ANEXOS

Espectro y estados localizados en sistemas fermiónicos compuestos

Índice

1. ANEXO I: Códigos

#Definir primero num = longitud de la cadena; t0, t1, t2

Y en el caso de los aislantes: δ

1.1. Espectro metal

```
M = zeros(num);
[filas, columnas] = size(M)
for j=1:columnas-1
M(j,j+1)=t1;
end
for i=1:filas-1
M(i+1,i) = t1;
end
#Condiciones periodicas
M(1,columnas) = t1;
M(filas, 1) = t1;
E1des = eig(M);
```

1.2. Unión dos metales

```
A = zeros(num);
#metal 1
for j=1:columnas/2-1
A(j,j+1)=t1;
end
for i=1:filas/2-1
A(i+1,i) = t1;
end
#INTERSECCION
A(filas/2, columnas/2+1) = t0;
A(filas/2+1, columnas/2) = t0;
#metal 2
for k=columnas/2+1:columnas-1
A(k,k+1)=t2;
```

```
end
for l=filas/2+1: filas-1
A(l+1,l)=t2;
end
#Condiciones periódicas
A(1,columnas) = t0;
A(filas, 1) = t0;
Eb = eig(A);
```

1.3. Espectro aislante

```
A1 = zeros(num);
[filas, columnas] = size(A1);
for j=1:columnas-1
A1(j,j+1)=t1+(-1)^(j+1)*delta1;
end
for i=1:filas-1
A1(i+1,i) = t1+(-1)^(i+1)*delta1;
end
A1(1, columnas)= t1+(-1)^(filas+1)*delta1;
A1(filas, 1) = t1+(-1)^(filas+1)*delta1;
E1des = eig(A1);
# Unión metal-aislante y aislante-aislante análoga a metal-metal.
```

1.4. Cálculo localización

```
[vect, diag] = eig(A);
#denominador
for indice=1:num
denominador(indice) = 0;
end
for columna = 1:num
for fila = 1:num
denominador(columna) = denominador(columna) + vect(fila, columna)*vect(fila,columna);
end
```

```
end
#numerador
for indice=1:num
numerador1(indice) = 0;
numerador2(indice) = 0;
end
for columna = 1:num
for indiced=100:199
numerador1(columna) = numerador1(columna) + vect(indiced, columna)*vect(indiced,columna);
numerador2(columna) = numerador2(columna) + vect(indiced+300, columna)*vect(indiced+300,columna);
end
end
numerador = numerador1 + numerador2;
for ii = 1:num
localizacion(ii) = numerador(ii)/denominador(ii);
end
```

1.5. Cálculo distribución

```
[vect, diag] = eig(J);
for indice=1:num
energias(indice) = diag(indice, indice);
end
#vector con energias
for indice=1:num
energias(indice) = diag(indice, indice);
end
#denominador for indice=1:num
denominador(indice) = 0;
end
for columna = 1:num
for fila = 1:num
denominador(columna) = denominador(columna) + vect(fila, columna)*vect(fila,columna);
end
```

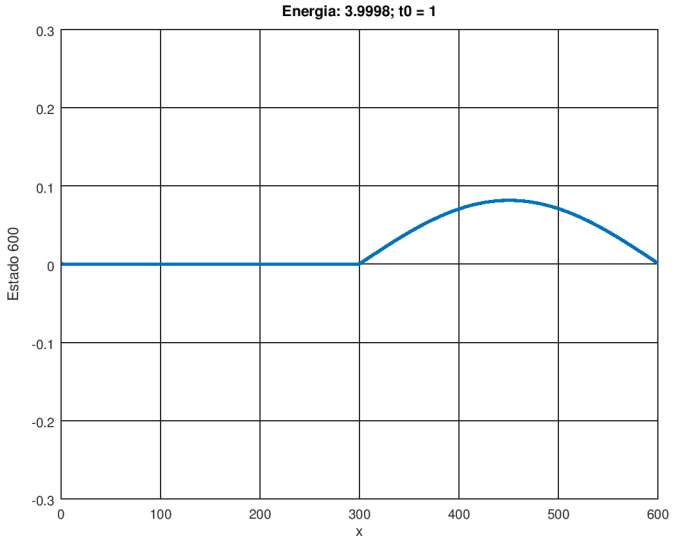
```
end
num6 = num/6;
#numerador
for indice=1:num
numerador1(indice) = 0;
numerador2(indice) = 0;
end
for columna = 1:num
for indiced=1:(num/2)
numerador1(columna) = numerador1(columna) + vect(indiced, columna)*vect(indiced,columna);
numerador2(columna) = numerador2(columna) +
+ vect(indiced+num/2, columna)*vect(indiced+num/2,columna);
end
end
numerador2menos = -numerador2;
distribucion = numerador1 + numerador2menos;
```

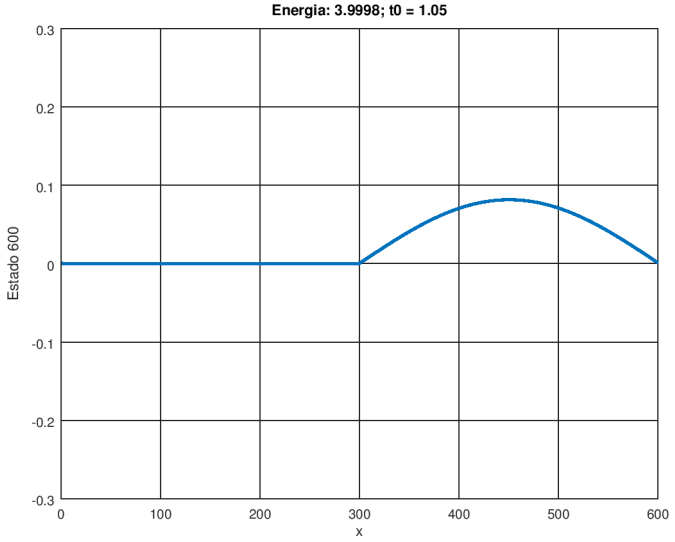
1.6. Cálculo penetración

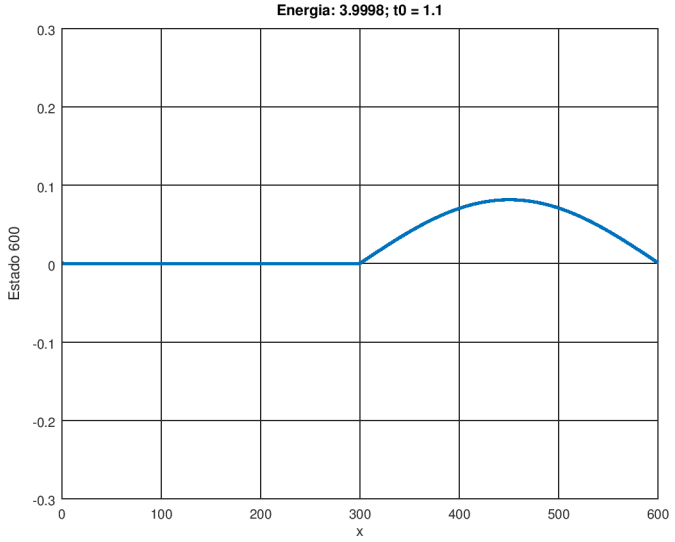
```
[vect, diag] = eig(J);
for indice=1:num
energias(indice) = diag(indice, indice);
end
#demonidador
for indice=1:num
denominador(indice) = 0;
end
for columna = 1:num
for fila = 1:num
denominador(columna) = denominador(columna) + vect(fila, columna)*vect(fila,columna);
end
end
num6 = num/6;
#numerador
```

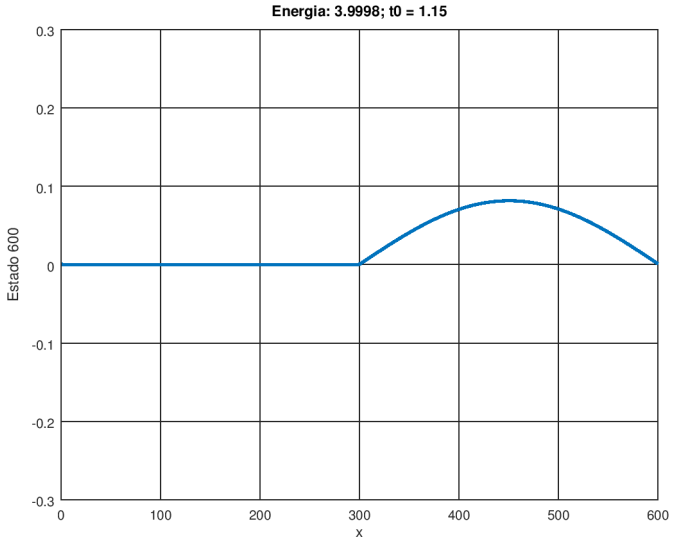
```
for indice=1:num
numerador(indice) = 0;
end
for columna = 1:num
for indiced=num/2+1:(num)
numerador(columna) = numerador(columna) + vect(indiced, columna)*vect(indiced,columna);
end
end
for ii = 1:num
entropia(ii) = numerador(ii)/denominador(ii);
end
```

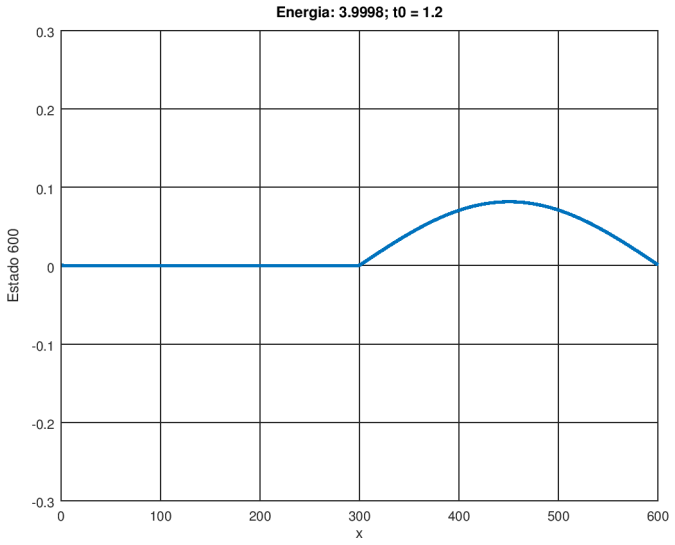
2. ANEXO II: Evolución estado de máxima energía, sistema metal-metal

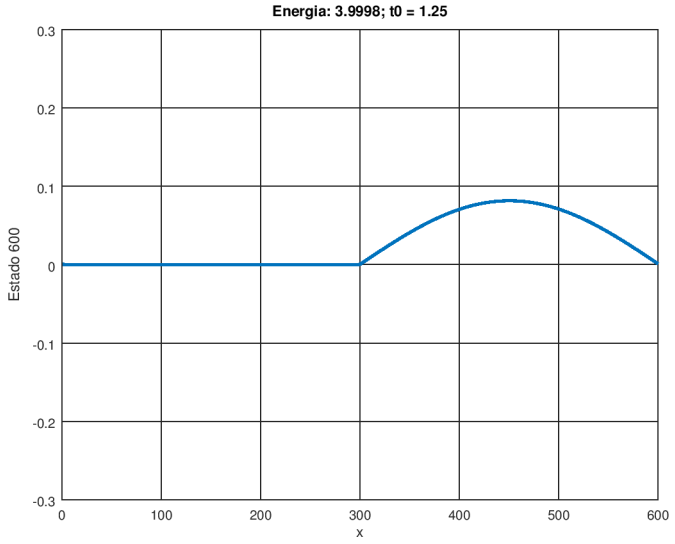


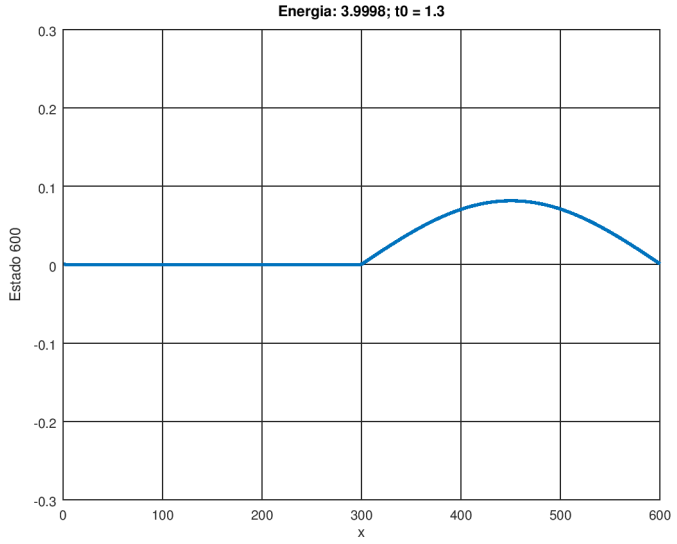


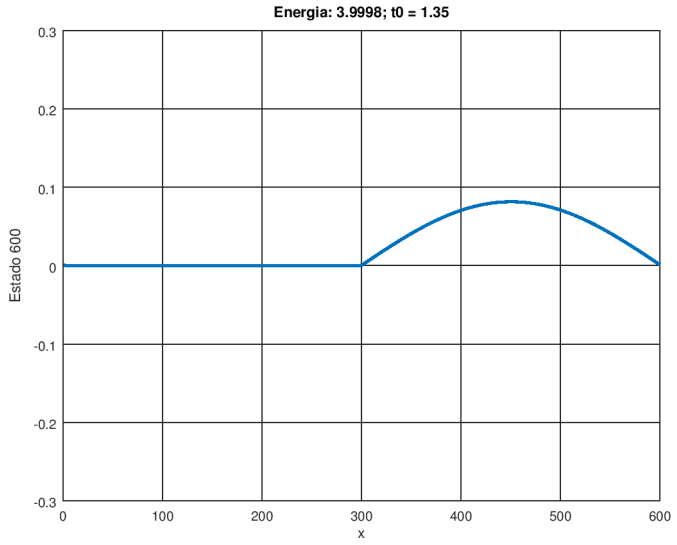


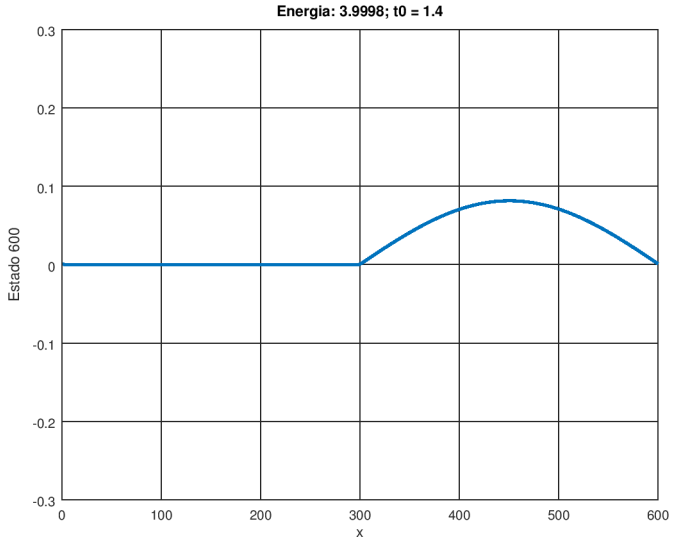

Energia: 3.9998; t0 = 1.15
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

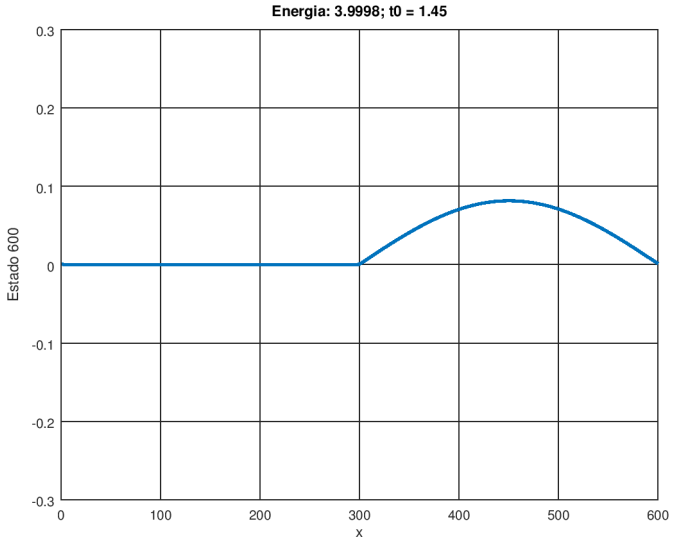

Energia: 3.9998; t0 = 1.2
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

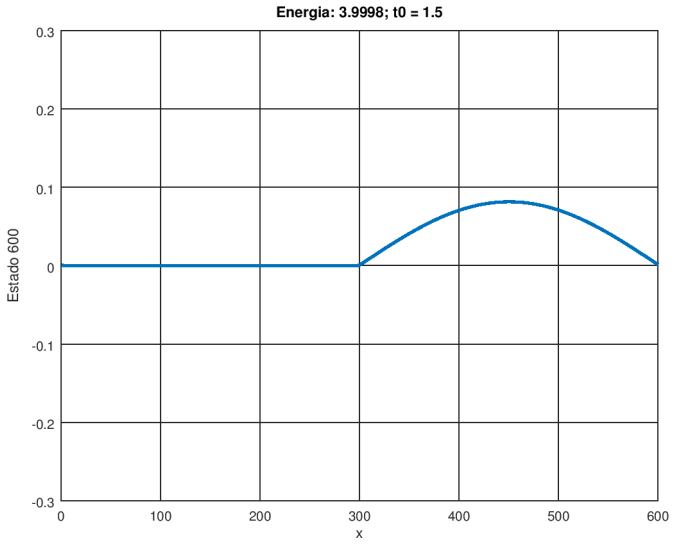

Energia: 3.9998; t0 = 1.25
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

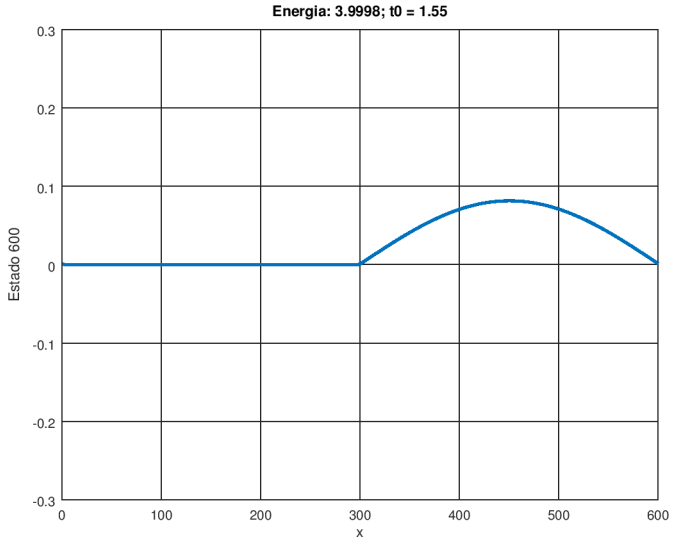

Energia: 3.9998; t0 = 1.3
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

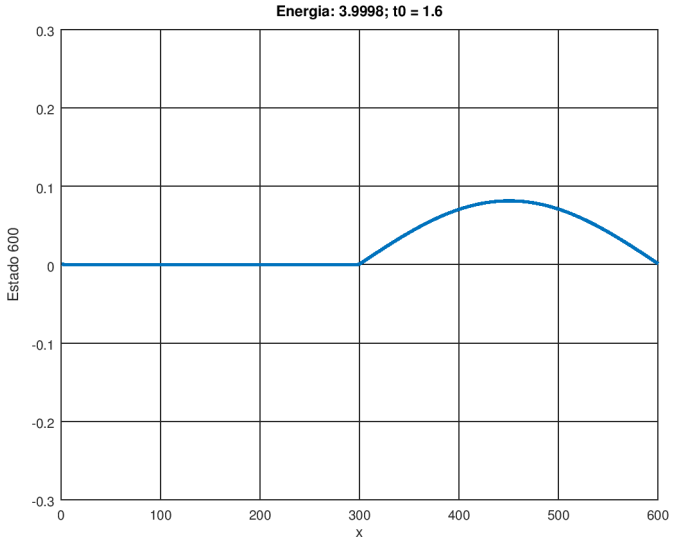

Energia: 3.9998; t0 = 1.35
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

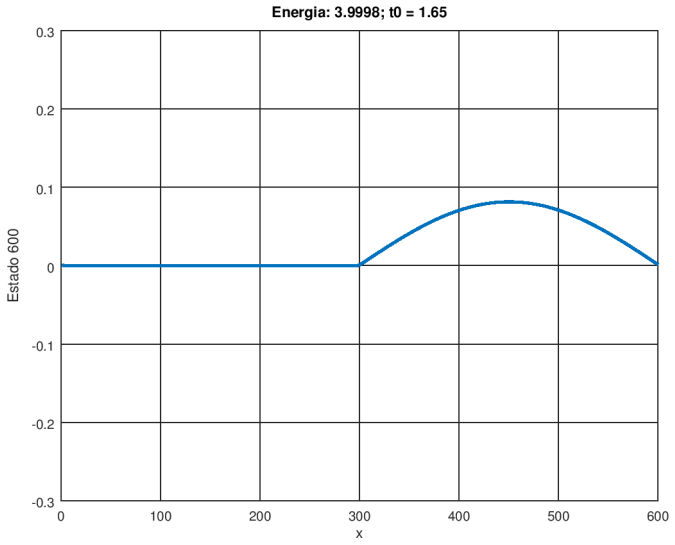

Energia: 3.9998; t0 = 1.4
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

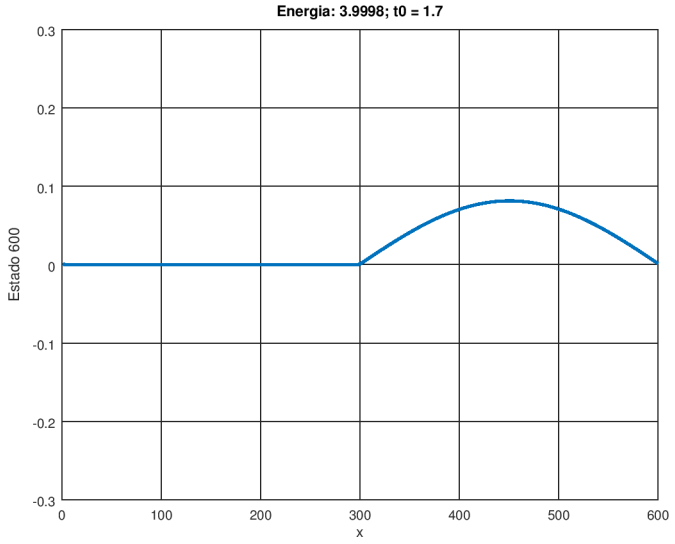

Energia: 3.9998; t0 = 1.45
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

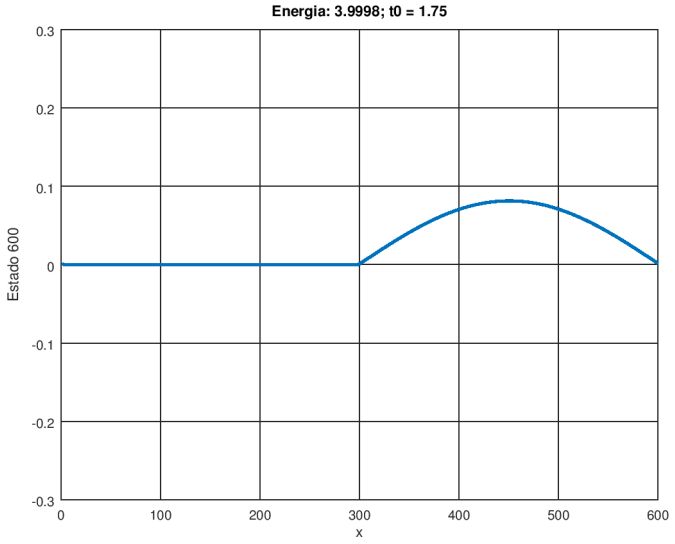

Energia: 3.9998; t0 = 1.5
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

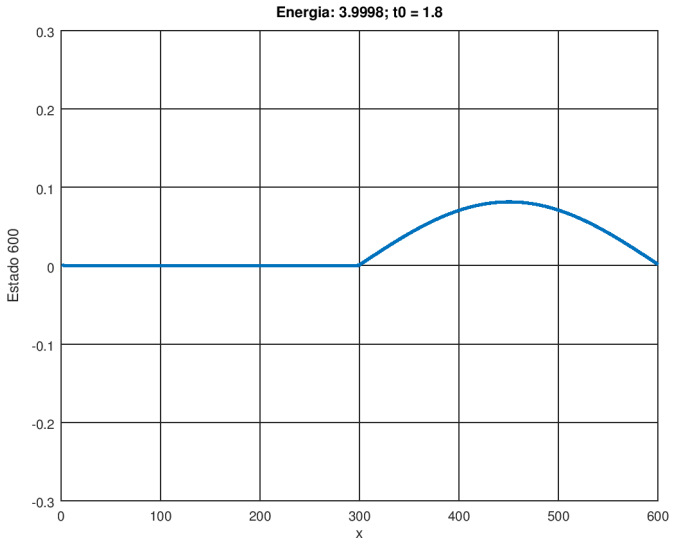

Energia: 3.9998; t0 = 1.55
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

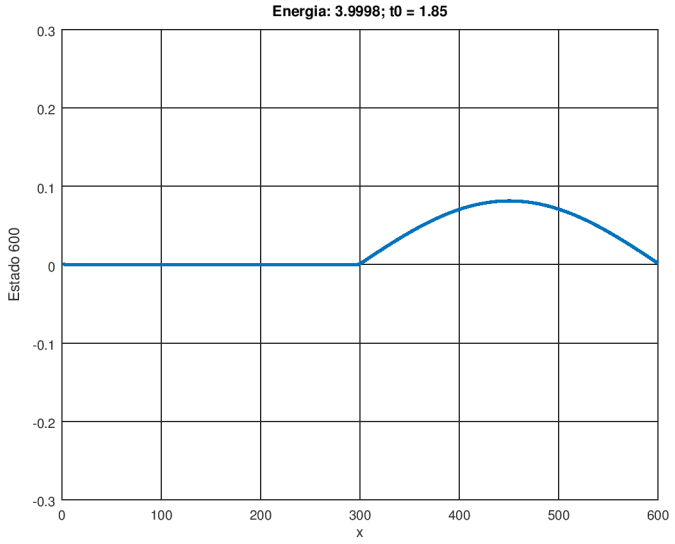

Energia: 3.9998; t0 = 1.6
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

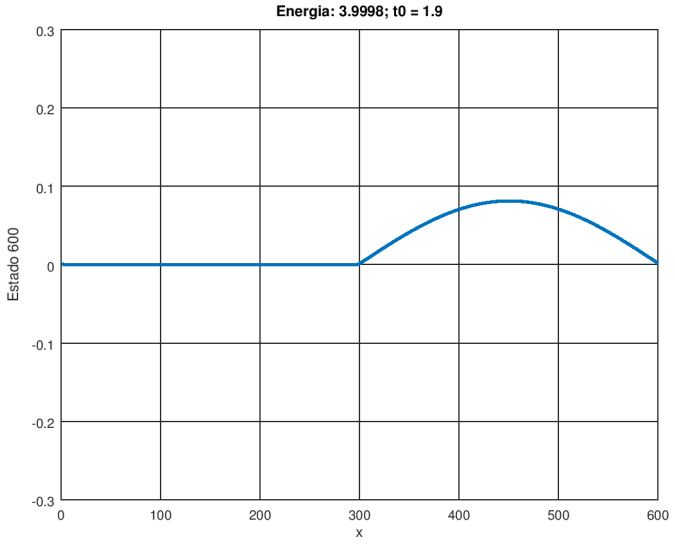

Energia: 3.9998; t0 = 1.65
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

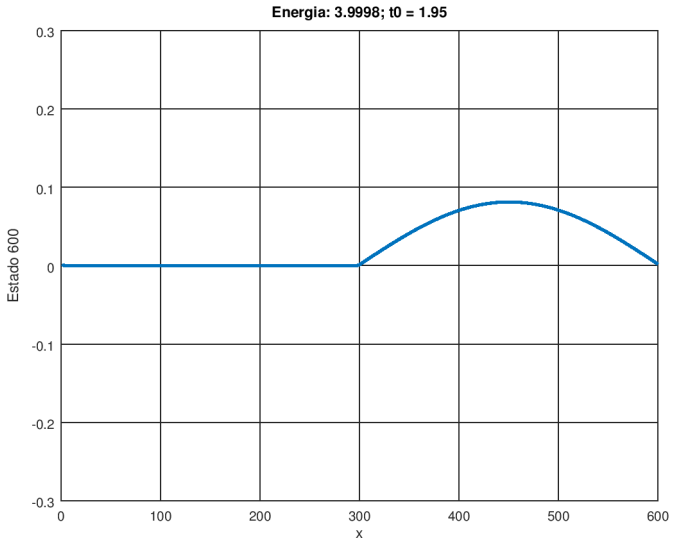

Energia: 3.9998; t0 = 1.7
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

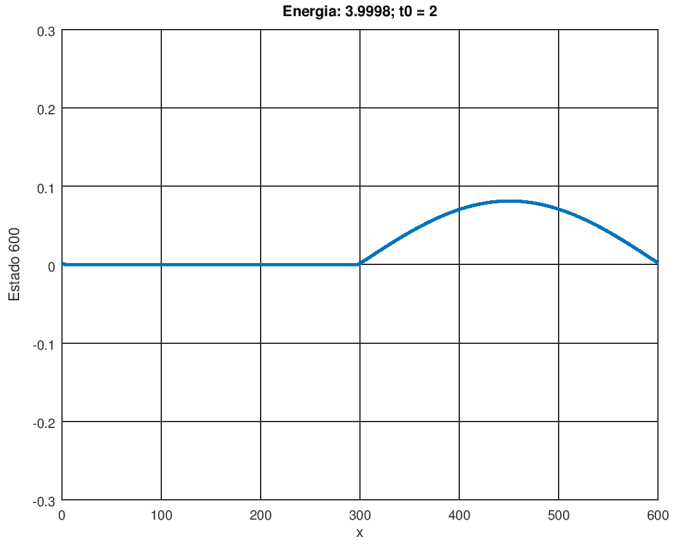

Energia: 3.9998; t0 = 1.75
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

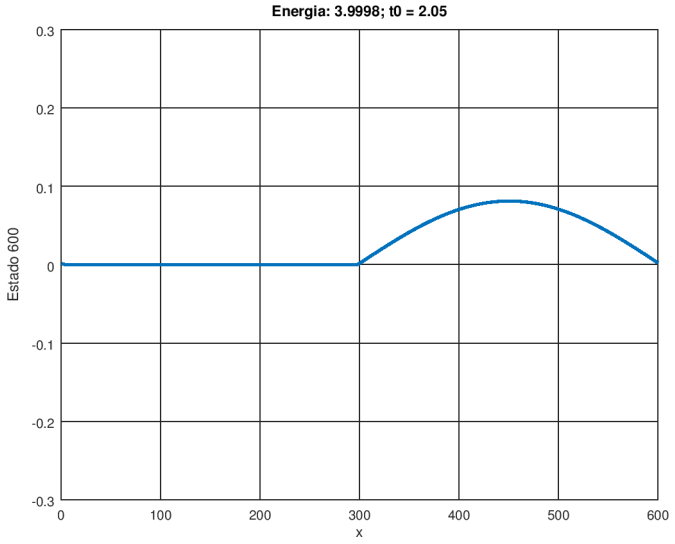

Energia: 3.9998; t0 = 1.8
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

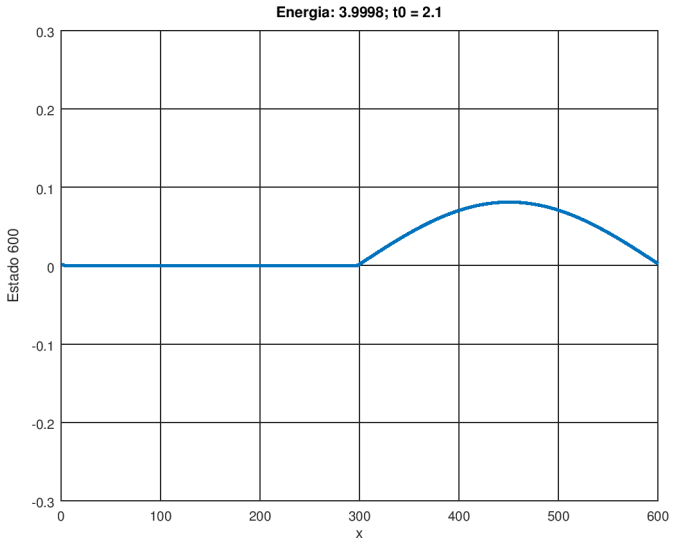

Energia: 3.9998; t0 = 1.85
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

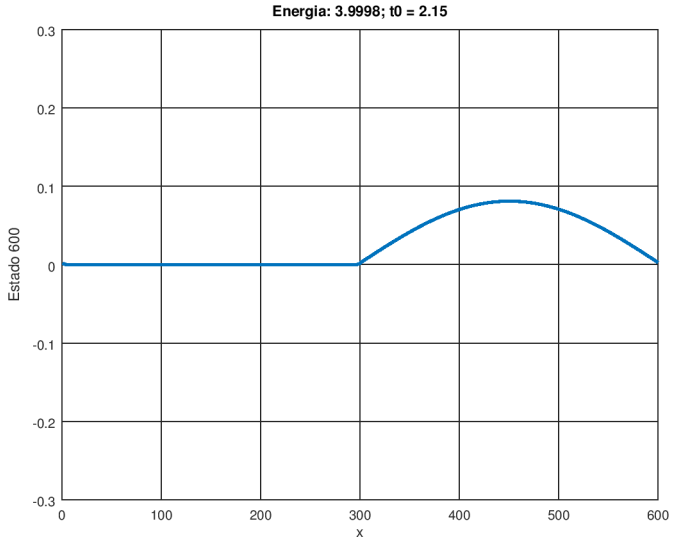

Energia: 3.9998; t0 = 1.9
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

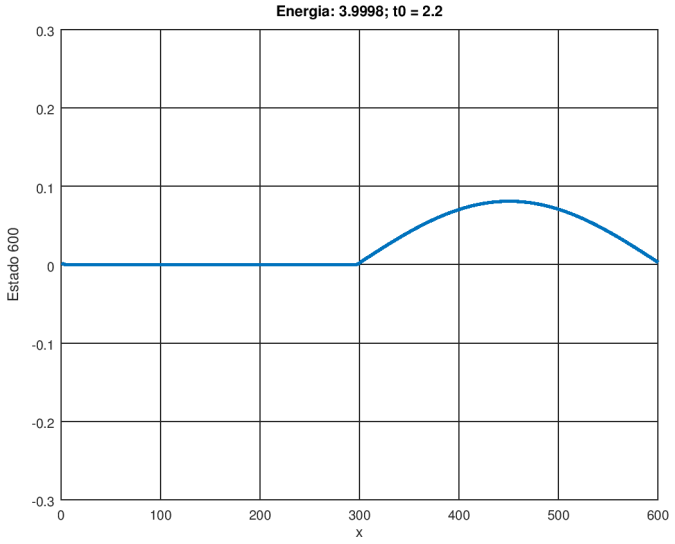

Energia: 3.9998; t0 = 1.95
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

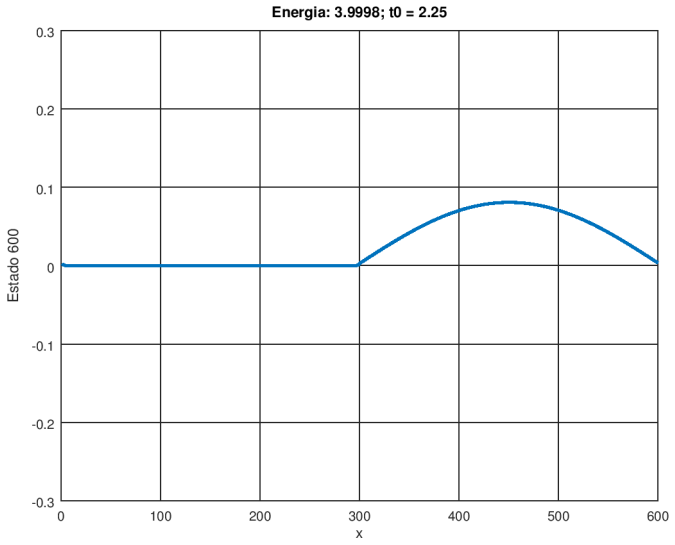

Energia: 3.9998; t0 = 2
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

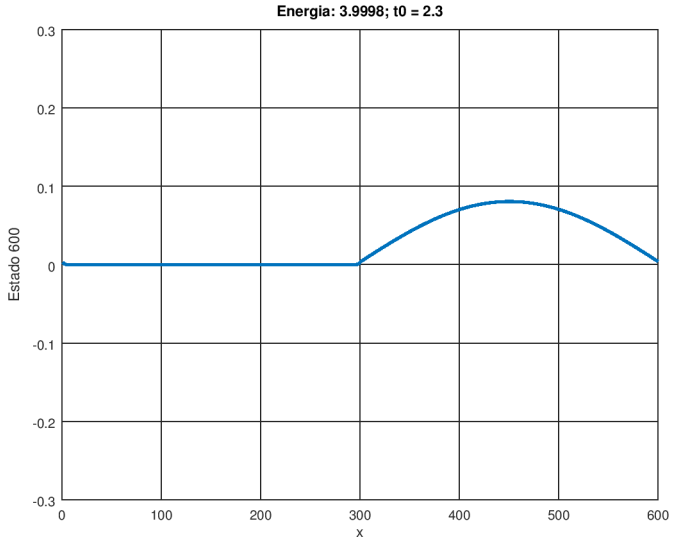

Energia: 3.9998; t0 = 2.05
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

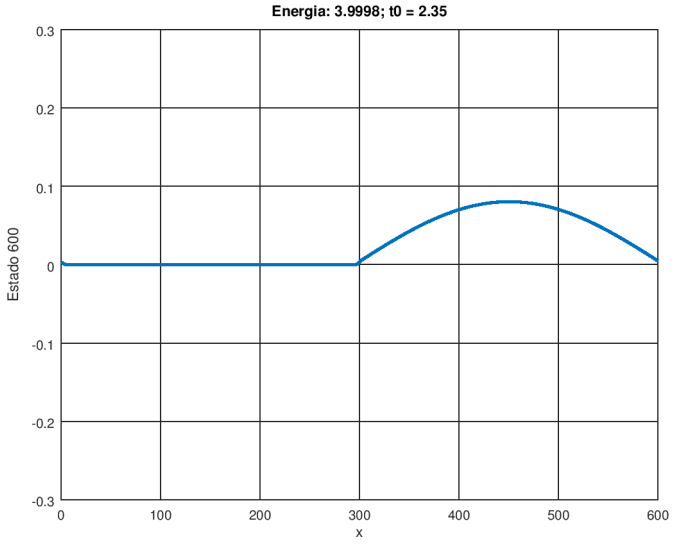

Energia: 3.9998; t0 = 2.1
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

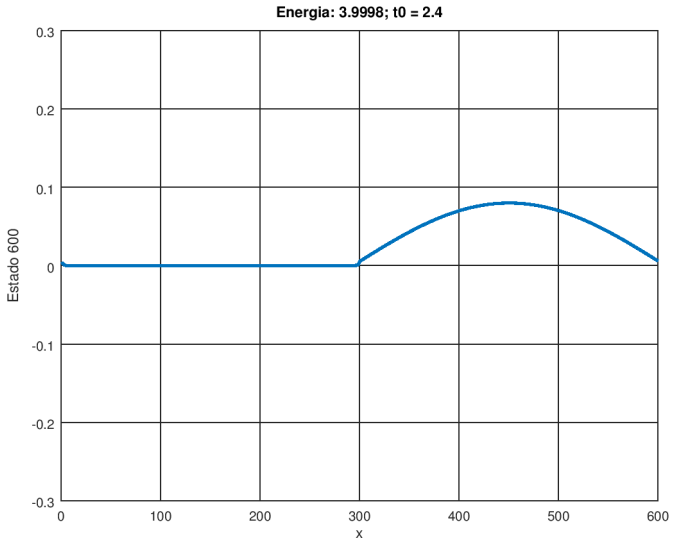

Energia: 3.9998; t0 = 2.15
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

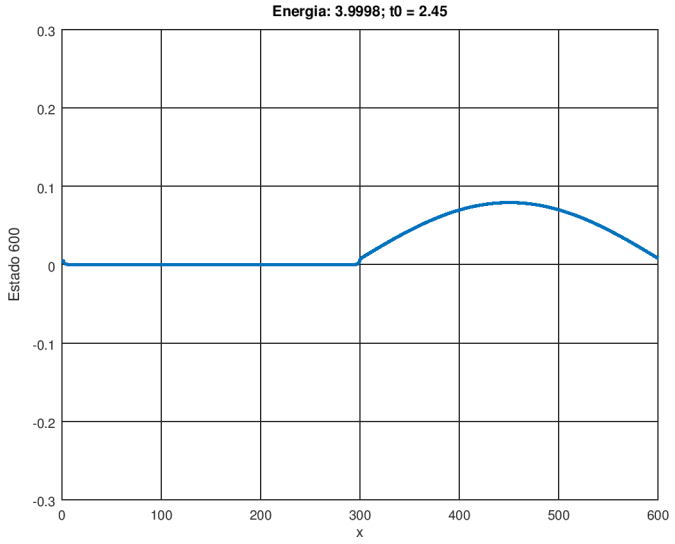

Energia: 3.9998; t0 = 2.2
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

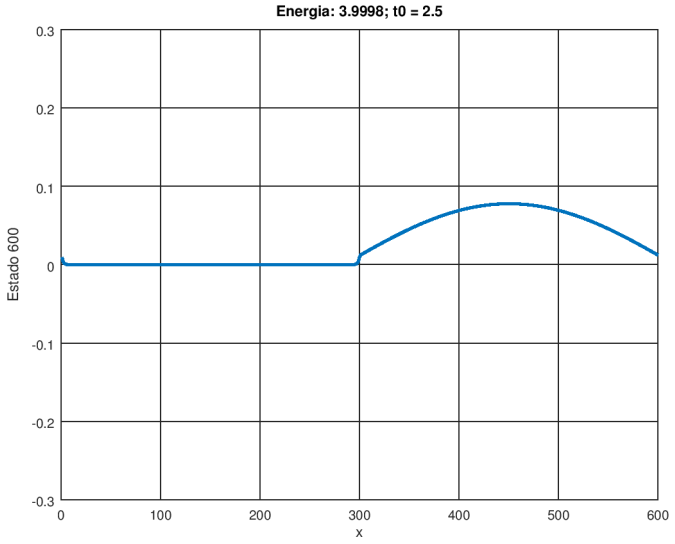

Energia: 3.9998; t0 = 2.25
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

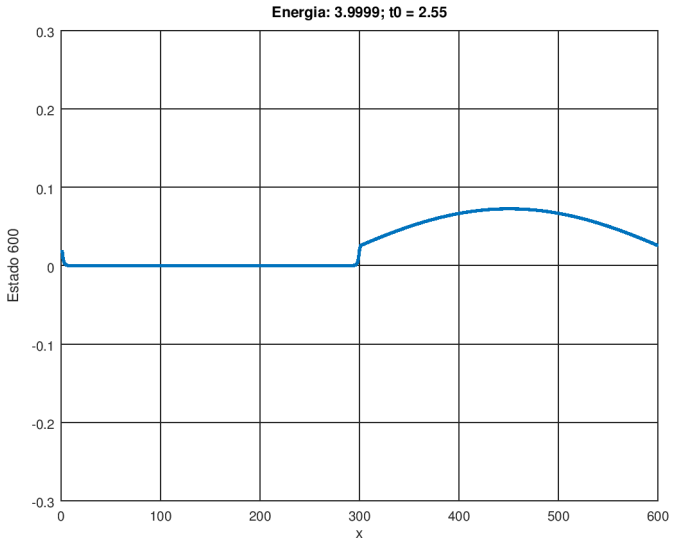

Energia: 3.9998; t0 = 2.3
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

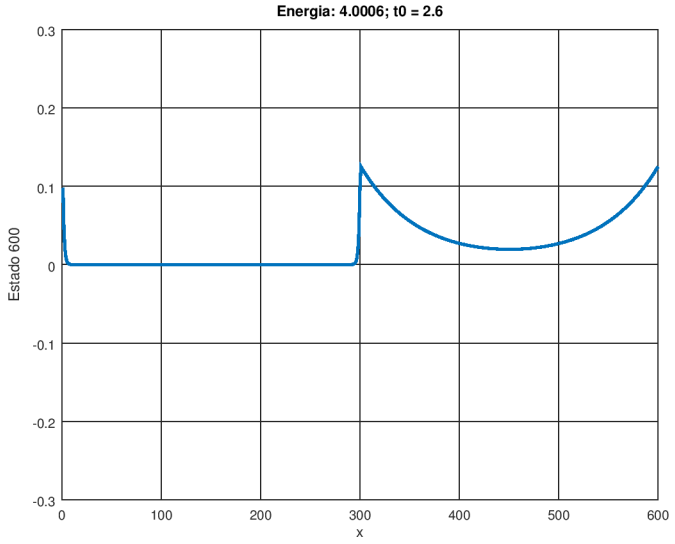

Energia: 3.9998; t0 = 2.35
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

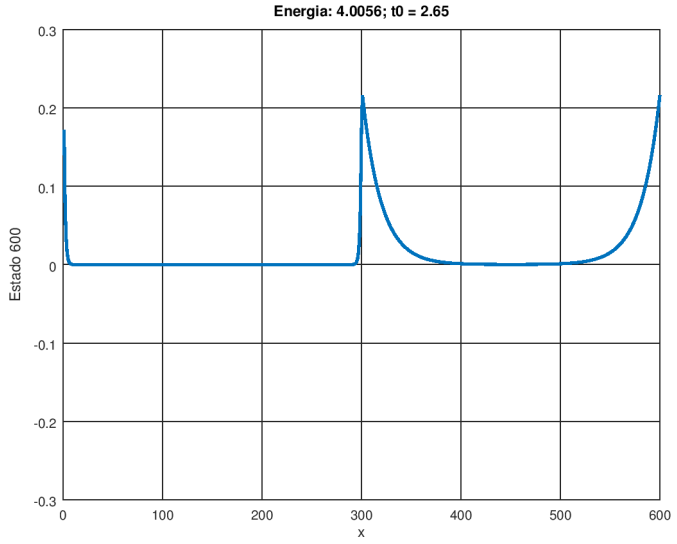

Energia: 3.9998; t0 = 2.4
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

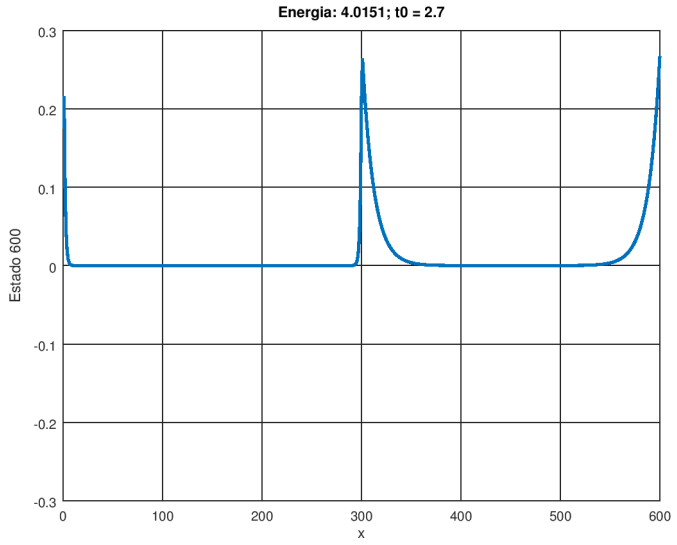

Energia: 3.9998; t0 = 2.45
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

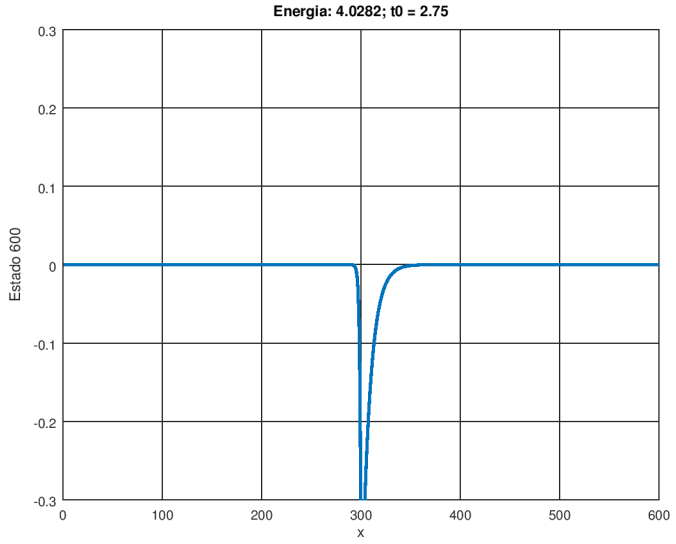

Energia: 3.9998; t0 = 2.5
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

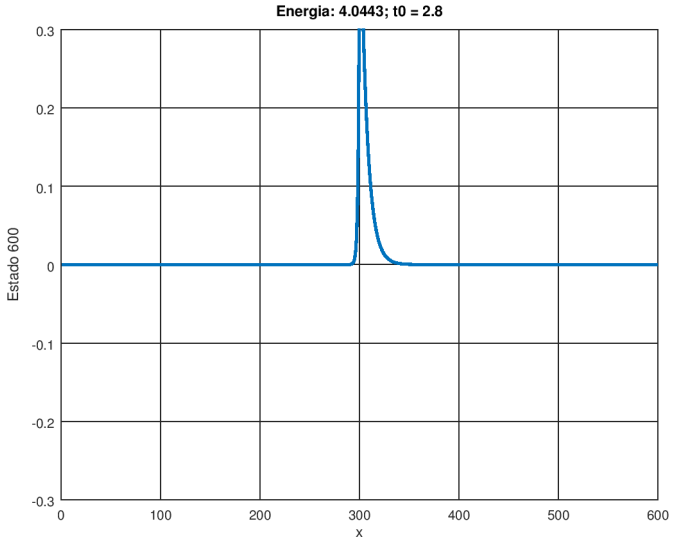

Energia: 3.9999; t0 = 2.55
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

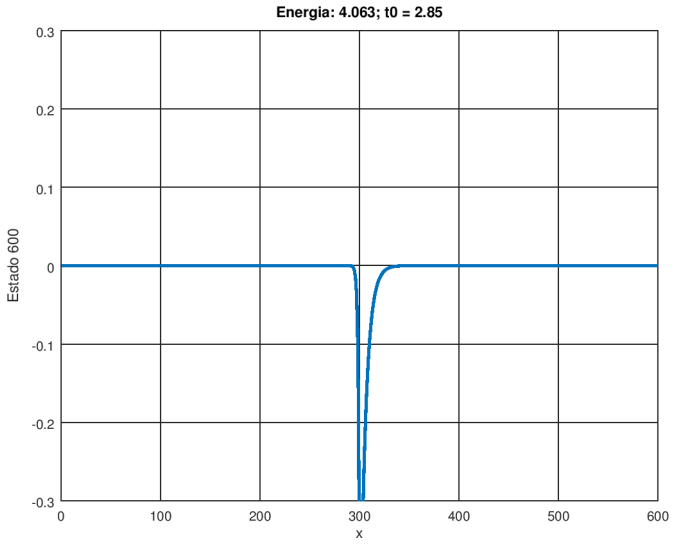

Energia: 4.0006; t0 = 2.6
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

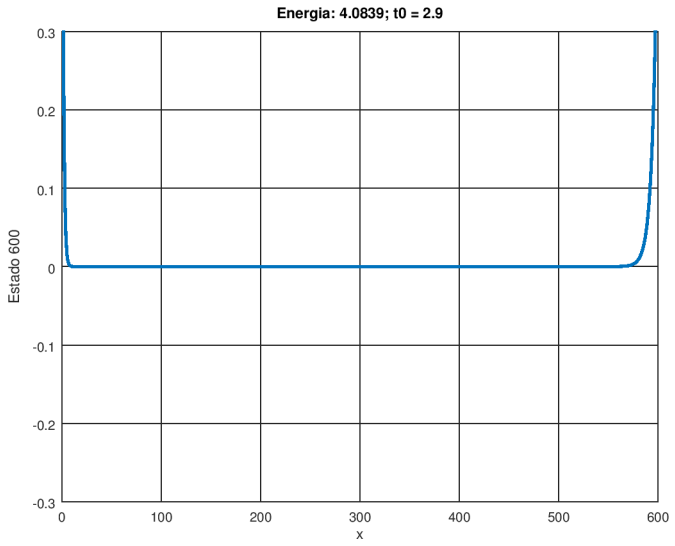

Energia: 4.0056; t0 = 2.65
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600


Energia: 4.0151; t0 = 2.7
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600


Energia: 4.0282; t0 = 2.75
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600


Energia: 4.0443; t0 = 2.8
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600


Energia: 4.063; t0 = 2.85
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600


Energia: 4.0839; t0 = 2.9
Estado 600
x
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
100
200
300
400
500
600

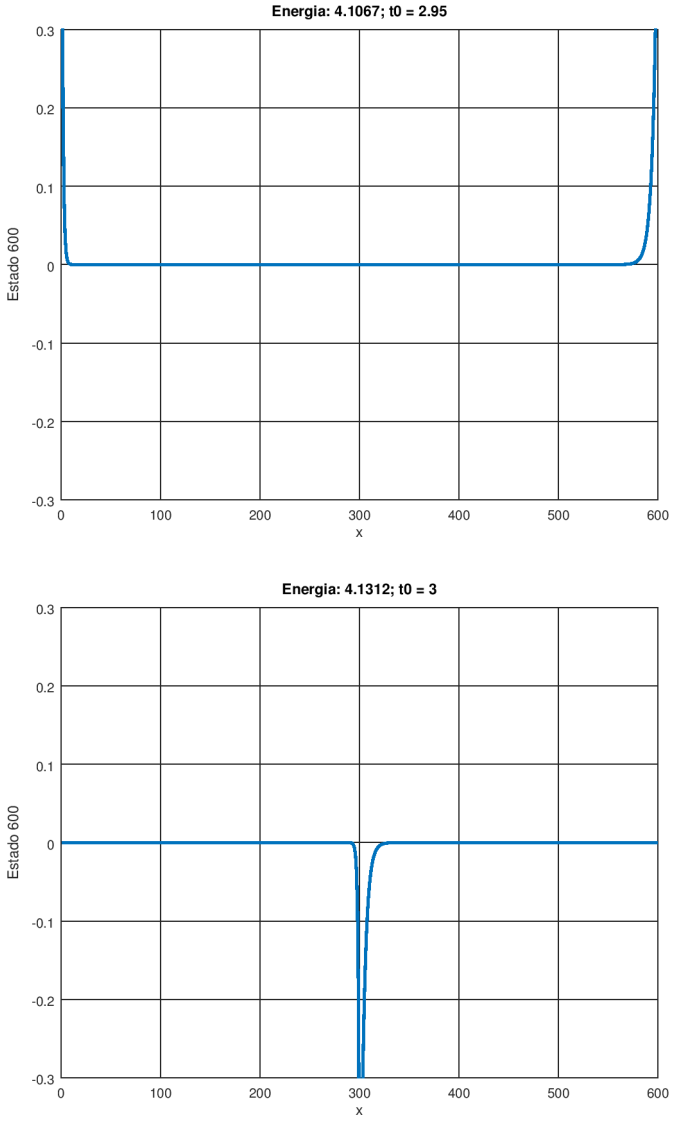
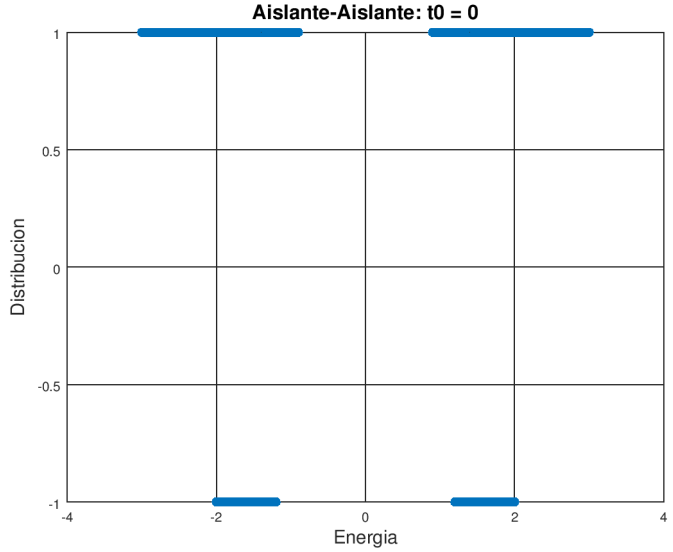
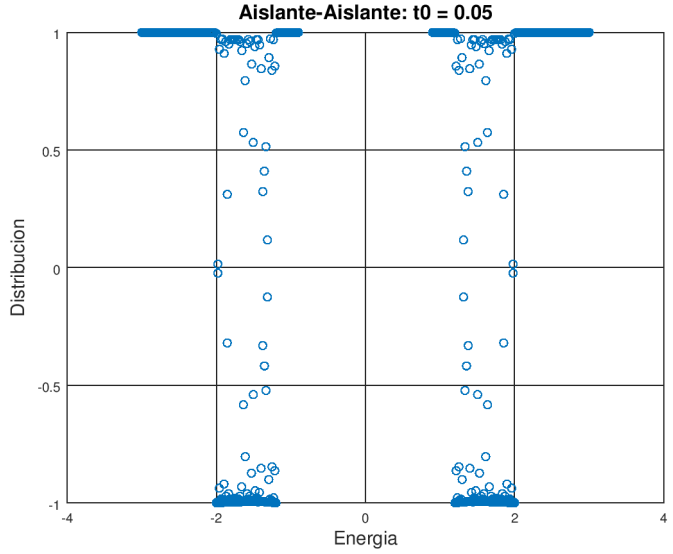
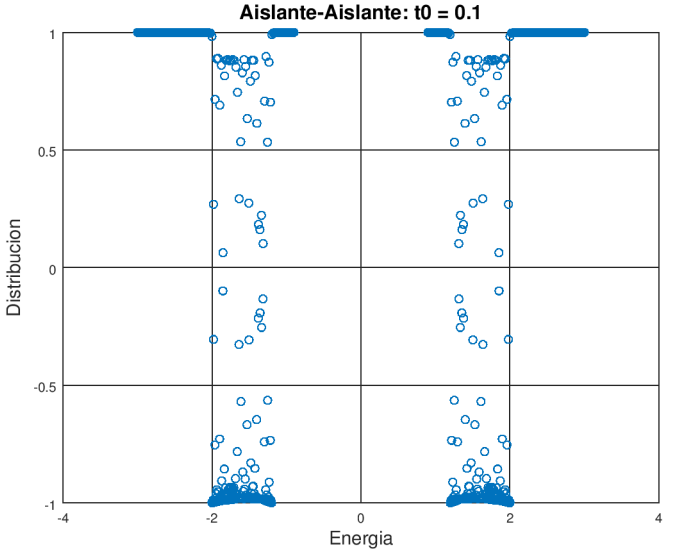


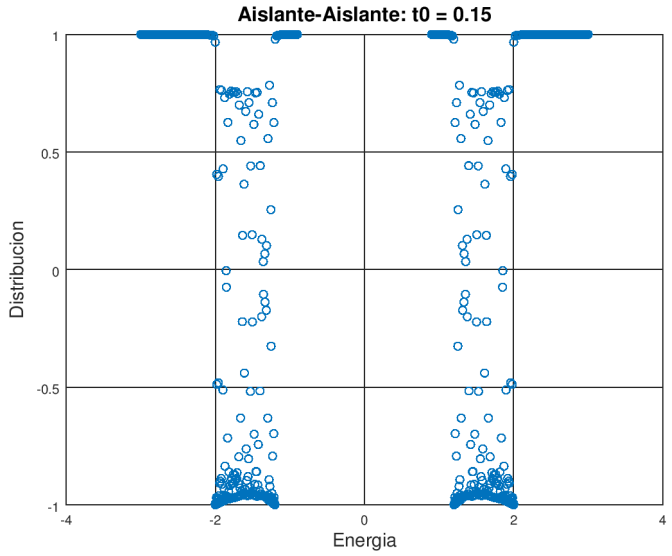
Figura 2.1: Evolución del estado de máxima energía en función del valor del contacto.

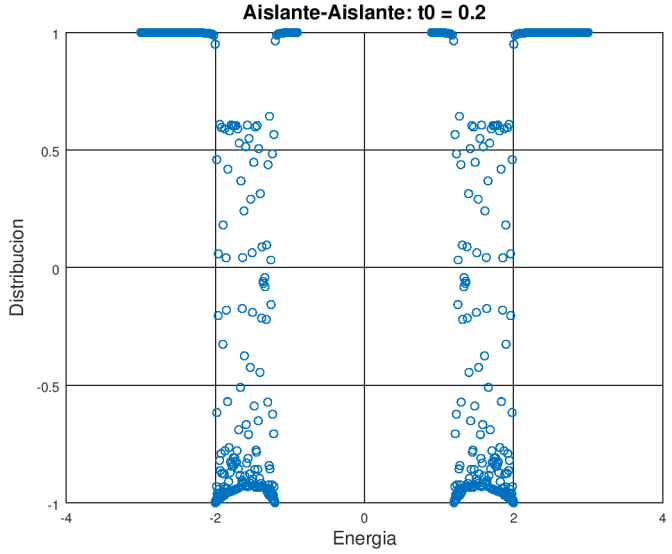
3. ANEXO III: Gráficas distribución

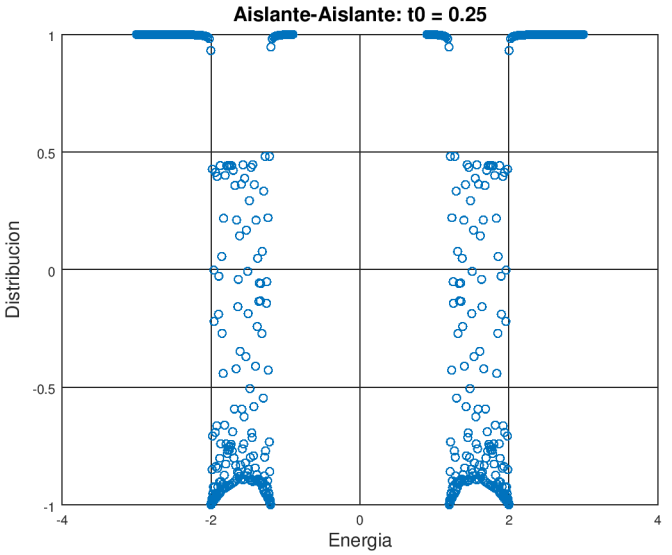


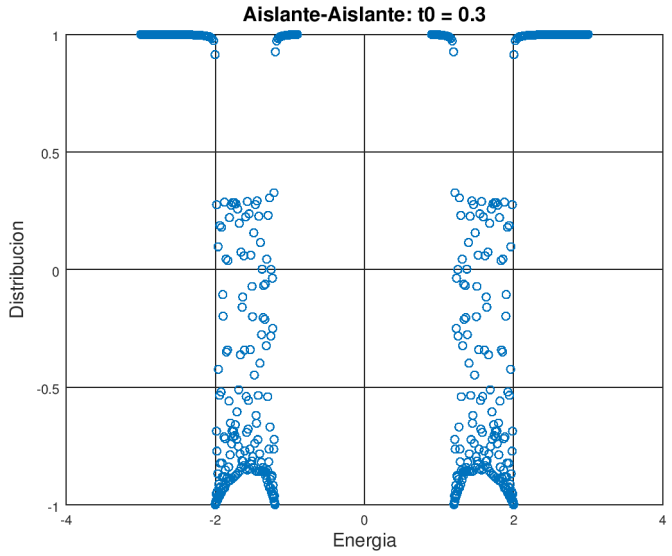


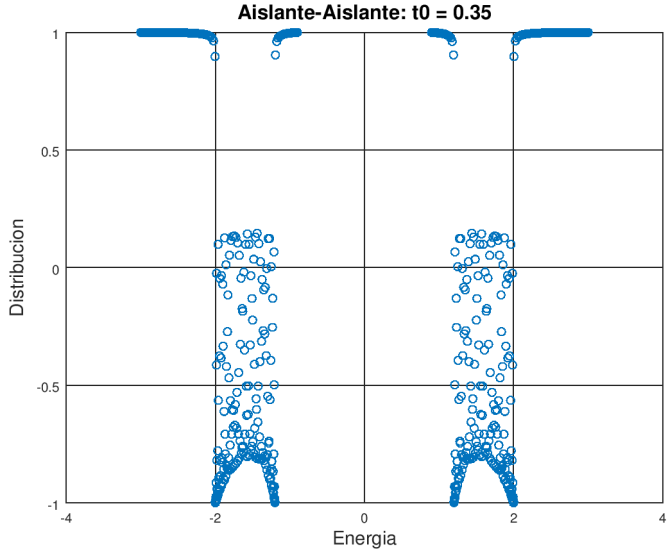


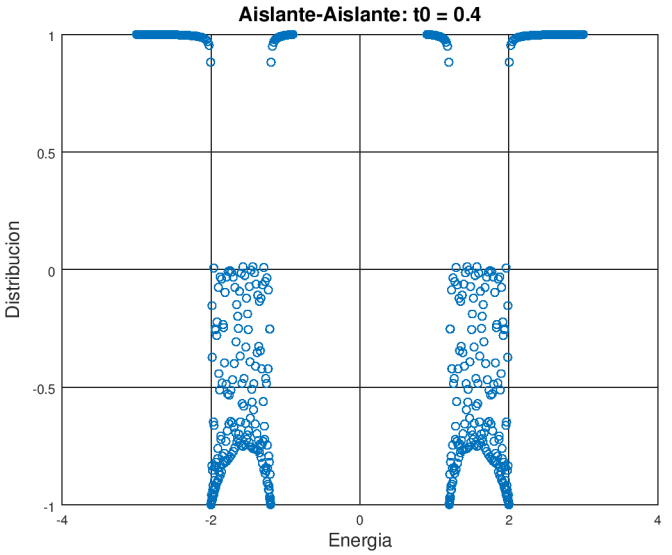

Aislante-Aislante: t0 = 0.15
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

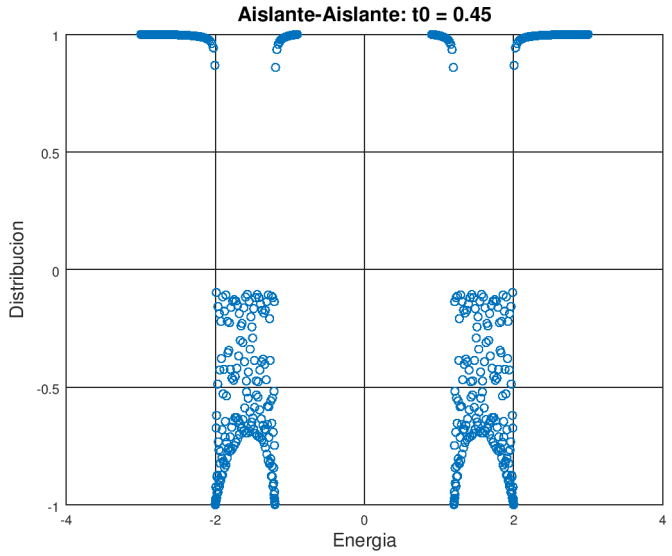

Aislante-Aislante: t0 = 0.2
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

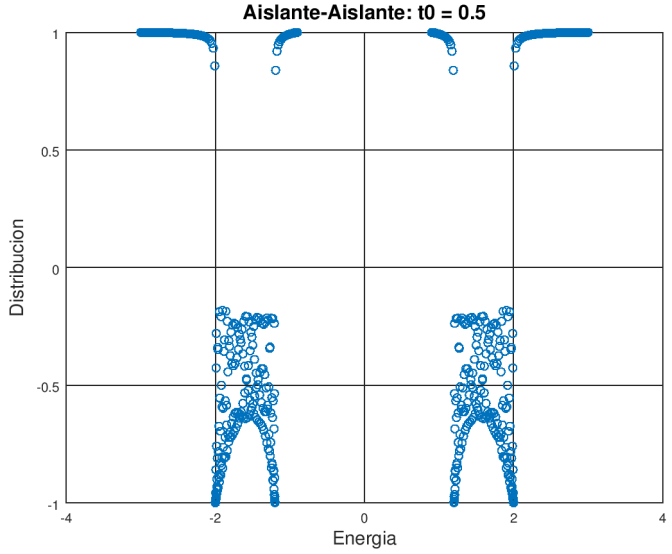

Aislante-Aislante: t0 = 0.25
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

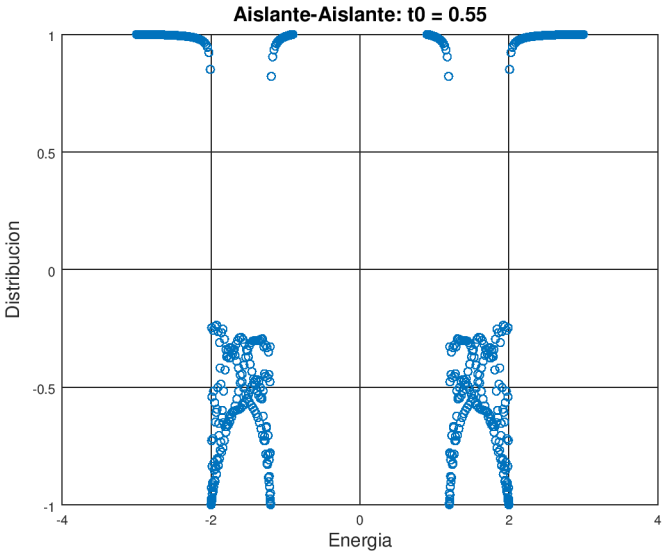

Aislante-Aislante: t0 = 0.3
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

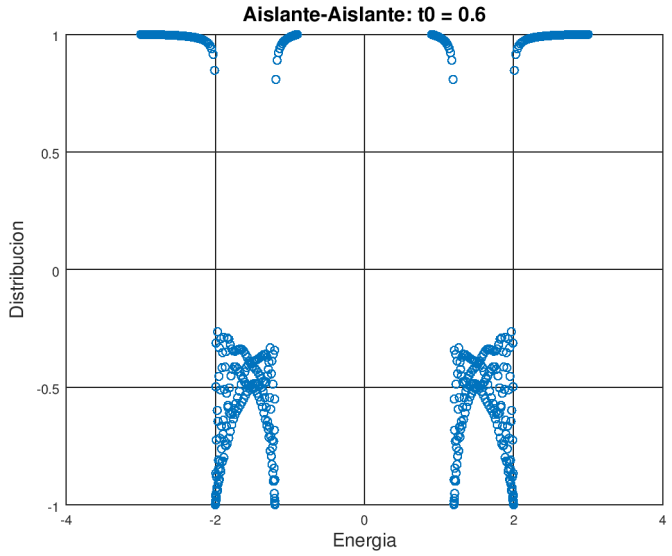

Aislante-Aislante: t0 = 0.35
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

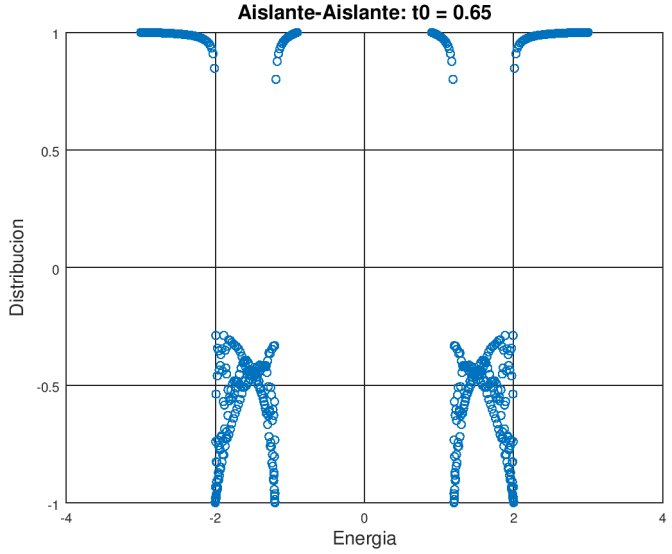

Aislante-Aislante: t0 = 0.4
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

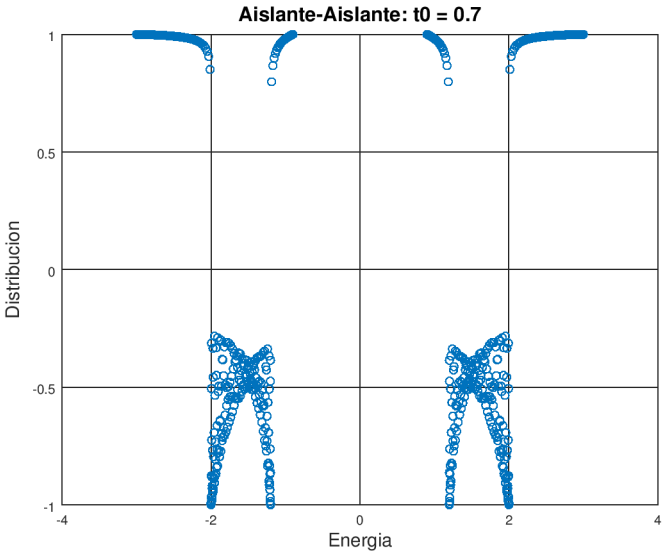

Aislante-Aislante: t0 = 0.45
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

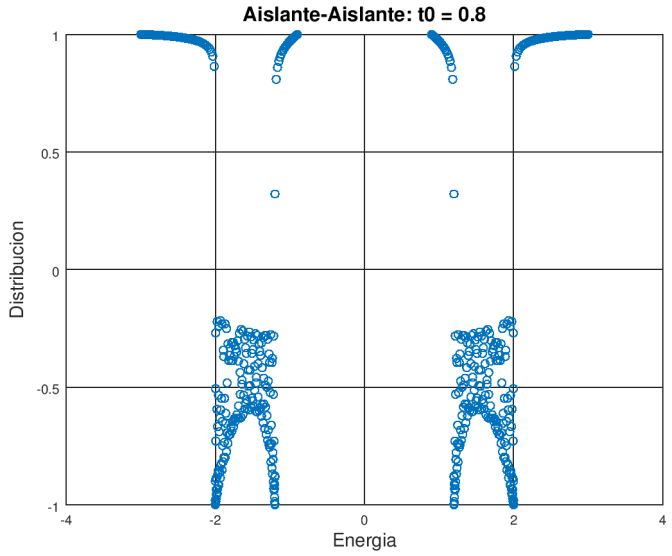

Aislante-Aislante: t0 = 0.5
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

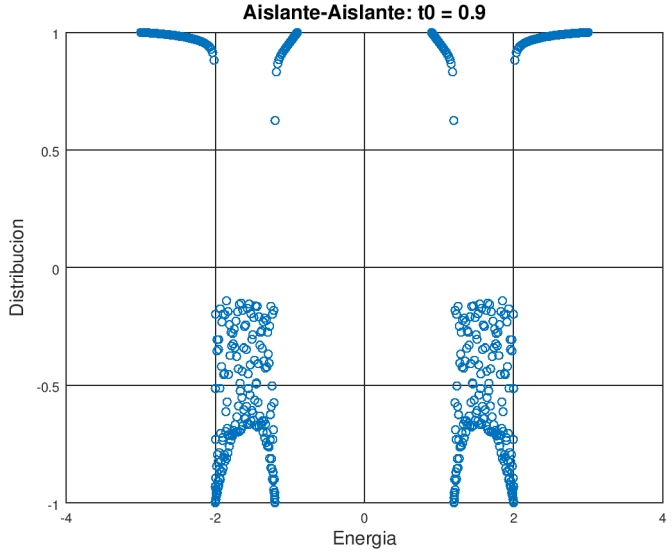

Aislante-Aislante: t0 = 0.55
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

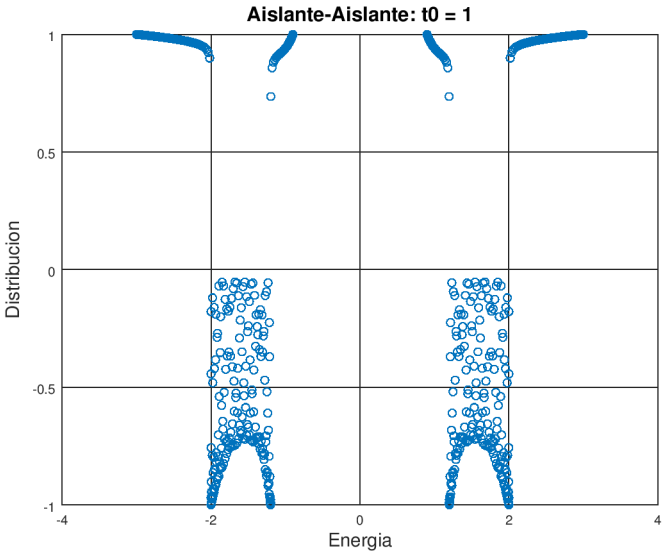

Aislante-Aislante: t0 = 0.6
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

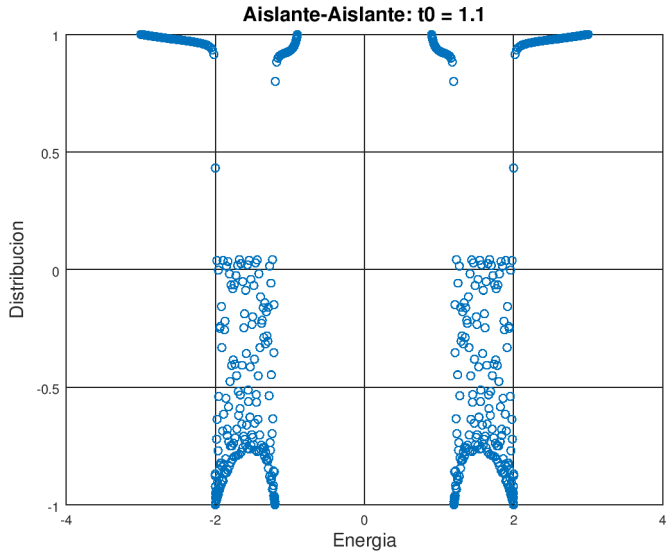

Aislante-Aislante: t0 = 0.65
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

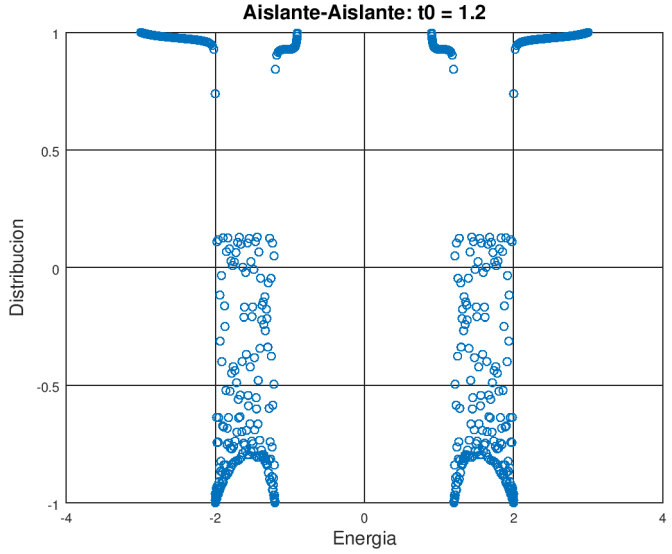

Aislante-Aislante: t0 = 0.7
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

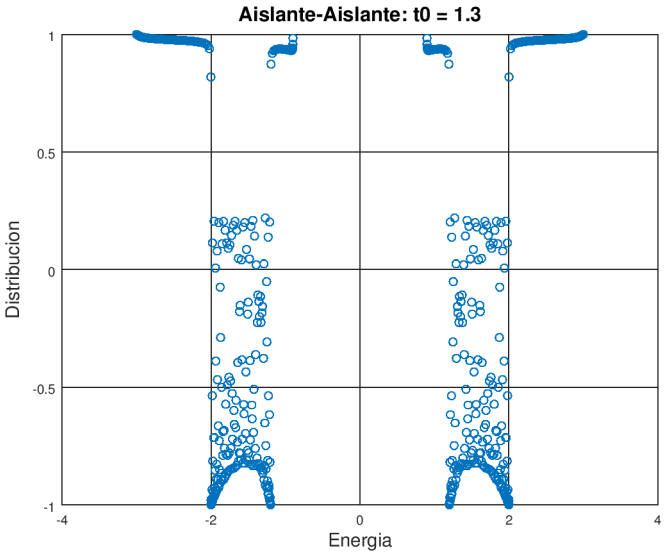

Aislante-Aislante: t0 = 0.8
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

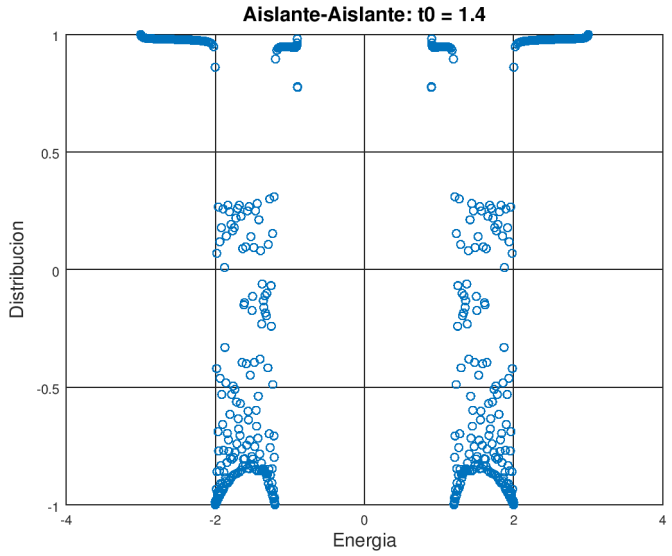

Aislante-Aislante: t0 = 0.9
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

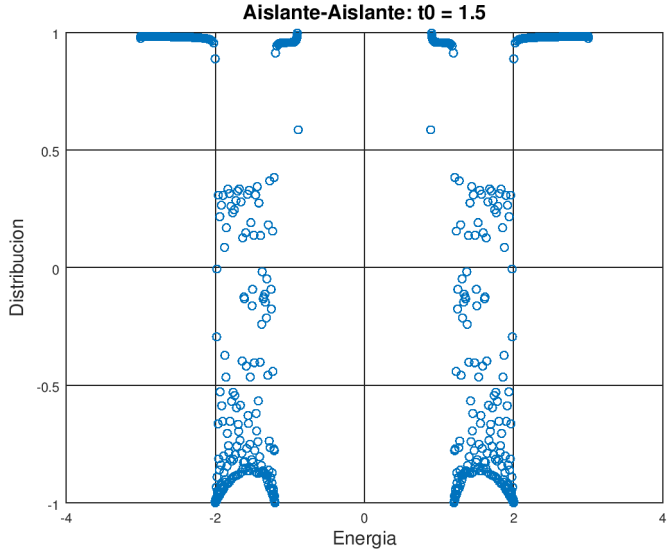

Aislante-Aislante: t0 = 1
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

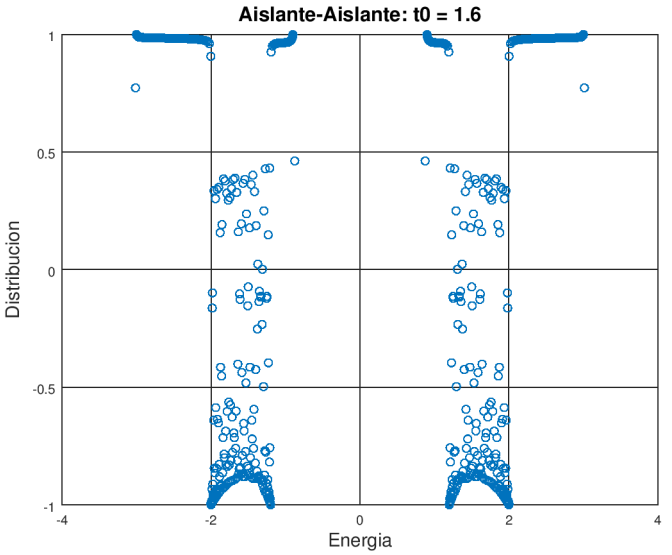

Aislante-Aislante: t0 = 1.1
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

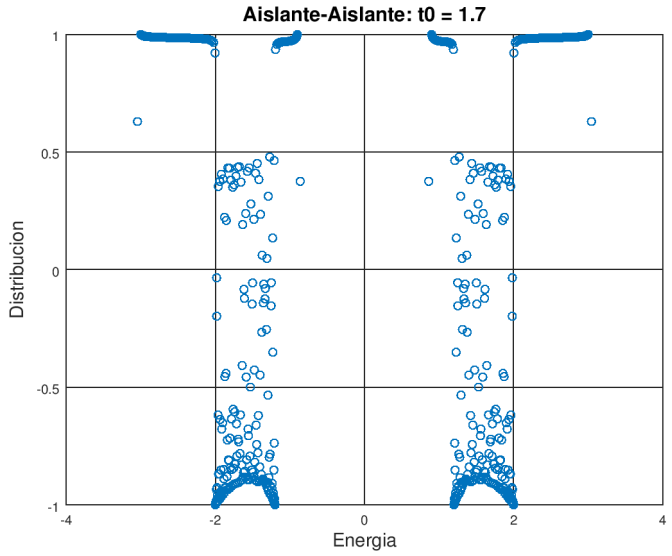

Aislante-Aislante: t0 = 1.2
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

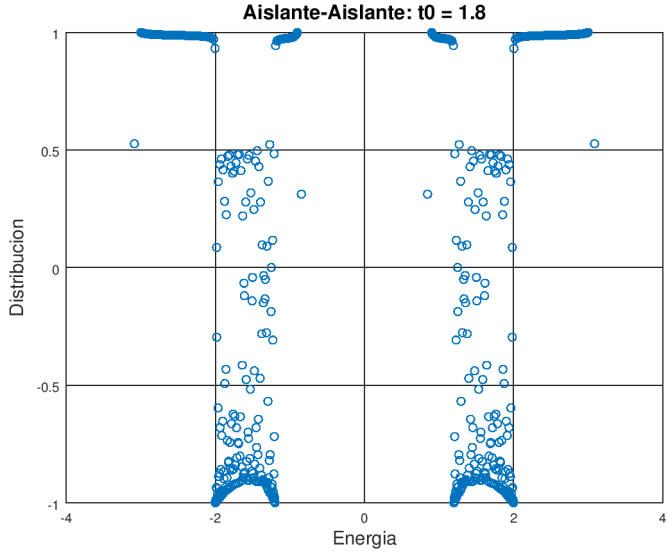

Aislante-Aislante: t0 = 1.3
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

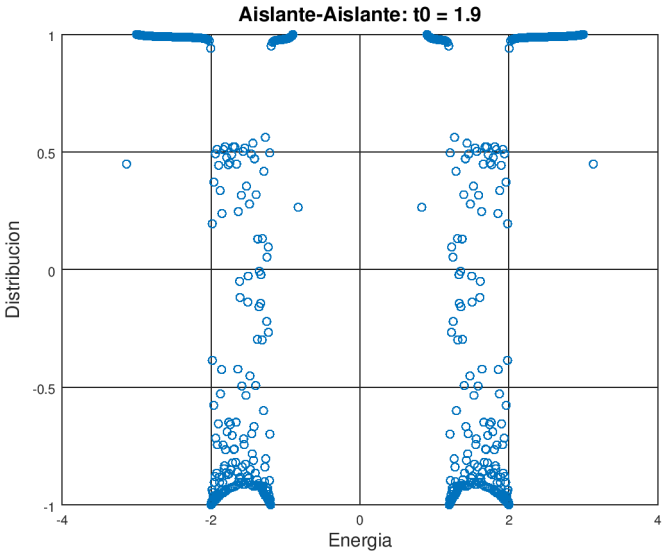

Aislante-Aislante: t0 = 1.4
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

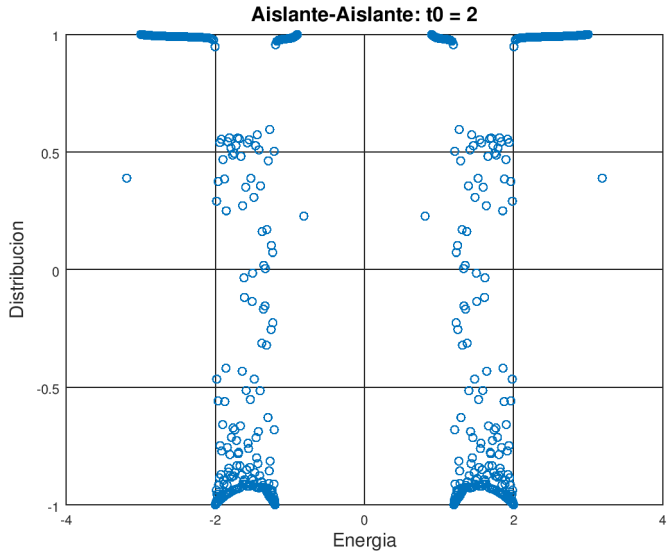

Aislante-Aislante: t0 = 1.5
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

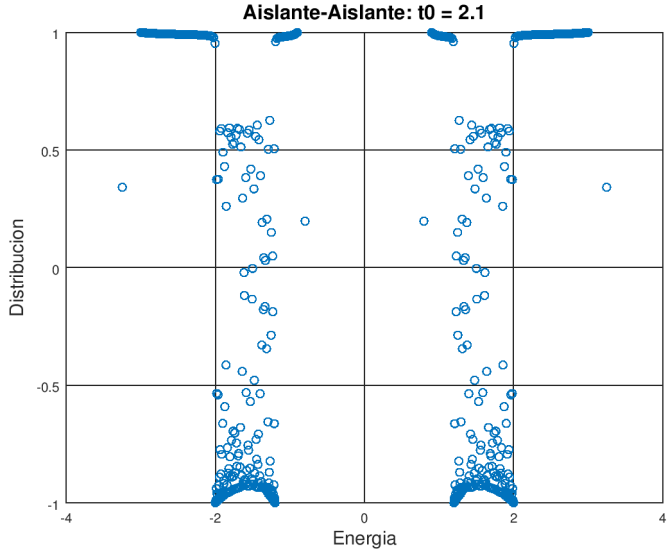

Aislante-Aislante: t0 = 1.6
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

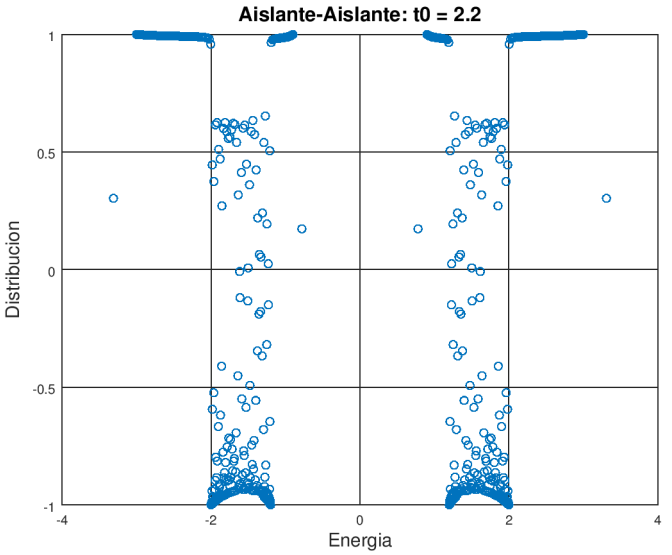

Aislante-Aislante: t0 = 1.7
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

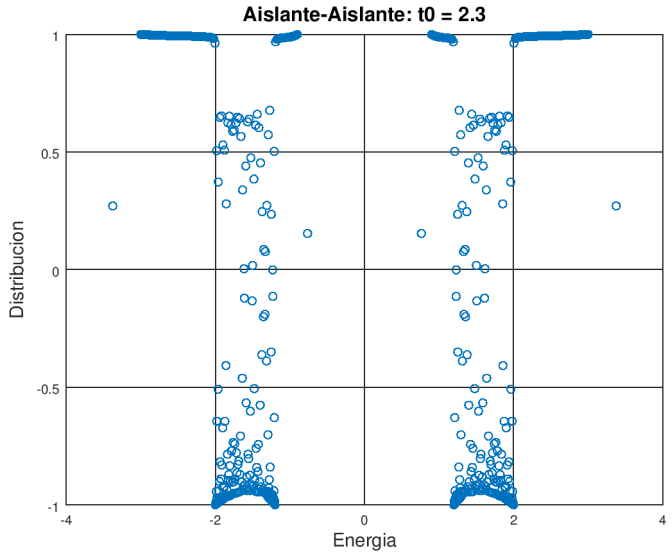

Aislante-Aislante: t0 = 1.8
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

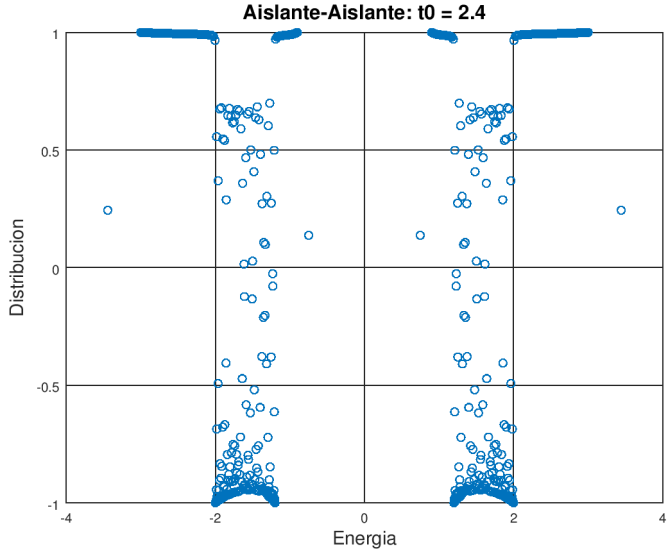

Aislante-Aislante: t0 = 1.9
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

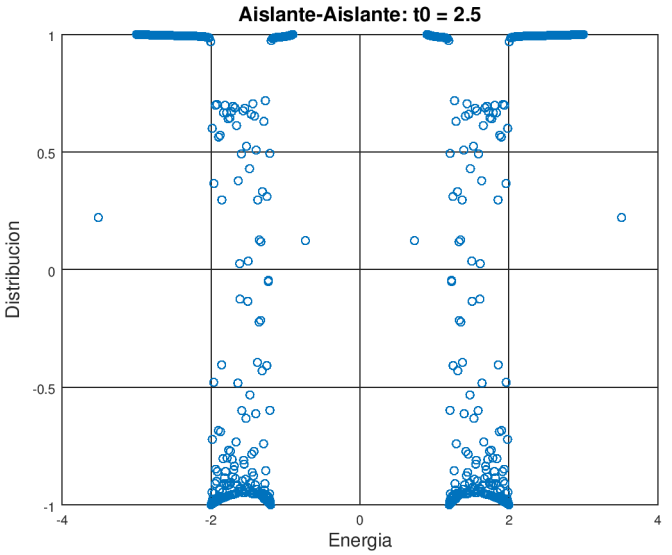

Aislante-Aislante: t0 = 2
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

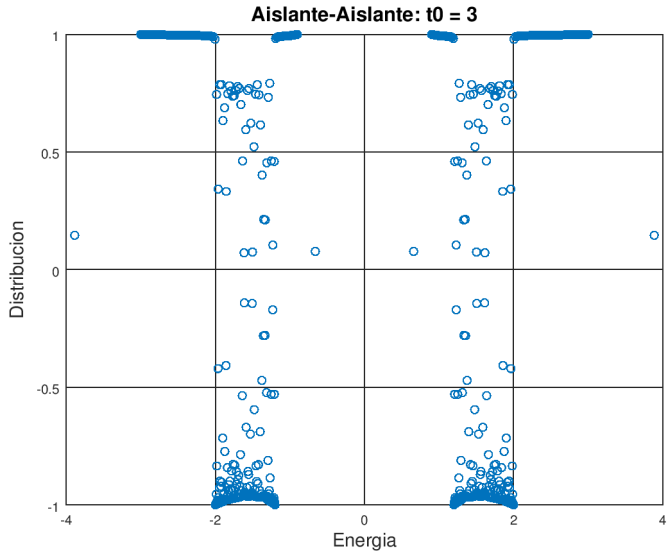

Aislante-Aislante: t0 = 2.1
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

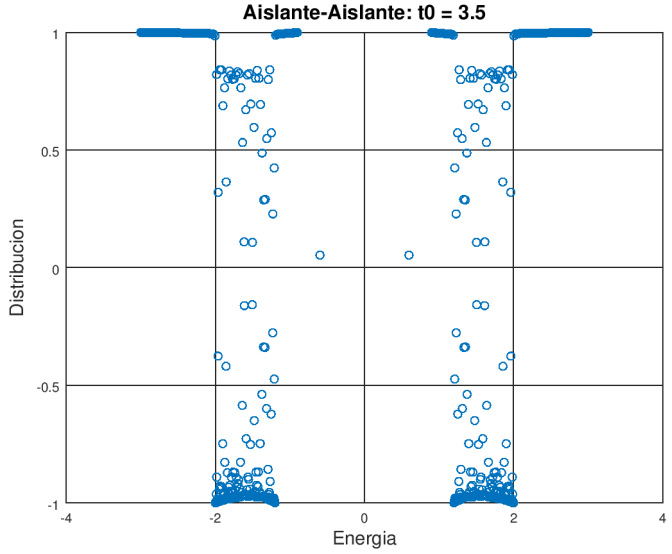

Aislante-Aislante: t0 = 2.2
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

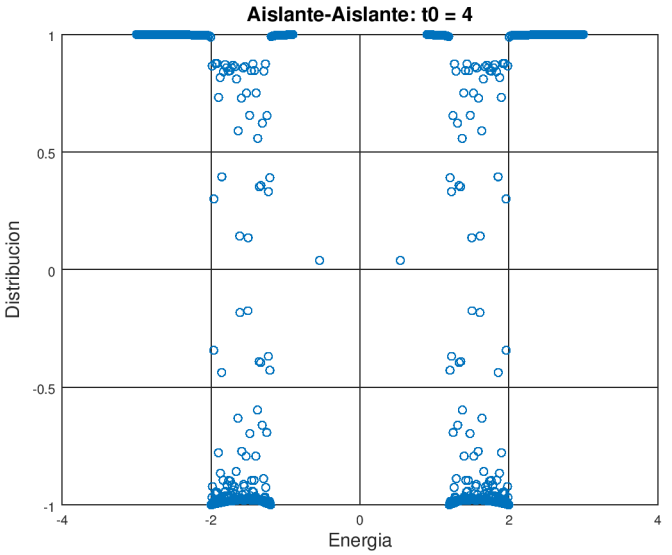

Aislante-Aislante: t0 = 2.3
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

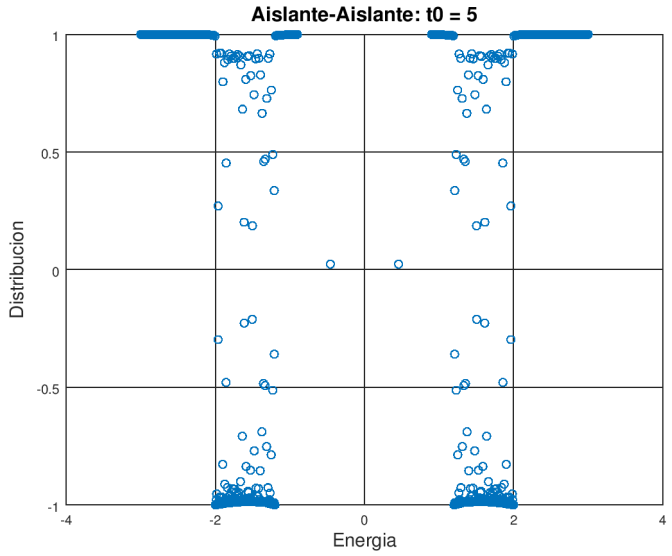

Aislante-Aislante: t0 = 2.4
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

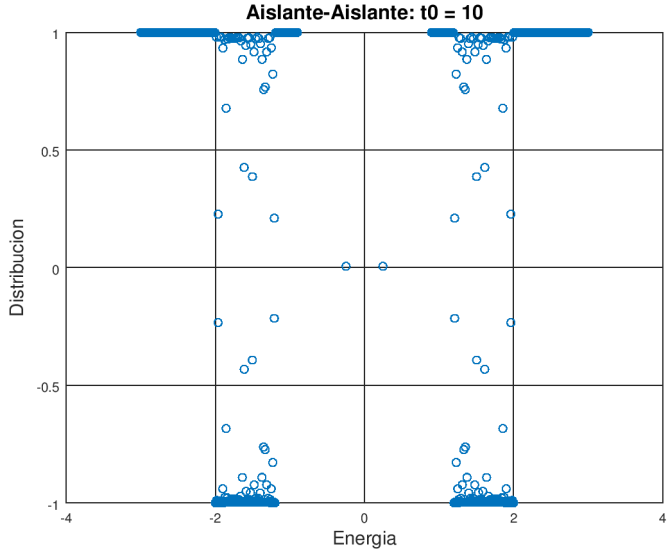

Aislante-Aislante: t0 = 2.5
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

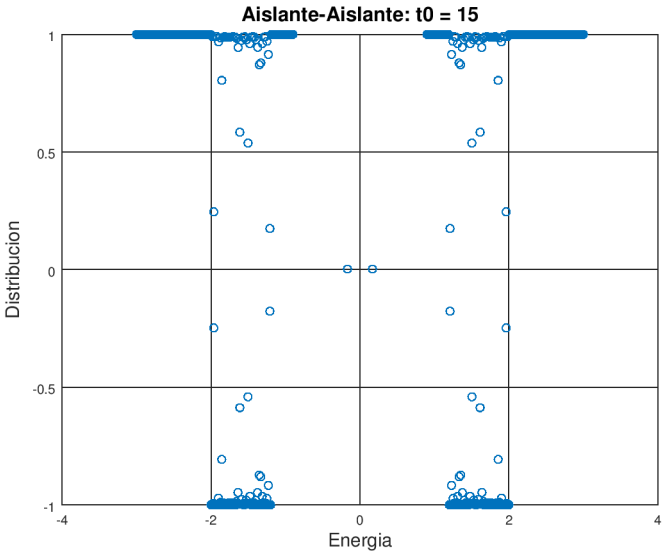

Aislante-Aislante: t0 = 3
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4


Aislante-Aislante: t0 = 3.5
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4


Aislante-Aislante: t0 = 4
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4


Aislante-Aislante: t0 = 5
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4


Aislante-Aislante: t0 = 10
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4


Aislante-Aislante: t0 = 15
Distribucion
Energia
1
0.5
0
-0.5
-1
-4
-2
0
2
4

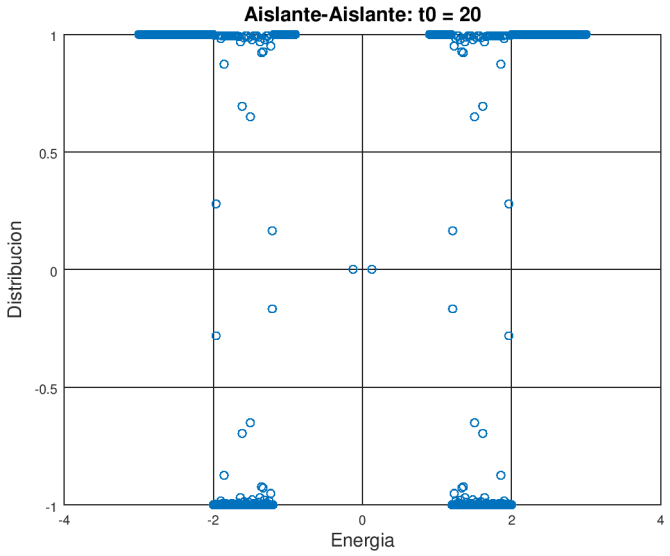
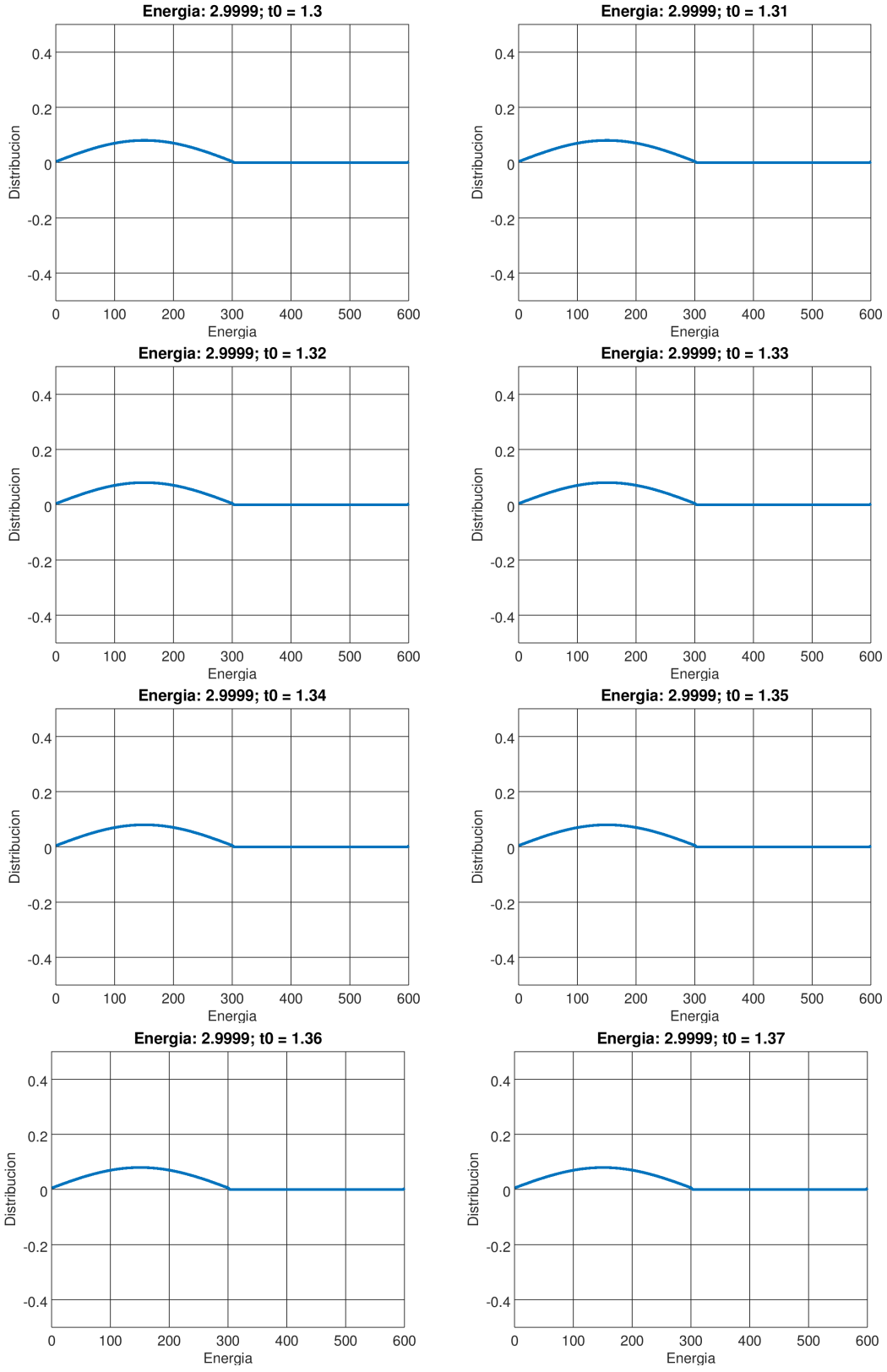
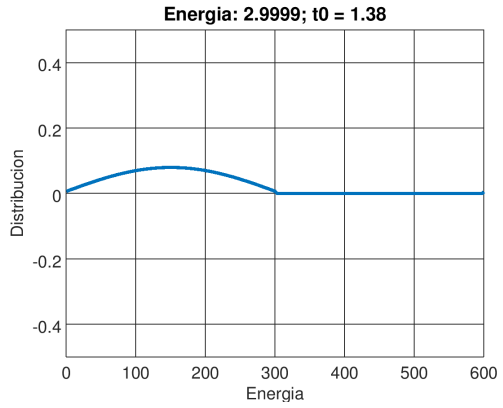
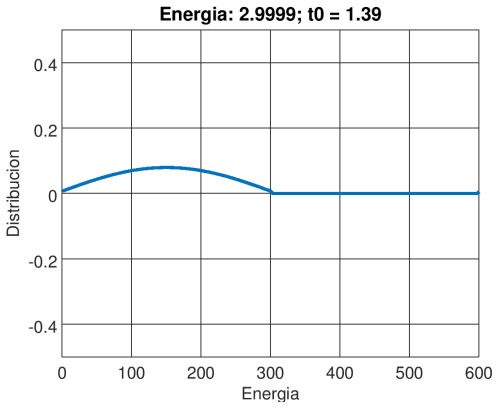


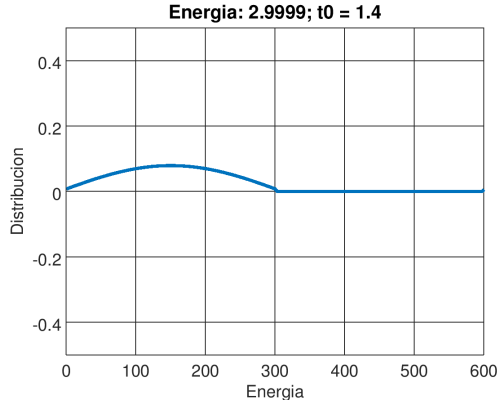
Figura 3.1: Evolución de la distribución en función del valor del contacto.

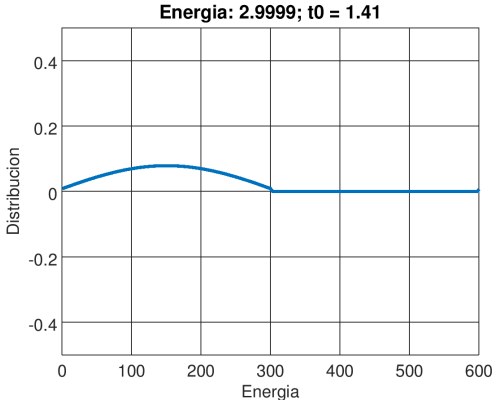
4. ANEXO IV: Evolución estado máxima energía

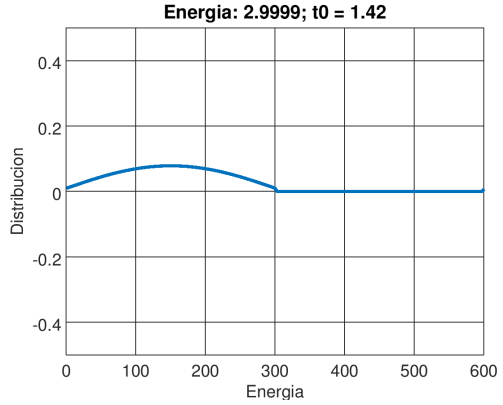


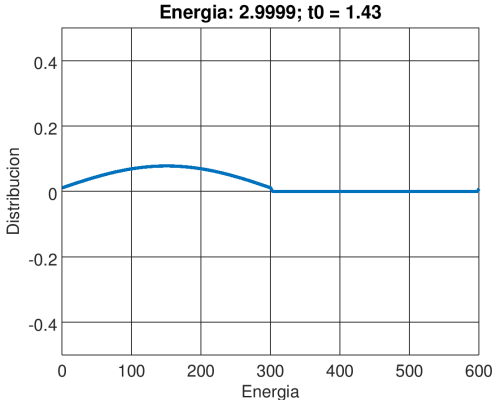

Energia: 2.9999; t0 = 1.38
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

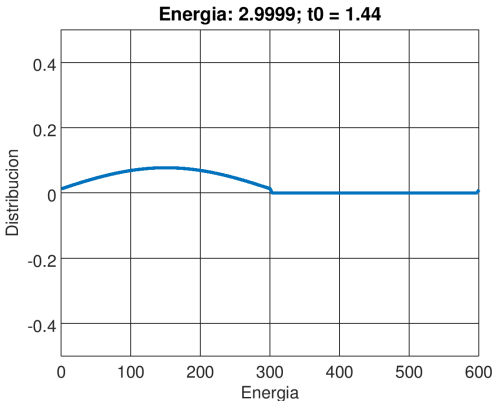

Energia: 2.9999; t0 = 1.39
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

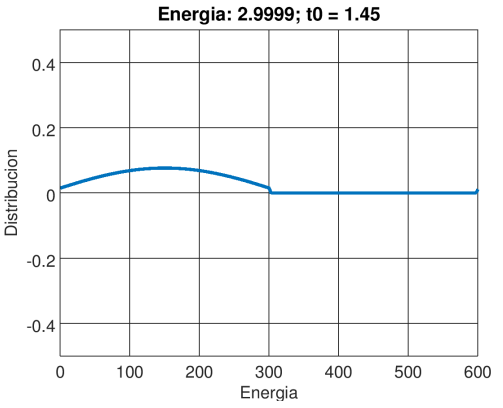

Energia: 2.9999; t0 = 1.4
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

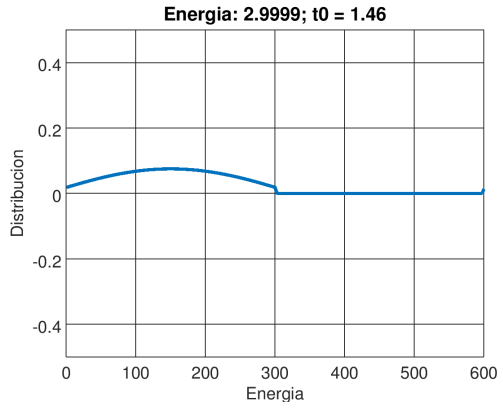

Energia: 2.9999; t0 = 1.41
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

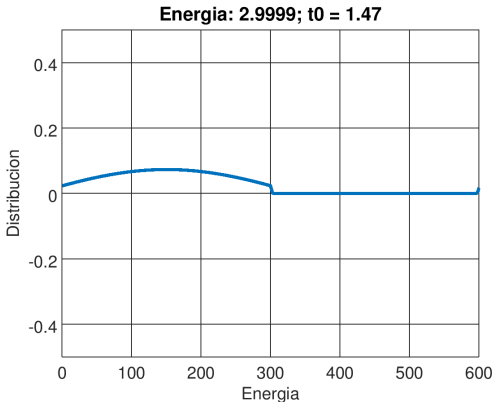

Energia: 2.9999; t0 = 1.42
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

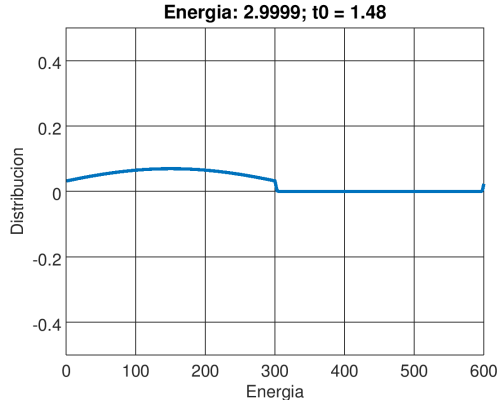

Energia: 2.9999; t0 = 1.43
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

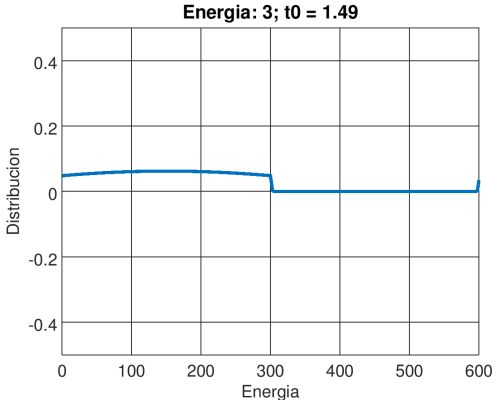

Energia: 2.9999; t0 = 1.44
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

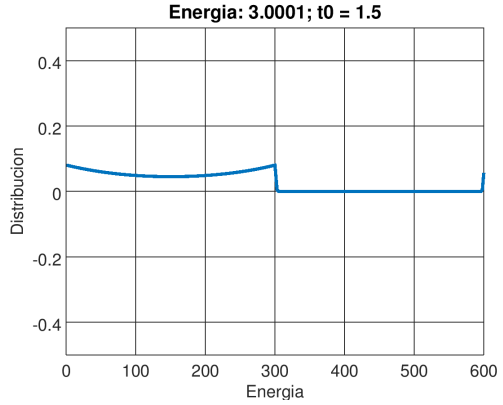

Energia: 2.9999; t0 = 1.45
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

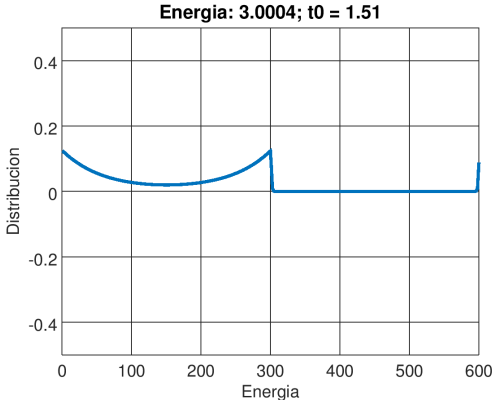

Energia: 2.9999; t0 = 1.46
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

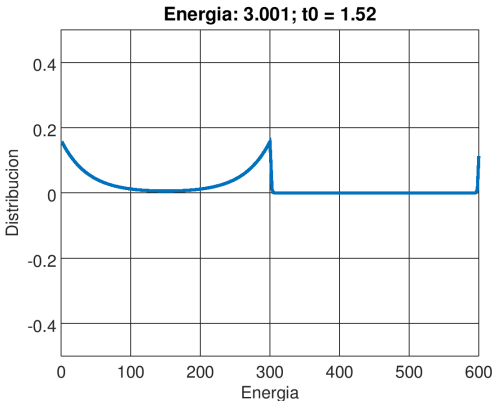

Energia: 2.9999; t0 = 1.47
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

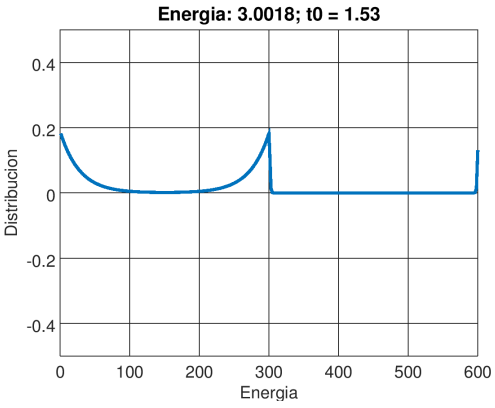

Energia: 2.9999; t0 = 1.48
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

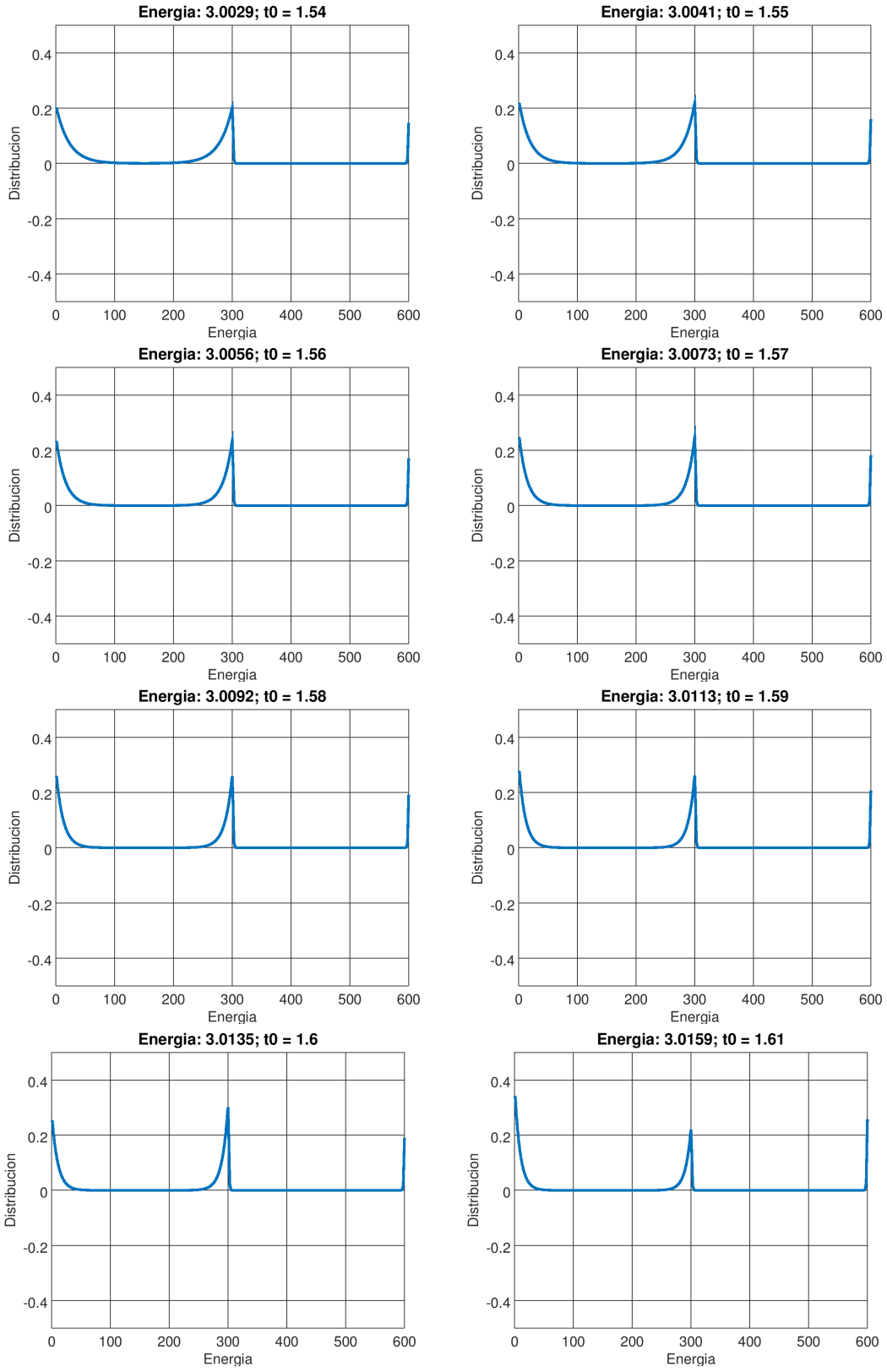

Energia: 3; t0 = 1.49
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

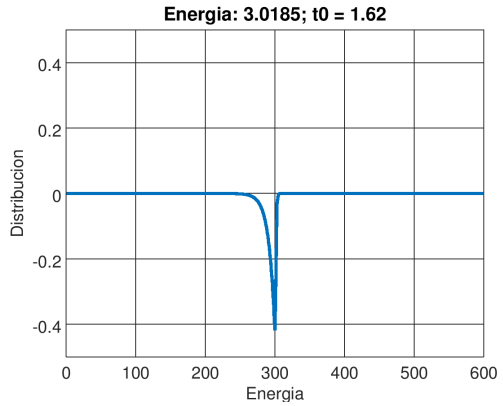

Energia: 3.0001; t0 = 1.5
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

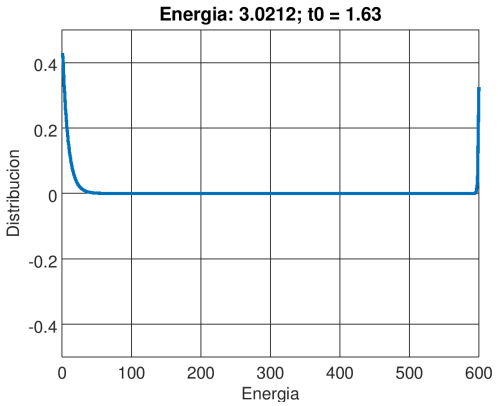

Energia: 3.0004; t0 = 1.51
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

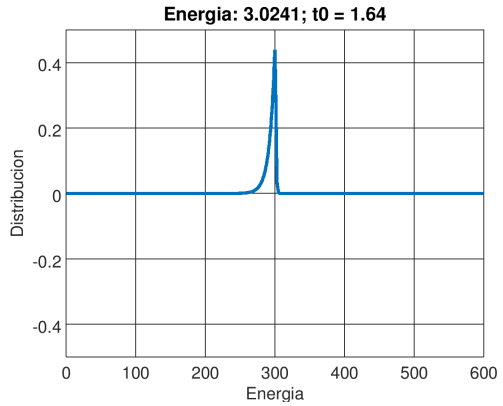

Energia: 3.001; t0 = 1.52
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

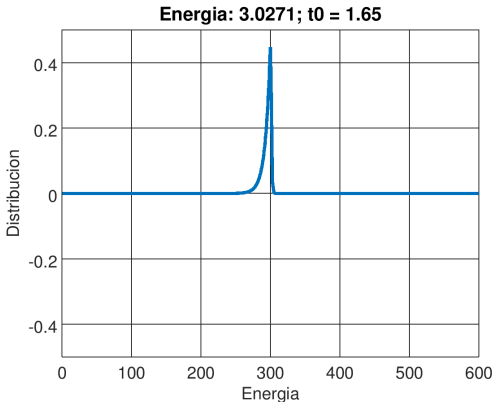

Energia: 3.0018; t0 = 1.53
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

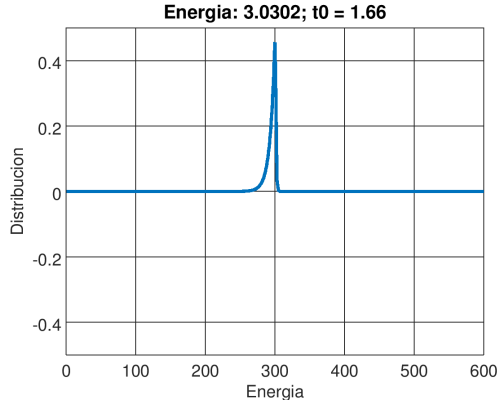

Energia: 3.0029; t0 = 1.54
Energia: 3.0041; t0 = 1.55
Energia: 3.0056; t0 = 1.56
Energia: 3.0073; t0 = 1.57
Energia: 3.0092; t0 = 1.58
Energia: 3.0113; t0 = 1.59
Energia: 3.0135; t0 = 1.6
Energia: 3.0159; t0 = 1.61
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

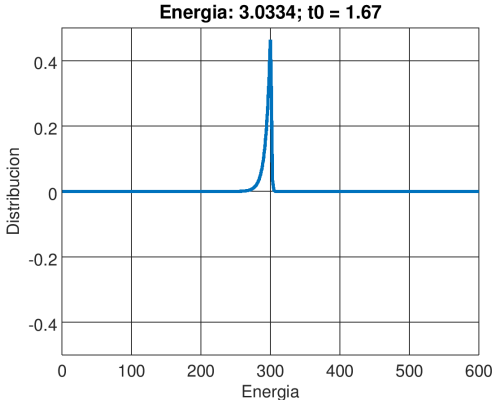

Energia: 3.0185; t0 = 1.62
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

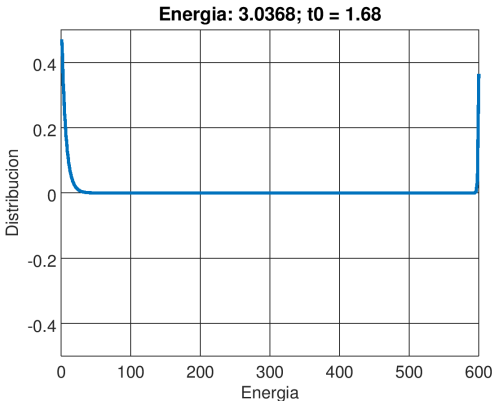

Energia: 3.0212; t0 = 1.63
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

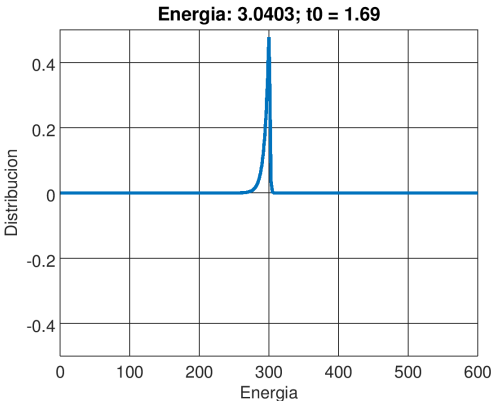

Energia: 3.0241; t0 = 1.64
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600


Energia: 3.0271; t0 = 1.65
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600


Energia: 3.0302; t0 = 1.66
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600


Energia: 3.0334; t0 = 1.67
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600


Energia: 3.0368; t0 = 1.68
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600


Energia: 3.0403; t0 = 1.69
Distribucion
Energia
0.4
0.2
0
-0.2
-0.4
0
100
200
300
400
500
600

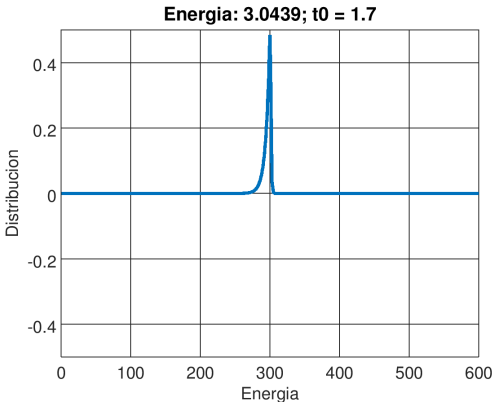


Figura 4.1: Evolución del estado de máxima energía de la banda de conducción en función del contacto.

5. ANEXO V: Casos concretos de la localización

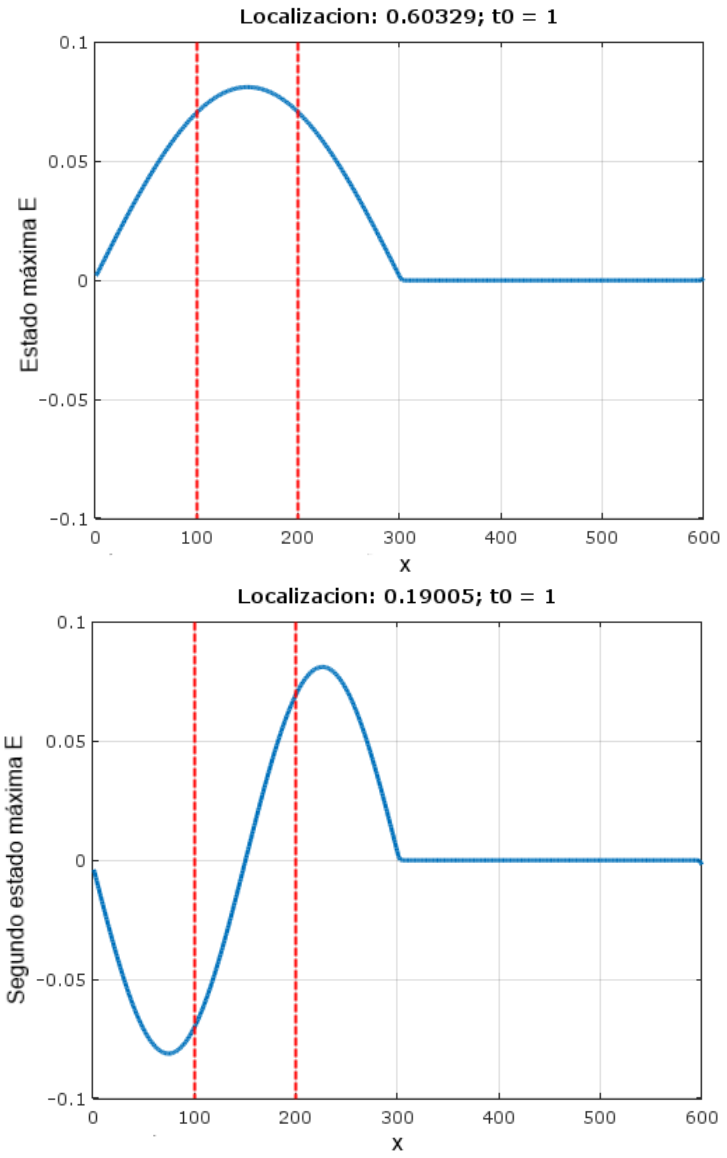


Figura 5.1: A pesar de que los estados están extendidos, el valor de su localización es distinto a 1/3.

6. ANEXO VI: Anchura de la transición variable con N

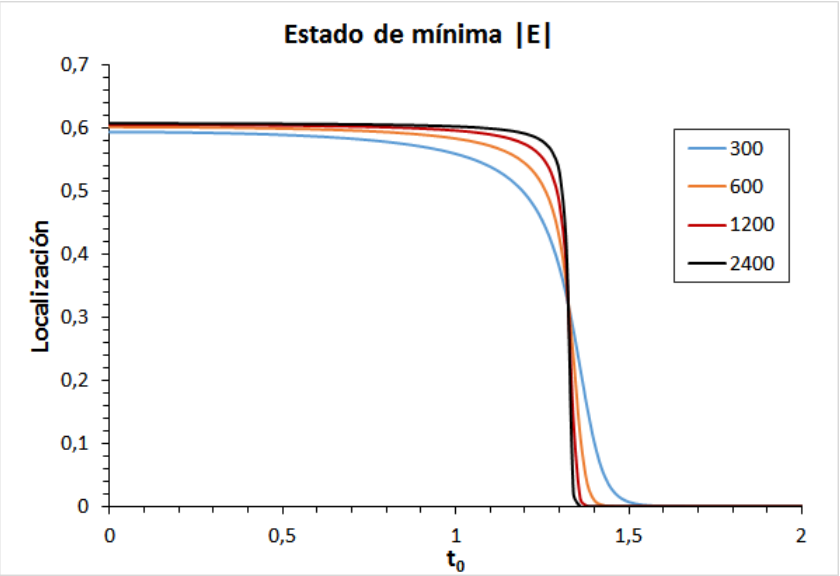


Figura 6.1: Evolución de la localización del estado de mínima energía de la banda de conducción.

7. ANEXO VII: Derivada de la energía en función del contacto

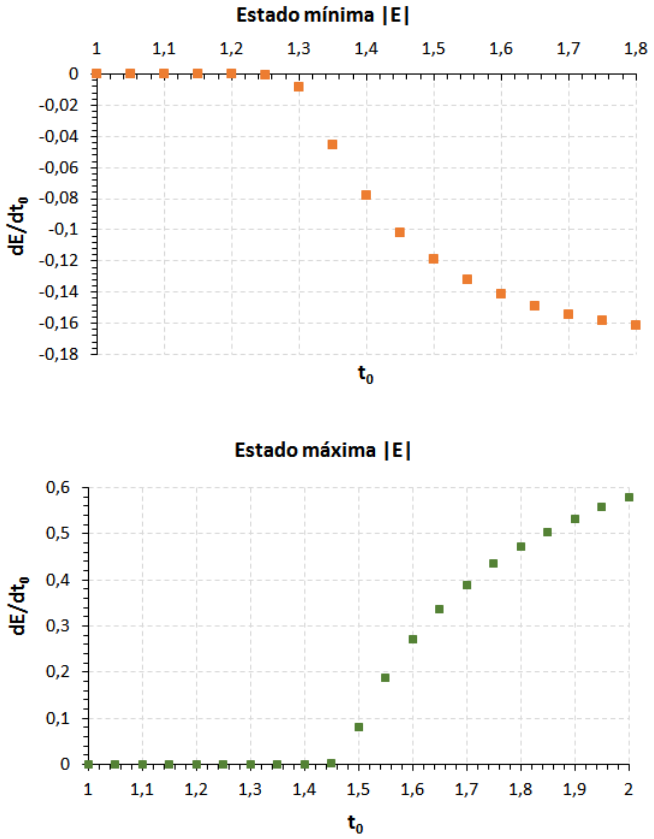


Figura 7.1: Arriba: evolución de la derivada de la energía del estado de mínima energía de la banda de conducción (301). Abajo: misma magnitud en el caso del estado de máxima energía (600)

8. ANEXO VIII: Evolución del gap para N = 600

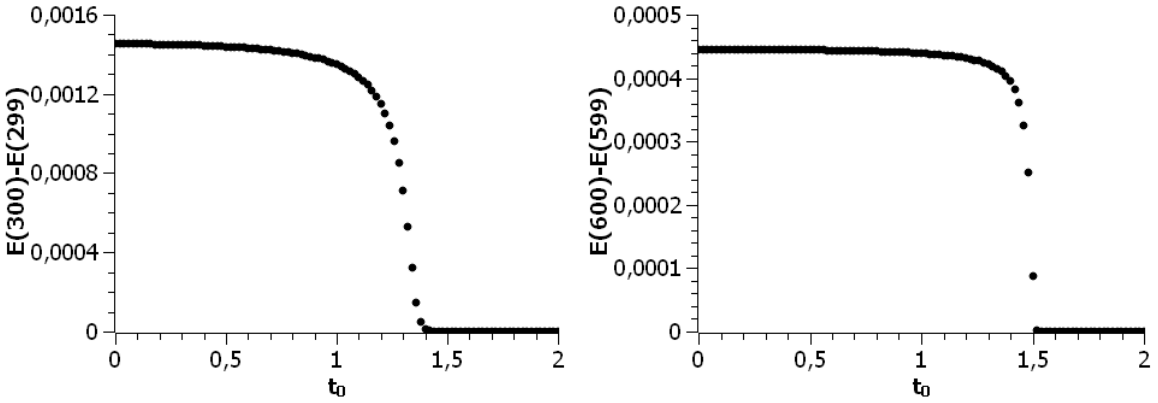


Figura 8.1: Izquierda: evolución del gap que existe entre los estados 300 y 299 en función del valor del contacto. Derecha: misma variación, pero para el caso de los estados 600 y 599.