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(* Parametros *)
dt = 0.005;
ħ = 1;
m = 1.9;
V0 = 0.21;
dx = 0.1;
xmin = -102.4;
xmax = 102.4;
Nn =  $\frac{x_{\max} - x_{\min}}{dx}$ ; (* Tamaño de los arrays *)

(* Array de espacios *)

$$xarray = Table\left[i, \left\{i, -\frac{1}{2} Nn dx, \frac{1}{2} Nn dx, dx\right\}\right];$$



$$dk = \frac{2 \pi}{Nn dx};$$


$$k0 = -\frac{1}{2} Nn dk;$$


$$karray = Table[k0 + i, \{i, 0, Nn dk, dk\}];$$


(* Potencial *)

$$L = \frac{\hbar}{\sqrt{2 m}};$$

ac = 3 L;

$$V[x_, a_, V0_] := (2 V0 / 3) (UnitStep[x + 2 a] - UnitStep[x + a]) +$$


$$(V0 / 2) (UnitStep[x + a] - UnitStep[x]) + V0 (UnitStep[x] - UnitStep[x - a]) +$$


$$(V0 / 2) (UnitStep[x - a] - UnitStep[x - 2 a]) +$$


$$(V0 / 8) (UnitStep[x - 2 a] - UnitStep[x - 4 a]);$$

varray = V[xarray, ac, V0];
zeroindex = 45;
Do[varray[[i]] = 1020, {i, 1, zeroindex}]
Do[varray[[i]] = 1020, {i, Length[varray] - zeroindex, Length[varray]}]

(* Array de funciones de onda *)
x0c = -60 L;

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$$p0c = \sqrt{2 m (0.2)} ;$$

$$dp2 = \frac{p0c^2}{80} ;$$

$$d = \frac{\hbar}{\sqrt{2 dp2}} ;$$

$$k0c = \frac{p0c}{\hbar} ;$$

$$\psi0x[x_, a_, x0_, k0_] := \frac{1}{\sqrt{a} \sqrt{\pi}} e^{-\frac{i}{2} \left(\frac{x-x0}{a}\right)^2 + i x k0} ;$$

$$\psi0xarray = \psi0x[xarray, d, x0c, k0c] ;$$

(* Para graficar *)

$$scalegauss = \frac{1}{\sqrt{d} \sqrt{\pi}} ;$$

$$scalev0 = v0 ;$$

$$scale = 0 ;$$

$$\text{If}[scalegauss > scalev0, scale = scalegauss, scale = scalev0] ;$$

[si]

(* Funciones *)

CF[ψxarray_] := Module[{ψtmp},
[módulo]

ψtmp = ψxarray;

Do[ψtmp[[i]] = 0.0, {i, 1, zeroindex}];

[repite]

Do[ψtmp[[i]] = 0.0, {i, Length[ψtmp] - zeroindex, Length[ψtmp]}];

[repite]

[longitud]

[longitud]

Return[ψtmp];

[retorna]

];

$$\text{Discretize}[\psi xarray_] := \psi xarray \frac{dx}{\sqrt{2 \pi}} e^{-i k0 xarray} ;$$

$$\text{Undiscretize}[\psi xarray_] := \psi xarray \frac{\sqrt{2 \pi}}{dx} e^{i k0 xarray} ;$$

$$\text{Step}\psi x[\psi xarray_ , dt_] := \psi xarray e^{-\frac{i}{2} \frac{varray}{\hbar} dt} ;$$

$$\text{Step}\psi k[\psi karray_ , dt_] := \psi karray e^{-\frac{i}{2} \frac{\hbar karray^2}{m} dt} ;$$

Stepψ[ψxarray_] := Module[{ψmx, ψmk},
[módulo]

ψmx = CF[ψxarray];

ψmx = Stepψx[ψmx, dt];

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     $\psi_{mk} = \text{Fourier}[\psi_{mx}] ;$ 
    [transformada de Fourier discreta]
     $\psi_{mk} = \text{Step}\psi_k[\psi_{mk}, dt] ;$ 
     $\psi_{mx} = \text{InverseFourier}[\psi_{mk}] ;$ 
    [transformada de Fourier discreta inversa]
     $\psi_{mx} = \text{Step}\psi_x[\psi_{mx}, dt] ;$ 
    Return[ $\psi_{mx}$ ] ;
    [retorna]
]
Step $\psi$ ForList[ $\psi_{xarray\_}$ ] := Module[{ $\psi_{mx}$ ,  $\psi_{mk}$ },
    [módulo]
     $\psi_{mx} = \text{CF}[\psi_{xarray}] ;$ 
     $\psi_{mx} = \text{Step}\psi_x[\text{Discretize}[\psi_{mx}], dt] ;$ 
     $\psi_{mk} = \text{Fourier}[\psi_{mx}] ;$ 
    [transformada de Fourier discreta]
     $\psi_{mk} = \text{Step}\psi_k[\psi_{mk}, dt] ;$ 
     $\psi_{mx} = \text{InverseFourier}[\psi_{mk}] ;$ 
    [transformada de Fourier discreta inversa]
     $\psi_{mx} = \text{Step}\psi_x[\psi_{mx}, dt] ;$ 
    Return[Undiscretize[ $\psi_{mx}$ ]] ;
    [retorna]
]
Evolve[ $\psi_{xarray\_}$ , iter_] := Module[{},
    [módulo]
    Print["t = " <> ToString[iter * dt]] ;
    [convierte a cadena de caracteres]
    Return[Undiscretize[Nest[Step $\psi$ , Discretize[ $\psi_{xarray}$ ], iter]]] ;
    [anida]
]
EvolveList[ $\psi_{xarray\_}$ , iter_] := Module[{},
    [módulo]
    Print["tmax = " <> ToString[iter * dt]] ;
    [convierte a cadena de caracteres]
    Return[NestList[Step $\psi$ ForList,  $\psi_{xarray}$ , iter]] ;
    [lista de resultados anidados]
]
ListLinePlot[{Abs[Evolve[ $\psi_{0xarray}$ , 2000]], varray},
    [gráfico de línea...] [valor absoluto]
    PlotRange → scale, PlotLegends → {"| $\psi(x,t)$ |", "V(x)"}]
    [leyendas de representación]

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