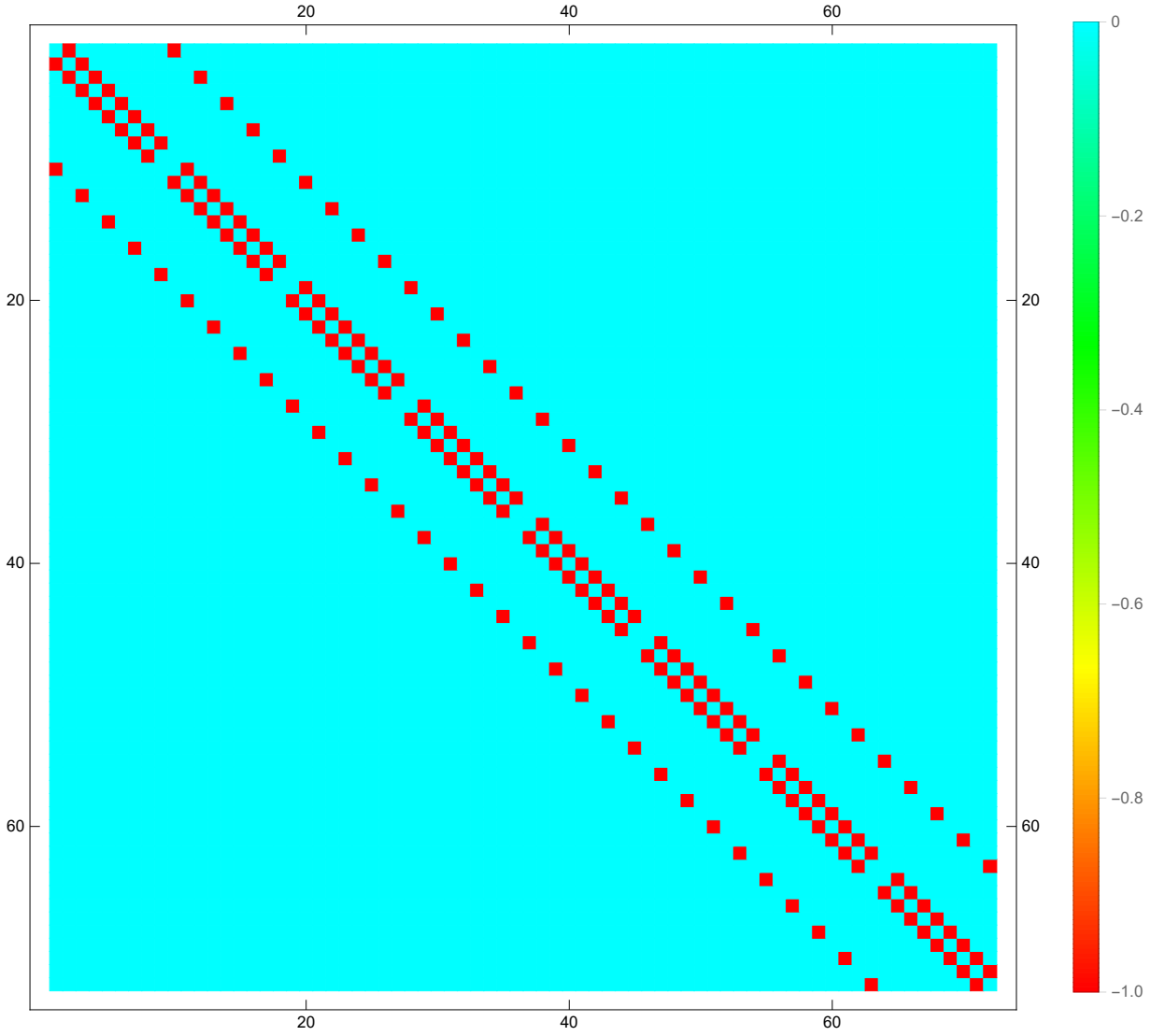
(2.85911)

Energias Exactas

$$\{\{En \to -2.85923\, t1\}, \{En \to -2.72777\, t1\}, \{En \to -2.63632\, t1\},$$
$$\{En \to (-2.53328 - 0.116669\, i)\, t1\}, \{En \to (-2.53328 + 0.116669\, i)\, t1\},$$
$$\{En \to (-2.35283 - 0.202545\, i)\, t1\}, \{En \to (-2.35283 + 0.202545\, i)\, t1\},$$
$$\{En \to (-2.15729 - 0.266044\, i)\, t1\}, \{En \to (-2.15729 + 0.266044\, i)\, t1\},$$
$$\{En \to (-1.95512 - 0.289793\, i)\, t1\}, \{En \to (-1.95512 + 0.289793\, i)\, t1\},$$
$$\{En \to (-1.75338 - 0.279317\, i)\, t1\}, \{En \to (-1.75338 + 0.279317\, i)\, t1\},$$
$$\{En \to -1.59922\, t1\}, \{En \to (-1.5669 - 0.251103\, i)\, t1\}, \{En \to (-1.5669 + 0.251103\, i)\, t1\},$$
$$\{En \to (-1.40334 - 0.138558\, i)\, t1\}, \{En \to (-1.40334 + 0.138558\, i)\, t1\},$$
$$\{En \to (-1.38489 - 0.223217\, i)\, t1\}, \{En \to (-1.38489 + 0.223217\, i)\, t1\},$$
$$\{En \to -1.36007\, t1\}, \{En \to (-1.23802 - 0.242747\, i)\, t1\}, \{En \to (-1.23802 + 0.242747\, i)\, t1\},$$
$$\{En \to (-1.12409 - 0.242117\, i)\, t1\}, \{En \to (-1.12409 + 0.242117\, i)\, t1\},$$
$$\{En \to (-1.03483 - 0.222828\, i)\, t1\}, \{En \to (-1.03483 + 0.222828\, i)\, t1\}, \{En \to -1.00442\, t1\},$$
$$\{En \to (-0.973345 - 0.191176\, i)\, t1\}, \{En \to (-0.973345 + 0.191176\, i)\, t1\}, \{En \to -0.945638\, t1\},$$
$$\{En \to (-0.928138 - 0.169418\, i)\, t1\}, \{En \to (-0.928138 + 0.169418\, i)\, t1\},$$
$$\{En \to (-0.874899 - 0.138161\, i)\, t1\}, \{En \to (-0.874899 + 0.138161\, i)\, t1\},$$
$$\{En \to (-0.828222 - 0.0881248\, i)\, t1\}, \{En \to (-0.828222 + 0.0881248\, i)\, t1\},$$
$$\{En \to (-0.776174 - 0.0187978\, i)\, t1\}, \{En \to (-0.776174 + 0.0187978\, i)\, t1\},$$
$$\{En \to -0.725686\, t1\}, \{En \to -0.649652\, t1\}, \{En \to -0.524734\, t1\}, \{En \to -0.32382\, t1\},$$
$$\{En \to -0.013183\, t1\}, \{En \to 0.013183\, t1\}, \{En \to 0.32382\, t1\}, \{En \to 0.524734\, t1\},$$
$$\{En \to 0.649652\, t1\}, \{En \to 0.725686\, t1\}, \{En \to (0.776174 - 0.0187978\, i)\, t1\},$$
$$\{En \to (0.776174 + 0.0187978\, i)\, t1\}, \{En \to (0.828222 - 0.0881248\, i)\, t1\},$$
$$\{En \to (0.828222 + 0.0881248\, i)\, t1\}, \{En \to (0.874899 - 0.138161\, i)\, t1\},$$
$$\{En \to (0.874899 + 0.138161\, i)\, t1\}, \{En \to (0.928138 - 0.169418\, i)\, t1\},$$
$$\{En \to (0.928138 + 0.169418\, i)\, t1\}, \{En \to 0.945638\, t1\}, \{En \to (0.973345 - 0.191176\, i)\, t1\},$$
$$\{En \to (0.973345 + 0.191176\, i)\, t1\}, \{En \to 1.00442\, t1\}, \{En \to (1.03483 - 0.222828\, i)\, t1\},$$
$$\{En \to (1.03483 + 0.222828\, i)\, t1\}, \{En \to (1.12409 - 0.242117\, i)\, t1\},$$
$$\{En \to (1.12409 + 0.242117\, i)\, t1\}, \{En \to (1.23802 - 0.242747\, i)\, t1\},$$
$$\{En \to (1.23802 + 0.242747\, i)\, t1\}, \{En \to 1.36007\, t1\}, \{En \to (1.38489 - 0.223217\, i)\, t1\},$$
$$\{En \to (1.38489 + 0.223217\, i)\, t1\}, \{En \to (1.40334 - 0.138558\, i)\, t1\},$$
$$\{En \to (1.40334 + 0.138558\, i)\, t1\}, \{En \to (1.5669 - 0.251103\, i)\, t1\},$$
$$\{En \to (1.5669 + 0.251103\, i)\, t1\}, \{En \to 1.59922\, t1\}, \{En \to (1.75338 - 0.279317\, i)\, t1\},$$
$$\{En \to (1.75338 + 0.279317\, i)\, t1\}, \{En \to (1.95512 - 0.289793\, i)\, t1\},$$
$$\{En \to (1.95512 + 0.289793\, i)\, t1\}, \{En \to (2.15729 - 0.266044\, i)\, t1\},$$
$$\{En \to (2.15729 + 0.266044\, i)\, t1\}, \{En \to (2.35283 - 0.202545\, i)\, t1\},$$
$$\{En \to (2.35283 + 0.202545\, i)\, t1\}, \{En \to (2.53328 - 0.116669\, i)\, t1\},$$
$$\{En \to (2.53328 + 0.116669\, i)\, t1\}, \{En \to 2.63632\, t1\}, \{En \to 2.72777\, t1\}, \{En \to 2.85923\, t1\}\}$$

```
(********************** ----- HAMILTONIANO
  en Espacio Real ----- **********************)
            real

(*Para este problema simplificado queda identico*)

HReal = HEdoBase ;
```

```
HEdoBase // MatrixForm;
            forma de matriz
MatrixPlot[HEdoBase , PlotTheme → "Detailed", ImageSize → Large, ColorFunction → Hue]
representación de matriz   tema de representación   tamaño de i···   grande   función de color   tonalidad


(* Para usar Green se requiere el
             verde
 Hamiltoniano discretiado (Matriz) en el espacio Real *)
                                                    real


(* Con Green obtendremos observables en función de la energía *)
       verde
Energia = En * IdentityMatrix[  Round[NEdos]  ];
             matriz identidad      entero más próximo


(* Se ingresa las posiciones atomicas que actuaran de Fuente y Drenante *)
PosicionFuente = Table[  i  , {i, 1, NZigzag, 1}];   (*Table[   i   ,{i,1,NZigzag,1}]*)
                 tabla                                 tabla
PosicionDrentante = Table[  NEdos - NZigzag + i  , {i, 1, NZigzag, 1}];
                    tabla

PosicionFuente =  Table  [  Round[{PosicionFuente[[i]] , PosicionFuente[[i]] }]  ,
                  tabla      entero más próximo
   {i, 1, Length[PosicionFuente], 1}];
          longitud
(* Genera las posiciones correspondientes a la matriz *)
PosicionDrentante =  Table  [  Round[{PosicionDrentante[[i]] , PosicionDrentante[[i]] }]  ,
                     tabla      entero más próximo
   {i, 1, Length[PosicionDrentante], 1}];
          longitud

(* Matrices de Autoenergías *)
   matrices
SigmaFuente = -i * tF *
   SparseArray[{    PosicionFuente → Table[1. , {i, 1, Length[PosicionFuente], 1} ]    },
   array disperso                   tabla                longitud
    {NEdos, NEdos}];
SigmaDrenante = -i * tD * SparseArray[{    PosicionDrentante →
                          array disperso
      Table[1. , {i, 1, Length[PosicionDrentante], 1} ]    }, {NEdos, NEdos}];
      tabla                longitud


tF = 1.;
tD = 1.;
t1 = 1.;
```




```
(********************** ----- I Operador ----- **********************)
```
número i

```
eval[[1]];
EdoBase = evec[[1]];
```

```
(*    I_i = i*(e/h)*2*π*( H Gn - Gn H )          Notacion:  b_{n+1}^† b_n {n;...} =
```

```
  √1 √0+1 {0,...,0,1-1,0+1,...,0;...} = {n+1;...} *)
(HEdoBase - SigmaFuente - SigmaDrenante) * GnMatrizDdensidad // MatrixForm;
                                                    forma de matriz

GnMatrizDensidad = Table[  Table[
                   tabla    tabla
    Conjugate[ EdoBase[[ j ]] ] * EdoBase[[ i ]]  , {i, 1, NEdos, 1}]  , {j, 1, NEdos, 1}];
    conjugado
GnMatrizDensidad // MatrixForm;
                    forma de matriz

IOperador = i * (  (HEdoBase  + SigmaDrenante) * GnMatrizDensidad  +
     GnMatrizDensidad  * (HEdoBase + SigmaDrenante)  ) ;

IVal = Im[IOperador];
       parte imaginaria
IVal // MatrixForm
        forma de matriz
```

```
ILocalY = Table[     Table[   -IVal[[il,  (jl - 1) * NZigzag + Mod[il - 1, NZigzag, 1] ]] +
          tabla      tabla                                    operación módulo
      IVal[[il,  (jl - 1) * NZigzag + Mod[il + 1, NZigzag, 1] ]]  ,
                                      operación módulo
    {il,  1 + (jl - 1) * NZigzag, jl * NZigzag, 1}]  , {jl, 1, NArmchair, 1}];
ILocalY = Flatten[ ILocalY];
          aplana

ILocalX =  Join[  Table[  IVal[[il, il + NZigzag ]]  ,
           junta  tabla
    {il, 1, NZigzag * (NArmchair - 1), 1} ] , Table[ 0., {jl, 1, NZigzag, 1}]  ];
                                                tabla

ILocal =
  Table[ {   { 1. + IntegerPart[  (i - 1) / (NZigzag ) ],  Mod[ i, NZigzag, 1.]  } ,
  tabla              parte entera                          operación módulo
    {ILocalX[[i]],  ILocalY[[i]] }  } ,  {i, 1, NEdos, 1.}];

ListVectorPlot[  ILocal  , ImageSize → Large, VectorColorFunction → "Rainbow",
representación vectorial de lista  tamaño de i···  grande  función de color de vector
 VectorPoints → 10, VectorScale → 0.08, PlotLegends → Automatic]
 número de puntos de ve··  escala de vector  leyendas de rep···  automático
ListStreamPlot[  ILocal  , ImageSize → Large, VectorColorFunction → "Rainbow",
representación de flujo de lista  tamaño de i···  grande  función de color de vector
```

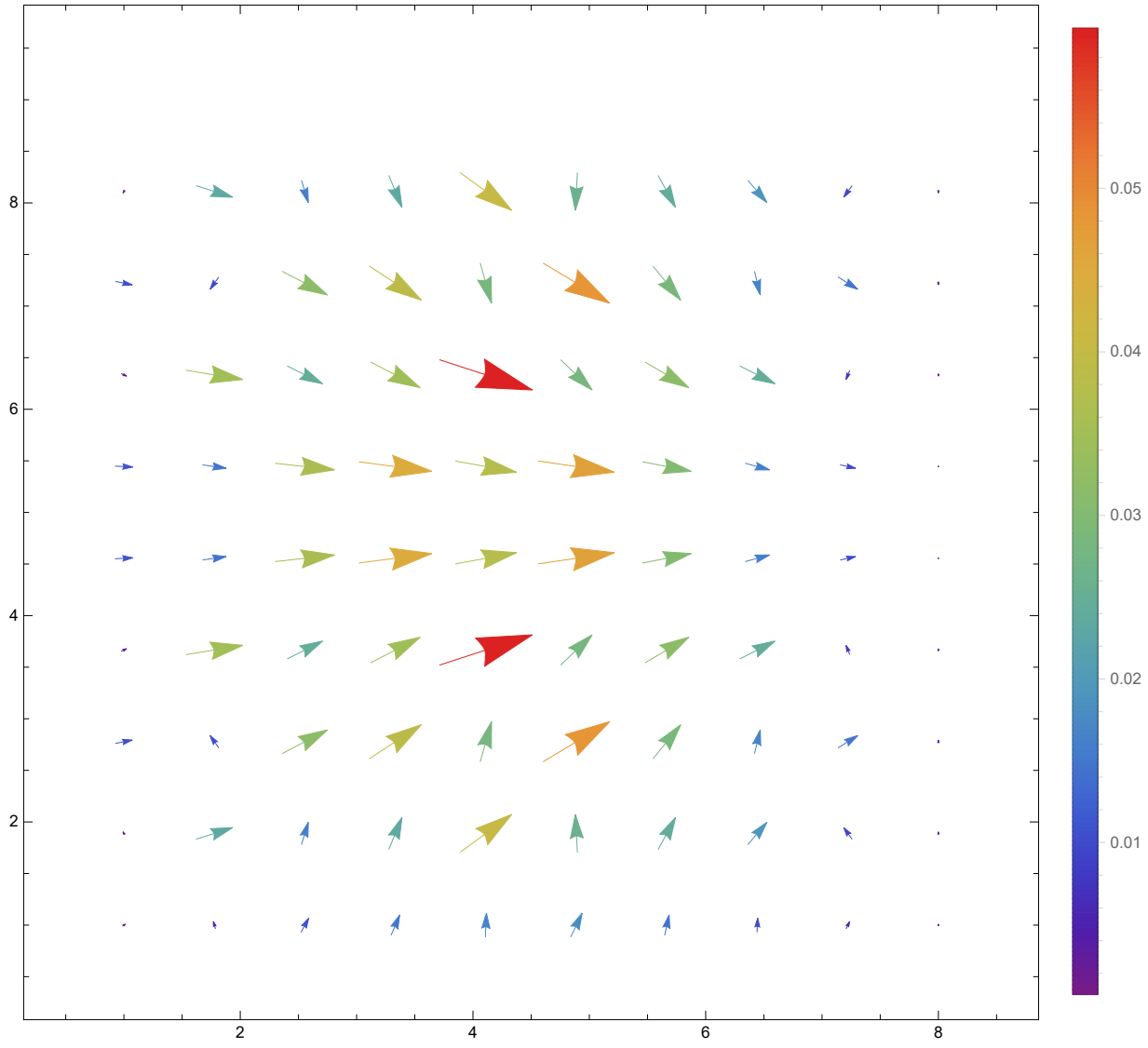
```
representación de flujo de lista    tamaño de f···  grande  función de color de vector
 VectorPoints → 10, VectorScale → 0.08, PlotLegends → Automatic]
                    escala de vector          leyendas de rep··· automático
```

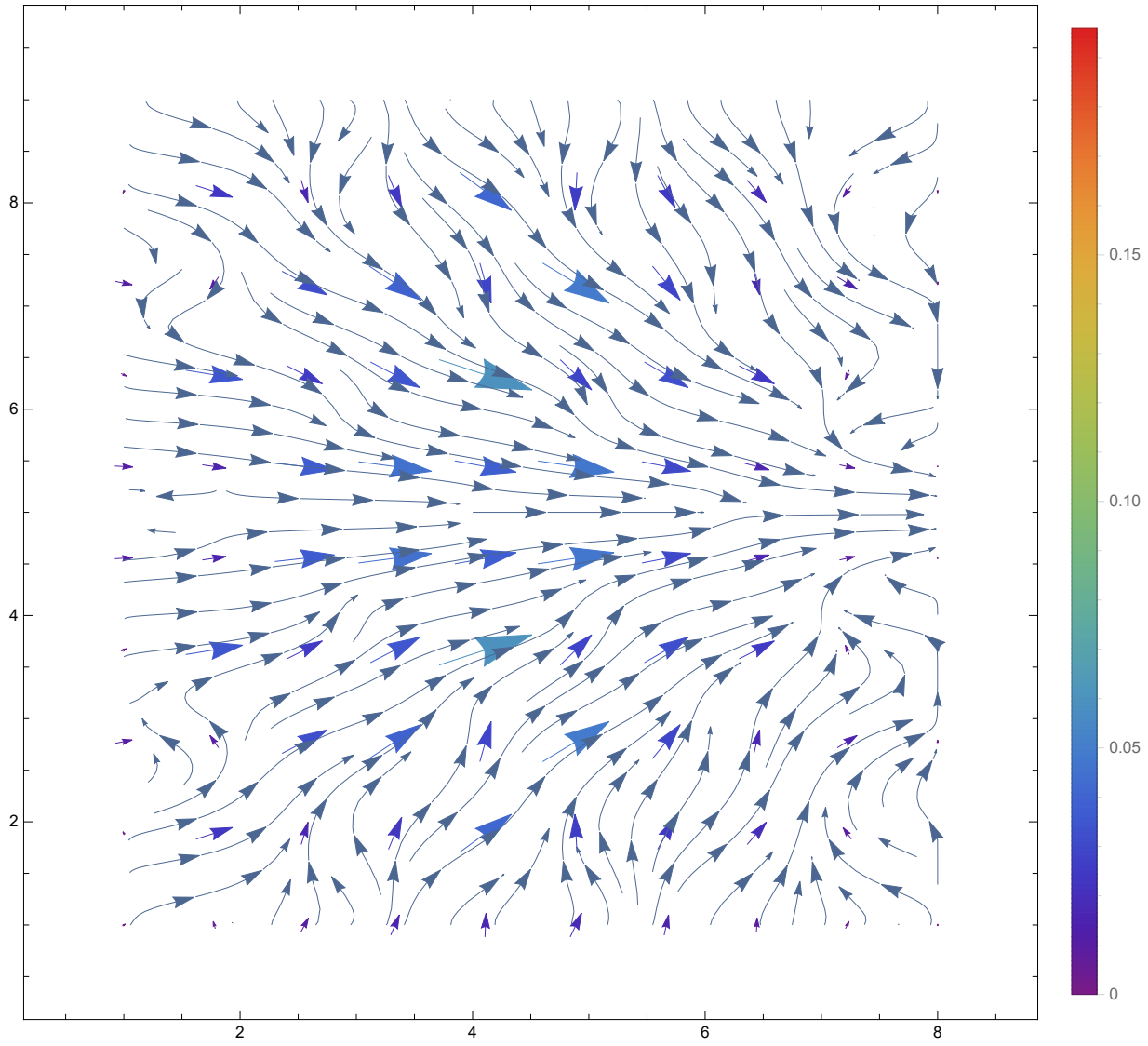
```
Clear[En]
borra
```

(* $J_i = 2*J*\left(b_{i+1}^{\dagger}\, b_i - b_{i-1}^{\dagger}\, b_i\right)$ Notacion: $b_{n+1}^{\dagger}\, b_n$ {n;...} = $\sqrt{1}\,\sqrt{0+1}$ {0,...,0,1-1,0+1,...,0;...} = {n+1;...} *)

0.	0.00140666	0.	0.	0.	0.	0.	0.
0.00140666	0.	0.00368269	0.	0.	0.	0.	0.
0.	0.00368269	0.	0.00595872	0.	0.	0.	0.
0.	0.	0.00595872	0.	0.00736538	0.	0.	0.
0.	0.	0.	0.00736538	0.	0.00736538	0.	0.
0.	0.	0.	0.	0.00736538	0.	0.00595872	0.
0.	0.	0.	0.	0.	0.00595872	0.	0.00368269
0.	0.	0.	0.	0.	0.	0.00368269	0.
0.	0.	0.	0.	0.	0.	0.	0.00140666
0.00177152	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.0121422	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.0185516	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.0121422	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.
0.	0.	0.	0.	0.	0.	0.	0.

```
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
0.      0.      0.      0.      0.      0.      0.      0.
```


8
6
4
2
2
4
6
8
0.05
0.04
0.03
0.02
0.01


8
6
4
2
2
4
6
8
0.15
0.10
0.05
0

```
(* Con Green obtendremos observables en función de la energía *)
EnMin = -4.;
EnMax = 4.;
NEnPuntos = 501.;

DEn = Abs[EnMax - EnMin] / (NEnPuntos - 1.);
EnergiasValores = Table[ (i) , {i, EnMin, EnMax, DEn} ];

Energia = Table[ (i) * IdentityMatrix[ Round[NEdos] ] , {i, EnMin, EnMax, DEn} ];

(*Broadening Matrix*)
GammaFuente = i * ( SigmaFuente - ConjugateTranspose[ SigmaFuente ]);
GammaDrenante = i * ( SigmaDrenante - ConjugateTranspose[ SigmaDrenante ]);

(*Funcion de Green del Nanosistema*)
FGreen = Table[ Inverse[
    Energia [[i]] - HEdoBase - SigmaFuente - SigmaDrenante ] , {i, 1, NEnPuntos, 1}];

(*Funcion de Transmision*)
Print[ Style["Función de Transmisión", 18, Bold, Purple] ]
FTranmision =
  Table[ { EnMin + DEn * (i - 1) , Tr[ GammaDrenante. FGreen[[i]] .GammaFuente.
      ConjugateTranspose[ FGreen[[i]] ] ] } , {i, 1, NEnPuntos, 1}];
```

```
ListPlot[  FTranmision  , PlotStyle → {{PointSize[0.01], Red}},
representación de lista   estilo de represe···  tamaño de punto  rojo
 LabelStyle → {14, Black}, AxesLabel → {"E" , "T(E)"}, ImageSize → Large,  Joined → True]
 estilo de etiqueta  negro  etiqueta de ejes  númer···  núme···  tamaño de i···  grande  unido  verdade
```

```
(*Función Espectral*)
A =  Table[
     tabla
   i * ( FGreen[[i]] - ConjugateTranspose[ FGreen[[i]] ] )   , {i, 1, NEnPuntos, 1}];
                       transpuesto conjugado
```

```
(*DOS: Densidad de Estados*)
Print[  Style["DOS", 18, Bold, Purple]  ]
escribe  estilo  negrita  púrpura
DOS =  Table[
       tabla
   { EnMin + DEn * (i - 1)  ,   Re[ Tr[ A[[i]] ] / (2 * π)  ] }  , {i, 1, NEnPuntos, 1}];
                                par···  traza
```

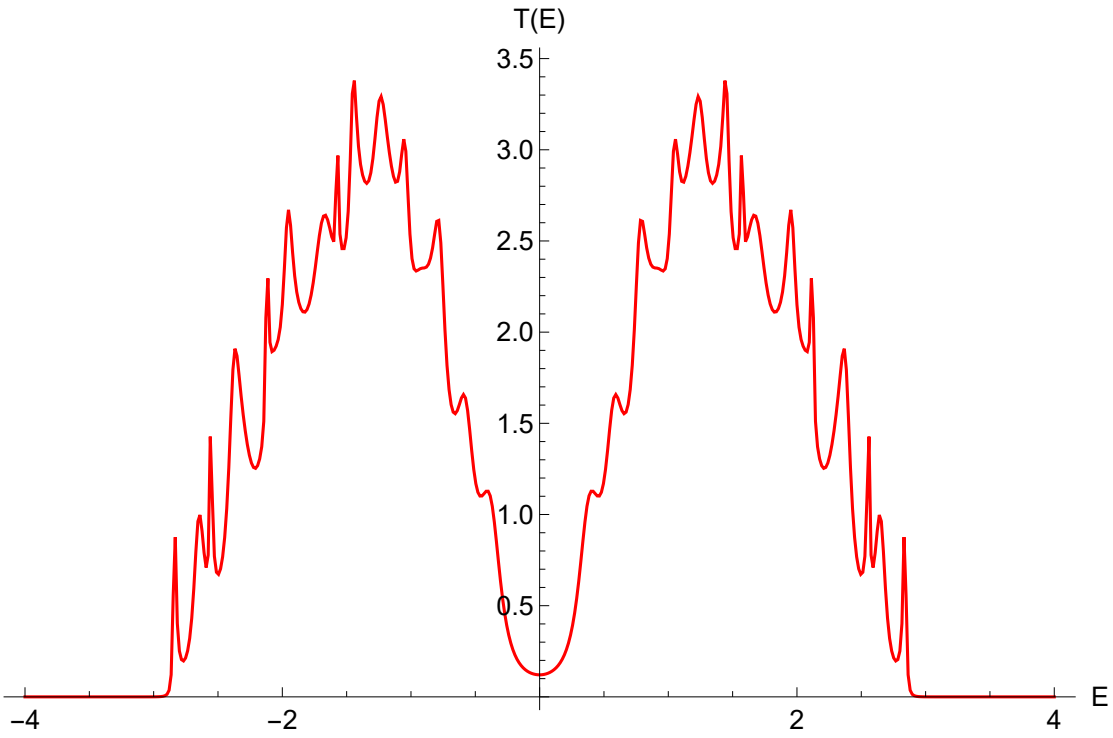
```
ListPlot[  DOS  , PlotStyle → {{PointSize[0.01], Red}}, LabelStyle → {14, Black},
representación de lista  estilo de represe···  tamaño de punto  rojo  estilo de etiqueta  negro
 AxesLabel → {"E" , "DOS(E)"}, ImageSize → Large,  Joined → True]
 etiqueta de ejes  número e  núme···  tamaño de i···  grande  unido  verdadero
```

```
(*LDOS: Densidad Local de Estados*)
Print[  Style["LDOS", 18, Bold, Purple]  ]
escribe  estilo  negrita  púrpura
LDOS =  Table[      Re[ Diagonal[ A[[i]] ] / (2 * π) ]     , {i, 1, NEnPuntos, 1}];
        tabla       pa···  diagonal
(*Los elementos de la Diagonal de A *)
                    diagonal
```

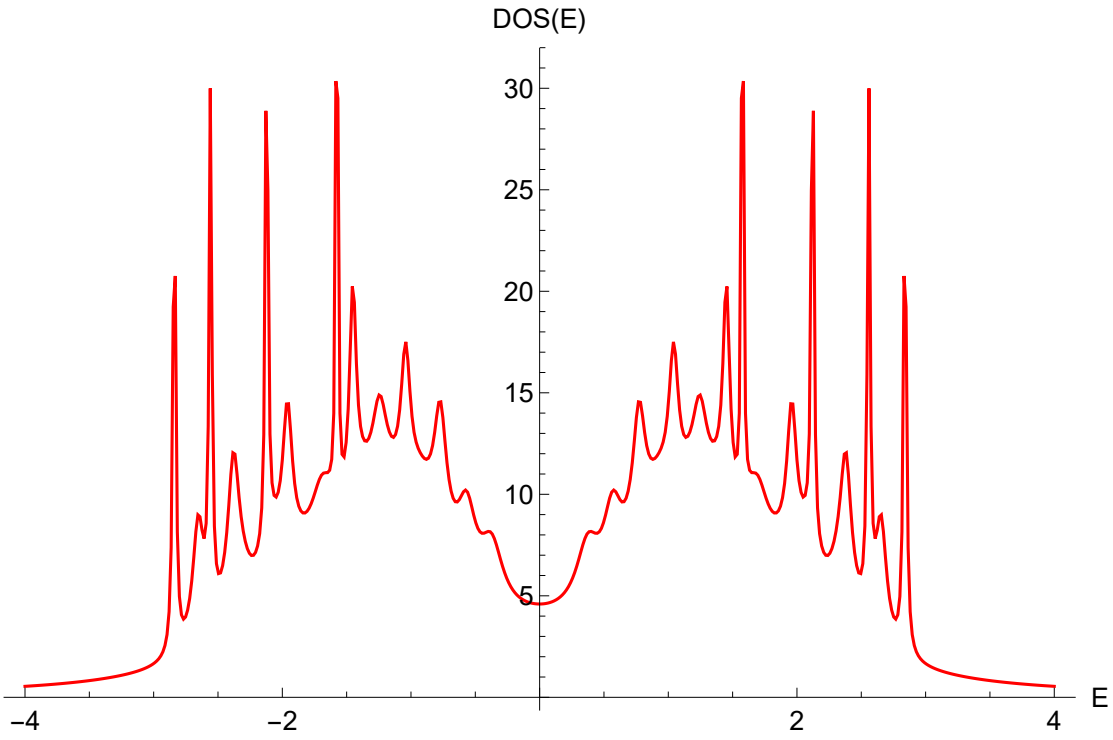
```
LDOSSitios = Table[        Table[   { EnMin + DEn * (i - 1)  ,   LDOS[[i, j]] }  ,
             tabla         tabla
    {i, 1, NEnPuntos, 1}]        ,  {j, 1, NEdos, 1}] ;
ListPlot[  LDOSSitios  , PlotStyle → {{PointSize[0.012], Blue},
representación de lista  estilo de represe··  tamaño de punto  azul
   {PointSize[0.015], Red}, {PointSize[0.01], Green}, {PointSize[0.006], Orange},
    tamaño de punto  rojo  tamaño de punto  verde  tamaño de punto  naranja
   {PointSize[0.003], Yellow}, {PointSize[0.008], Pink}}, LabelStyle → {14, Black},
    tamaño de punto  amarillo  tamaño de punto  rosa  estilo de etiqueta  negro
 AxesLabel → {"E" , "LDOS(E)"}, ImageSize → Large,  Joined → True]
             número e  núme···  tamaño de i···  grande  unido  verdadero
```

[Número e] [Nume] [Tamaño de f] [grande] [unido] [verdadero]

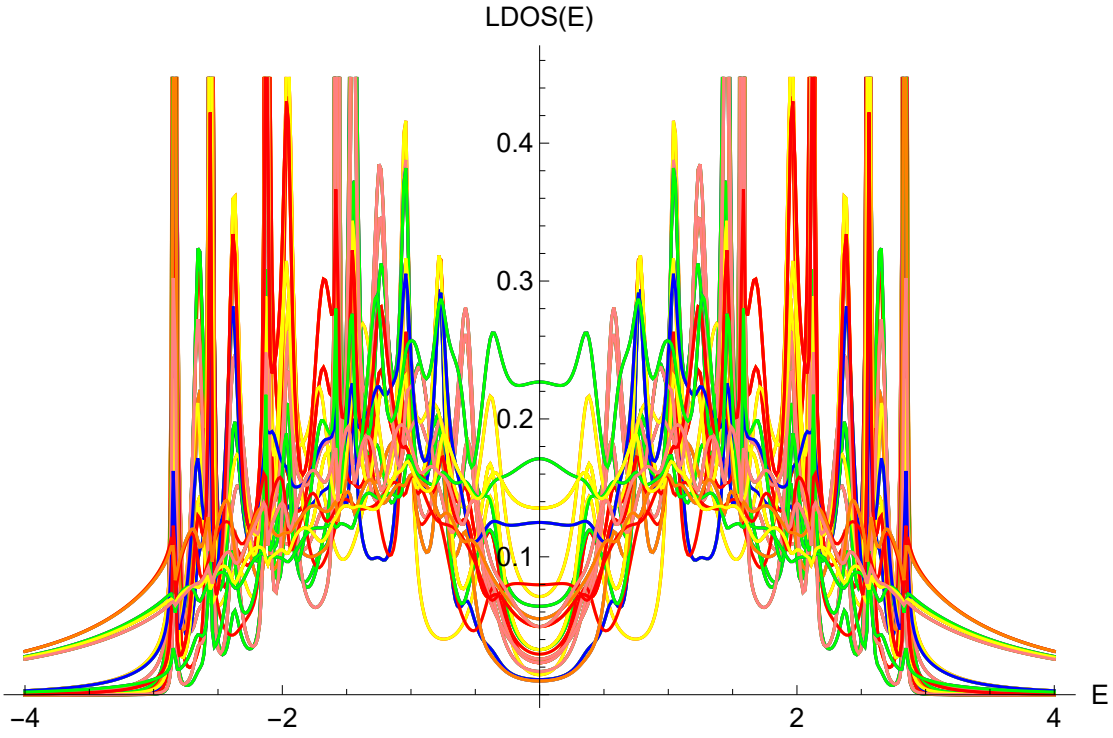
Función de Transmisión



DOS



LDOS

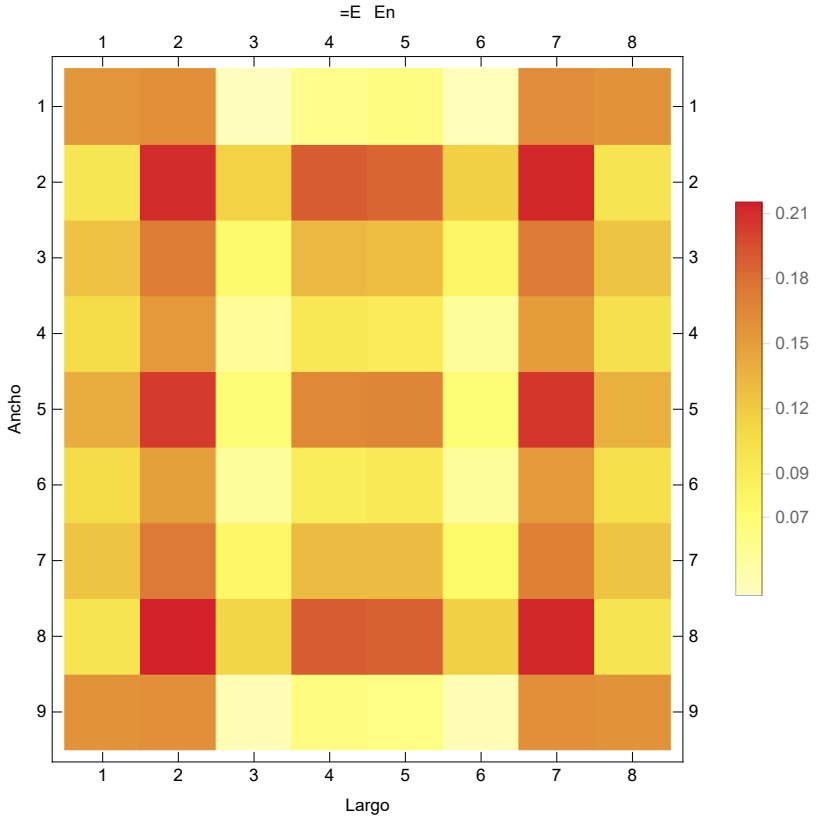


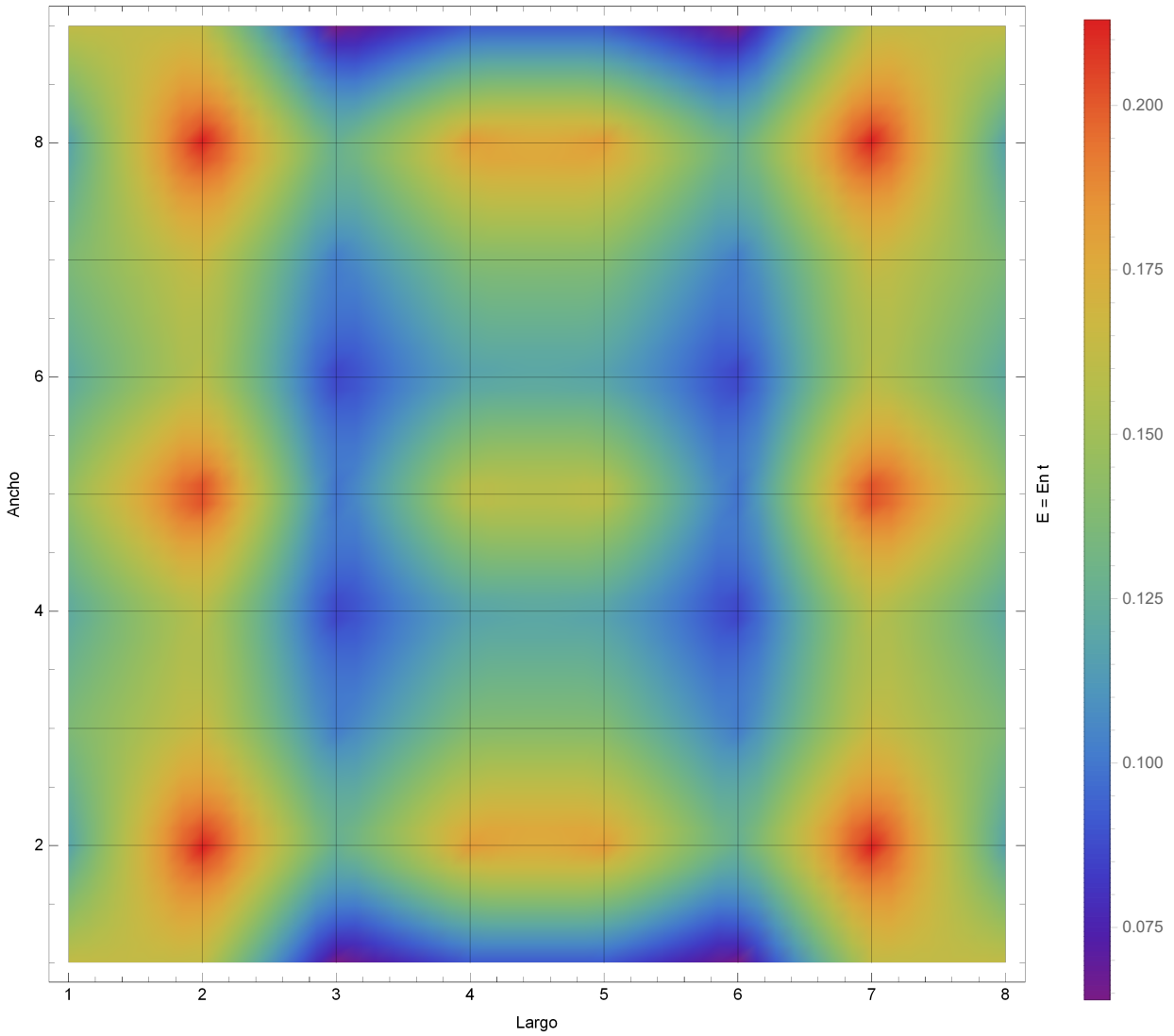
EnergiasValores

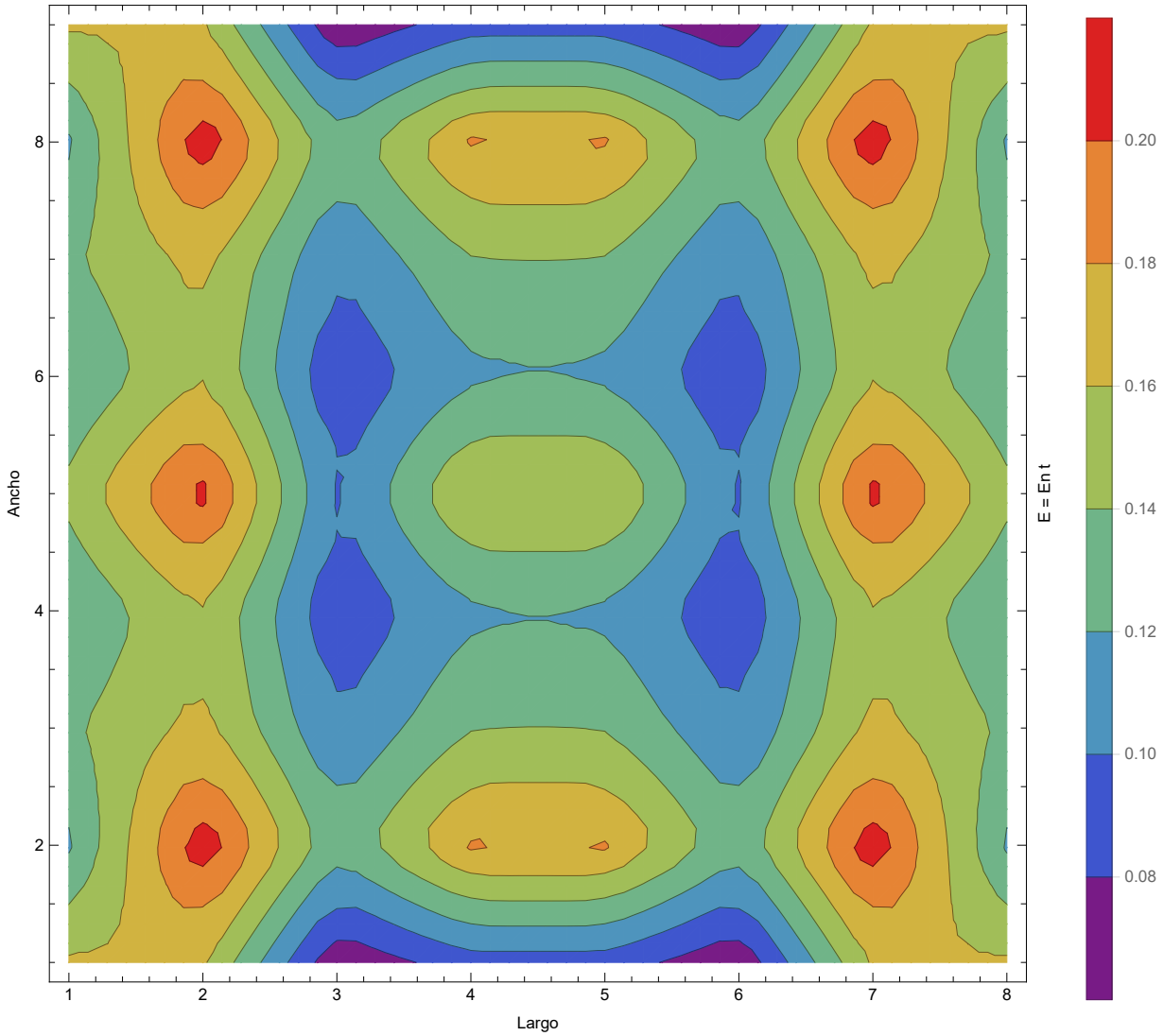
{−4., −3.984, −3.968, −3.952, −3.936, −3.92, −3.904, −3.888, −3.872, −3.856, −3.84,
−3.824, −3.808, −3.792, −3.776, −3.76, −3.744, −3.728, −3.712, −3.696, −3.68, −3.664,
−3.648, −3.632, −3.616, −3.6, −3.584, −3.568, −3.552, −3.536, −3.52, −3.504, −3.488,
−3.472, −3.456, −3.44, −3.424, −3.408, −3.392, −3.376, −3.36, −3.344, −3.328, −3.312,
−3.296, −3.28, −3.264, −3.248, −3.232, −3.216, −3.2, −3.184, −3.168, −3.152, −3.136,
−3.12, −3.104, −3.088, −3.072, −3.056, −3.04, −3.024, −3.008, −2.992, −2.976,
−2.96, −2.944, −2.928, −2.912, −2.896, −2.88, −2.864, −2.848, −2.832, −2.816, −2.8,
−2.784, −2.768, −2.752, −2.736, −2.72, −2.704, −2.688, −2.672, −2.656, −2.64,
−2.624, −2.608, −2.592, −2.576, −2.56, −2.544, −2.528, −2.512, −2.496, −2.48,
−2.464, −2.448, −2.432, −2.416, −2.4, −2.384, −2.368, −2.352, −2.336, −2.32, −2.304,
−2.288, −2.272, −2.256, −2.24, −2.224, −2.208, −2.192, −2.176, −2.16, −2.144,
−2.128, −2.112, −2.096, −2.08, −2.064, −2.048, −2.032, −2.016, −2., −1.984, −1.968,
−1.952, −1.936, −1.92, −1.904, −1.888, −1.872, −1.856, −1.84, −1.824, −1.808,
−1.792, −1.776, −1.76, −1.744, −1.728, −1.712, −1.696, −1.68, −1.664, −1.648,
−1.632, −1.616, −1.6, −1.584, −1.568, −1.552, −1.536, −1.52, −1.504, −1.488, −1.472,
−1.456, −1.44, −1.424, −1.408, −1.392, −1.376, −1.36, −1.344, −1.328, −1.312,
−1.296, −1.28, −1.264, −1.248, −1.232, −1.216, −1.2, −1.184, −1.168, −1.152, −1.136,
−1.12, −1.104, −1.088, −1.072, −1.056, −1.04, −1.024, −1.008, −0.992, −0.976,
−0.96, −0.944, −0.928, −0.912, −0.896, −0.88, −0.864, −0.848, −0.832, −0.816, −0.8,
−0.784, −0.768, −0.752, −0.736, −0.72, −0.704, −0.688, −0.672, −0.656, −0.64,
−0.624, −0.608, −0.592, −0.576, −0.56, −0.544, −0.528, −0.512, −0.496, −0.48, −0.464,
−0.448, −0.432, −0.416, −0.4, −0.384, −0.368, −0.352, −0.336, −0.32, −0.304, −0.288,
−0.272, −0.256, −0.24, −0.224, −0.208, −0.192, −0.176, −0.16, −0.144, −0.128, −0.112,
−0.096, −0.08, −0.064, −0.048, −0.032, −0.016, 0., 0.016, 0.032, 0.048, 0.064, 0.08,
0.096, 0.112, 0.128, 0.144, 0.16, 0.176, 0.192, 0.208, 0.224, 0.24, 0.256, 0.272, 0.288,
0.304, 0.32, 0.336, 0.352, 0.368, 0.384, 0.4, 0.416, 0.432, 0.448, 0.464, 0.48, 0.496,
0.512, 0.528, 0.544, 0.56, 0.576, 0.592, 0.608, 0.624, 0.64, 0.656, 0.672, 0.688, 0.704,
0.72, 0.736, 0.752, 0.768, 0.784, 0.8, 0.816, 0.832, 0.848, 0.864, 0.88, 0.896, 0.912,
0.928, 0.944, 0.96, 0.976, 0.992, 1.008, 1.024, 1.04, 1.056, 1.072, 1.088, 1.104, 1.12,
1.136, 1.152, 1.168, 1.184, 1.2, 1.216, 1.232, 1.248, 1.264, 1.28, 1.296, 1.312, 1.328,
1.344, 1.36, 1.376, 1.392, 1.408, 1.424, 1.44, 1.456, 1.472, 1.488, 1.504, 1.52, 1.536,
1.552, 1.568, 1.584, 1.6, 1.616, 1.632, 1.648, 1.664, 1.68, 1.696, 1.712, 1.728, 1.744,
1.76, 1.776, 1.792, 1.808, 1.824, 1.84, 1.856, 1.872, 1.888, 1.904, 1.92, 1.936, 1.952,
1.968, 1.984, 2., 2.016, 2.032, 2.048, 2.064, 2.08, 2.096, 2.112, 2.128, 2.144, 2.16,
2.176, 2.192, 2.208, 2.224, 2.24, 2.256, 2.272, 2.288, 2.304, 2.32, 2.336, 2.352, 2.368,
2.384, 2.4, 2.416, 2.432, 2.448, 2.464, 2.48, 2.496, 2.512, 2.528, 2.544, 2.56, 2.576,
2.592, 2.608, 2.624, 2.64, 2.656, 2.672, 2.688, 2.704, 2.72, 2.736, 2.752, 2.768, 2.784,
2.8, 2.816, 2.832, 2.848, 2.864, 2.88, 2.896, 2.912, 2.928, 2.944, 2.96, 2.976, 2.992,
3.008, 3.024, 3.04, 3.056, 3.072, 3.088, 3.104, 3.12, 3.136, 3.152, 3.168, 3.184, 3.2,
3.216, 3.232, 3.248, 3.264, 3.28, 3.296, 3.312, 3.328, 3.344, 3.36, 3.376, 3.392,
3.408, 3.424, 3.44, 3.456, 3.472, 3.488, 3.504, 3.52, 3.536, 3.552, 3.568, 3.584, 3.6,
3.616, 3.632, 3.648, 3.664, 3.68, 3.696, 3.712, 3.728, 3.744, 3.76, 3.776, 3.792,
3.808, 3.824, 3.84, 3.856, 3.872, 3.888, 3.904, 3.92, 3.936, 3.952, 3.968, 3.984, 4.}

```
(*LDOS en Espacio REAL*)
Print[  Style["LDOS", 18, Bold, Purple]  ]
escribe  estilo  negrita  púrpura
EnVal = -1.76;
NEn = 1. + ( EnVal - EnMin ) / DEn;


LDOSRealMatrix =  Table[
                  tabla
   SparseArray[ {{i_, i_} → 0.}, {NZigzag, NArmchair} ]    , {j, 1, NEnPuntos, 1}];
   array disperso
Do[  Do[  LDOSRealMatrix [[j,  Mod[ i, NZigzag, 1.] ,
repite  repite                 operación módulo
     1. + IntegerPart[  (i - 1) / NZigzag  ]  ]] = Re[ LDOS [[j, i]] ]  ,
        parte entera                          parte real
   {i, 1, NEdos, 1.}]    , {j, 1, NEnPuntos, 1}];

MatrixPlot[  LDOSRealMatrix [[NEn]] ,
representación de matriz
 PlotTheme → "Detailed", ColorFunction -> "TemperatureMap",
 tema de representación  función de color
 FrameLabel → {{"Largo", HoldForm["=E  "] En}, {"Ancho", None}}]
                         forma sin eva··  número e  ninguno


LDOSRealDensity =
  Table[  Table[ { 1. + IntegerPart[  (i - 1) / NZigzag ],  Mod[ i, NZigzag, 1.],
  tabla  tabla   parte entera                               operación módulo
     Re[ LDOS [[j, i]] ]} ,  {i, 1, NEdos, 1.}]    , {j, 1, NEnPuntos, 1}];
     parte real

ListDensityPlot[  LDOSRealDensity [[NEn]]  ,
representación de densidad de lista
 FrameLabel → {{"Ancho", StringTemplate["E = `1` t"][En]}, {"Largo", None}},
 etiqueta de marco  plantilla de cadena ···  número e  ninguno
 ImageSize → Large, ColorFunction → "Rainbow", InterpolationOrder → 1,
             grande  función de color  orden de interpolación
 MaxPlotPoints → 50, Mesh → {6, 7}, PlotLegends → Automatic]
 máximo número de punto··  malla  leyendas de rep···  automático
ListContourPlot[  LDOSRealDensity [[NEn]]  ,
representación de contornos de lista
 FrameLabel → {{"Ancho", StringTemplate["E = `1` t"][En]}, {"Largo", None}},
                         plantilla de cadena ···  número e  ninguno
 ImageSize → Large, ColorFunction → "Rainbow", InterpolationOrder → 1,
             grande  función de color  orden de interpolación
 MaxPlotPoints → 50, Mesh → {6, 7}, PlotLegends → Automatic]
                     malla  leyendas de rep···  automático
```

LDOS

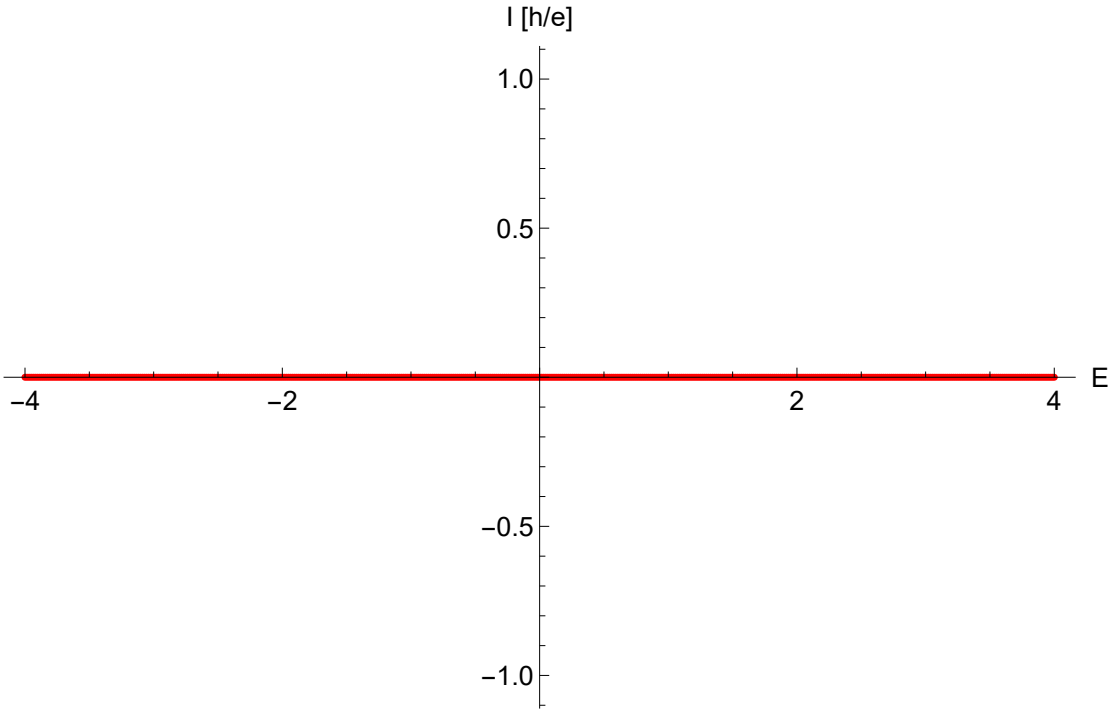



Ancho
Largo
E = En t
1
2
3
4
5
6
7
8
0.200
0.175
0.150
0.125
0.100
0.075


Ancho
Largo
E = En t
1
2
3
4
5
6
7
8
0.20
0.18
0.16
0.14
0.12
0.10
0.08

```
(********** -------- Corriente -------- **********)
Print[  Style["Corriente Total", 18, Bold, Purple]   ]
escribe  estilo  total  negrita púrpura
fFermi2 = 1;     (*Suponiendo Funciones de Fermi iguales a 1*)
SigmaDispersiva = GammaDrenante;    (*Energías de Dispersión, In-Scattering*)
                                                    entrada
FGreenIn =
  Table[      FGreen[[i]] . SigmaDispersiva. ConjugateTranspose[ FGreen[[i]] ]     ,
  tabla                                      transpuesto conjugado
   {i, 1, NEnPuntos, 1}];    (*Funcion de Green de Dispersión*)
                                          verde
IVal =  Table[      Im[ 2 * FGreenIn[[i]] * fFermi2 ]     , {i, 1, NEnPuntos, 1}];
        tabla       parte imaginaria
(*Matrices con los valores de las corrientes*)
  matrices
ITotal =  Table[
          tabla
   { EnMin + DEn * (i - 1)  ,     Tr[ IVal[[i]] ]   }     , {i, 1, NEnPuntos, 1}];
                                  traza
(*Corriente Total en Función de la Energía: Unidades (h/e)*)
            total
ListPlot[   ITotal   , PlotStyle → {{PointSize[0.0065], Red}},
representación de lista  estilo de represe··· tamaño de punto  rojo
 LabelStyle → {14, Black}, AxesLabel → {"E" , "I [h/e]"}, ImageSize → Large]
                  negro  etiqueta de ejes  nú···  número i  tamaño de i···  grande
```

Corriente Total


I [h/e]
1.0
0.5
−0.5
−1.0
−4
−2
2
4
E

EnergiasValores

```
{-4., -3.984, -3.968, -3.952, -3.936, -3.92, -3.904, -3.888, -3.872, -3.856, -3.84,
 -3.824, -3.808, -3.792, -3.776, -3.76, -3.744, -3.728, -3.712, -3.696, -3.68, -3.664,
 -3.648, -3.632, -3.616, -3.6, -3.584, -3.568, -3.552, -3.536, -3.52, -3.504, -3.488,
 -3.472, -3.456, -3.44, -3.424, -3.408, -3.392, -3.376, -3.36, -3.344, -3.328, -3.312,
 -3.296, -3.28, -3.264, -3.248, -3.232, -3.216, -3.2, -3.184, -3.168, -3.152, -3.136,
 -3.12, -3.104, -3.088, -3.072, -3.056, -3.04, -3.024, -3.008, -2.992, -2.976,
 -2.96, -2.944, -2.928, -2.912, -2.896, -2.88, -2.864, -2.848, -2.832, -2.816, -2.8,
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3.008, 3.024, 3.04, 3.056, 3.072, 3.088, 3.104, 3.12, 3.136, 3.152, 3.168, 3.184, 3.2,
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3.616, 3.632, 3.648, 3.664, 3.68, 3.696, 3.712, 3.728, 3.744, 3.76, 3.776, 3.792,
3.808, 3.824, 3.84, 3.856, 3.872, 3.888, 3.904, 3.92, 3.936, 3.952, 3.968, 3.984, 4.}
```
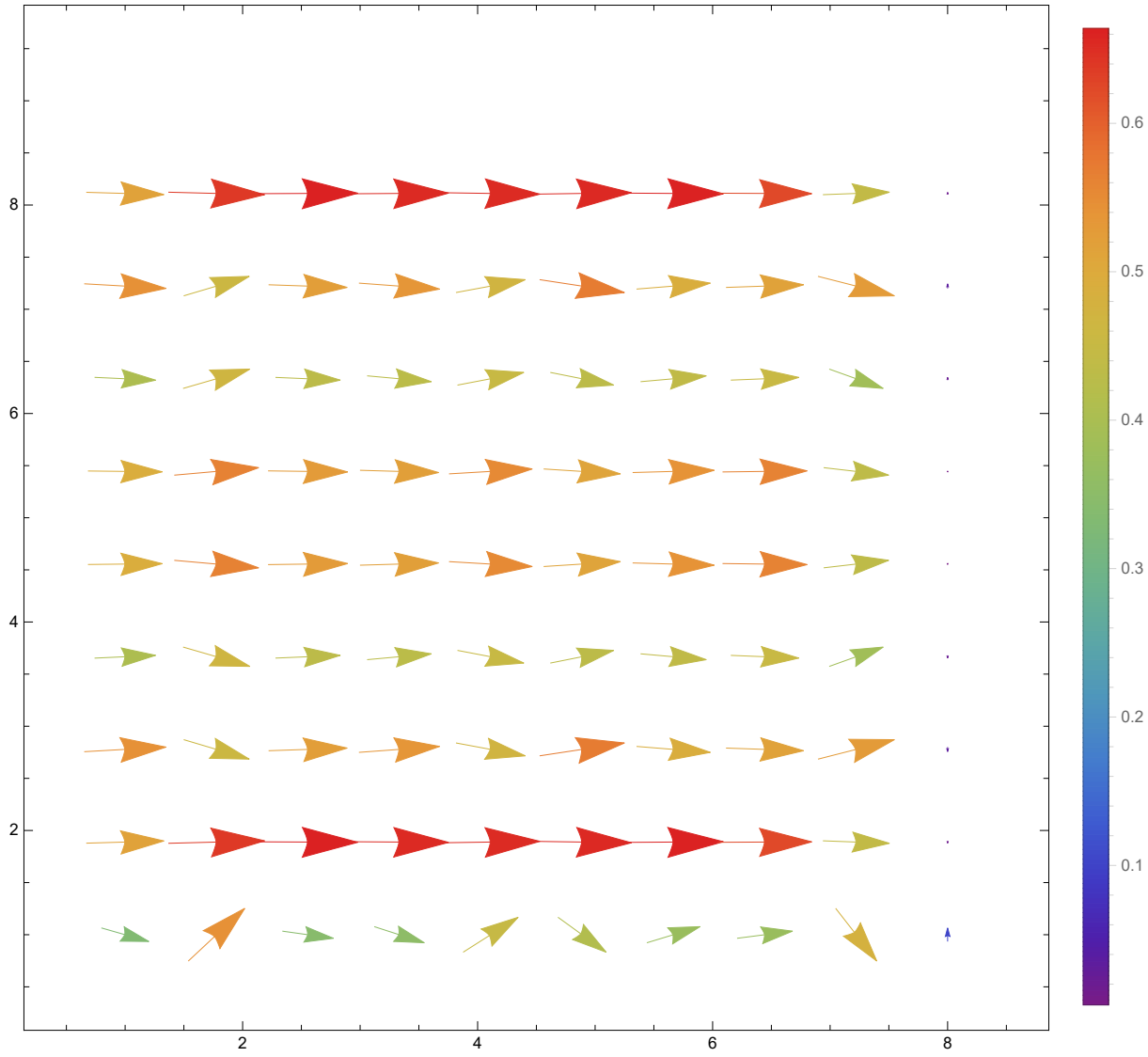
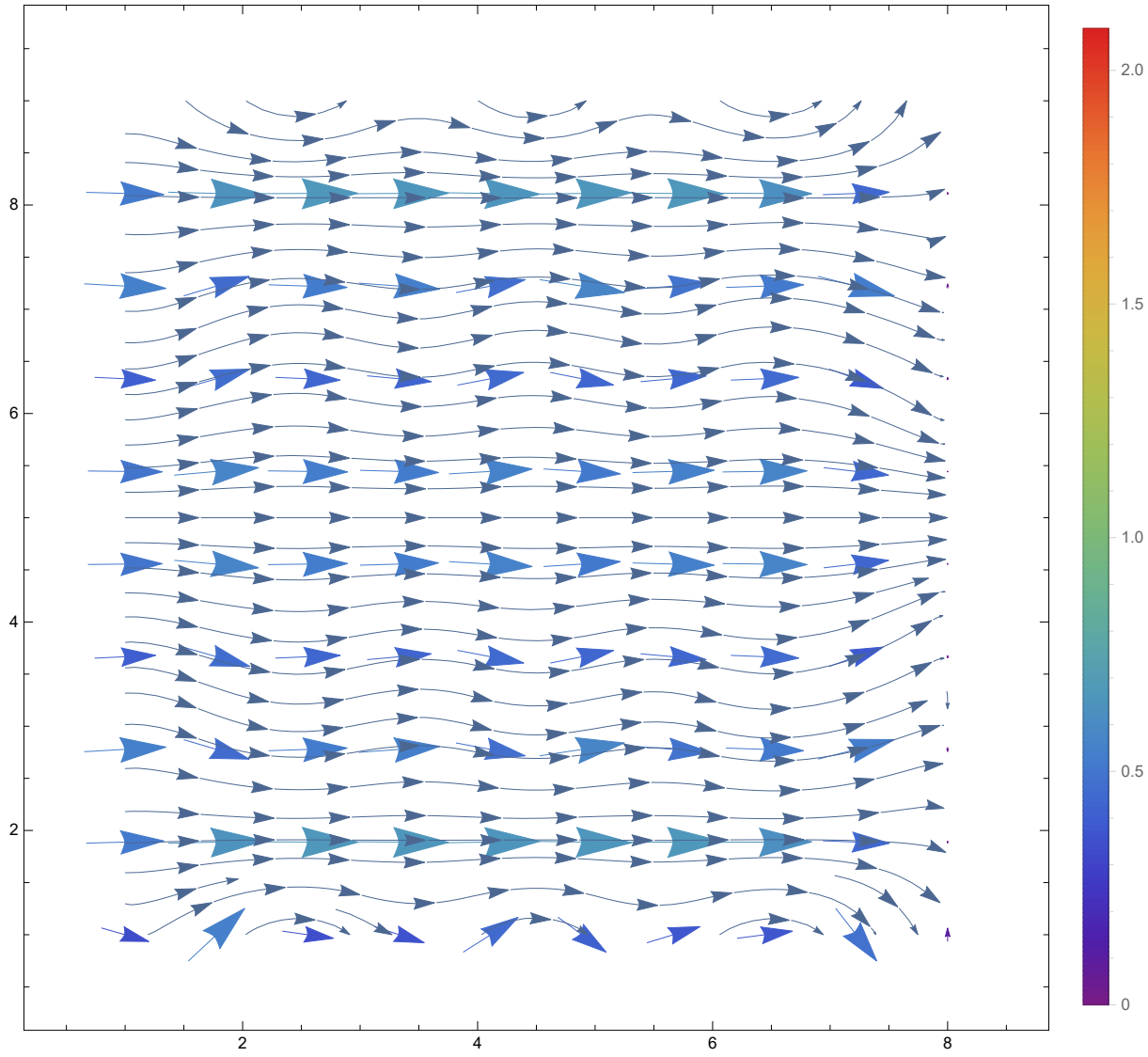

```
(*Corriente LOCAL*)
EnVal = -1.76;
NEn = 1. + ( EnVal - EnMin ) / DEn;

IVal[[ NEn ]] // MatrixForm;
                 forma de matriz


ILocalY = Table[     Table[   -IVal[[NEn, il,  (jl - 1) * NZigzag + Mod[il - 1, NZigzag, 1] ]] +
          tabla      tabla                                  operación módulo
      IVal[[NEn, il,  (jl - 1) * NZigzag + Mod[il + 1, NZigzag, 1] ]]  ,
                                  operación módulo
    {il,  1 + (jl - 1) * NZigzag, jl * NZigzag, 1}]  , {jl, 1, NArmchair, 1}];
ILocalY = Flatten[ ILocalY];
          aplana

ILocalX =  Join[  Table[  IVal[[NEn, il, il + NZigzag ]]  ,
           junta  tabla
    {il, 1, NZigzag * (NArmchair - 1), 1} ] , Table[ 0., {jl, 1, NZigzag, 1}]  ];
                                                tabla



ILocal =
  Table[ {   { 1. + IntegerPart[  (i - 1) / (NZigzag ) ],  Mod[ i, NZigzag, 1.]  } ,
  tabla              parte entera                          operación módulo
    {ILocalX[[i]],  ILocalY[[i]] }  } ,  {i, 1, NEdos, 1.}];


ListVectorPlot[   ILocal   , ImageSize → Large, VectorColorFunction → "Rainbow",
representación vectorial de lista   tamaño de i···  grande  función de color de vector
 VectorPoints → 10, VectorScale → 0.08, PlotLegends → Automatic]
                    escala de vector     leyendas de rep···  automático
ListStreamPlot[   ILocal   , ImageSize → Large, VectorColorFunction → "Rainbow",
                             tamaño de i···  grande  función de color de vector
 VectorPoints → 10, VectorScale → 0.08, PlotLegends → Automatic]
                    escala de vector     leyendas de rep···  automático
```


8
6
4
2
2
4
6
8
0.6
0.5
0.4
0.3
0.2
0.1


2
4
6
8
2
4
6
8
2.0
1.5
1.0
0.5
0