

```
In[1]:= Clear["Global`*"];
```

Problem

Solve numerically the differential equation (in atomic units $\hbar = 1$, $m_e = 1$)

$$i \frac{\partial \psi(x, t)}{\partial t} = -\frac{1}{2\mu} \frac{\partial^2 \psi(x, t)}{\partial x^2} \quad (1)$$

with the following initial condition

$$\psi(x, 0) = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-(x-x_0)^2/(4\sigma^2) + ipx} \quad (2)$$

and Dirichlet boundary conditions

$$\begin{aligned} u(-\infty, t) &= 0 \\ u(+\infty, t) &= 0 \end{aligned} \quad (3)$$

Exact solution

Initial normalized Gaussian packet :

```
In[2]:= psi0[x_, x0_, sigma_, p_] = 1 / (2 Pi sigma^2)^(1/4) Exp[(- (x - x0)^2 / (4 sigma^2) + i p x)];
Assuming[sigma > 0,
Integrate[psi0[x, x0, sigma, p] * psi0[x, x0, sigma, -p], {x, -Infinity, Infinity}]]
```

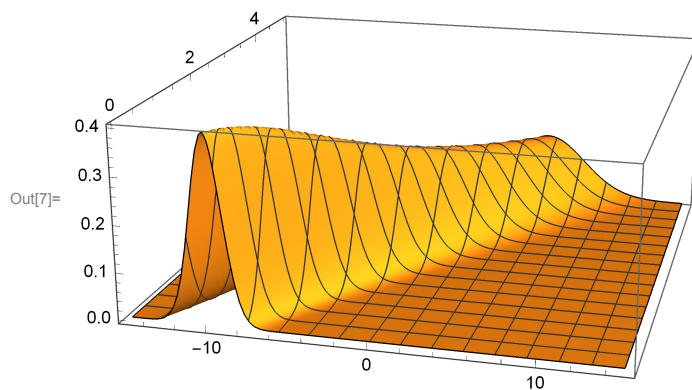
```
Out[3]= 1
```

Exact solution:

$$\text{psiExact}[x_, t_, x0_, \sigma_, p_, \mu_] = e^{\frac{-(x-x0)^2 \mu - 2 i p^2 t \sigma^2 + p (-2 t x0 + 4 i x \mu \sigma^2)}{2 i t + 4 \mu \sigma^2}} \left(\frac{2}{\pi}\right)^{1/4} \sqrt{\sigma} / \left(\sqrt{\frac{i t}{\mu} + 2 \sigma^2}\right);$$

Parameters:

```
In[5]:= pini = 3; mass = 1; xini = -10; sigma_i = 1;
xmin = -15; xmax = 15; tmax = 5;
Plot3D[Abs[psiExact[x, t, xini, sigma_i, pini, mass]^2],
{x, xmin, xmax}, {t, 0, tmax}, PlotRange -> All, PlotPoints -> 100]
```



Numerical solution in the FEM-DVR basis

Gauss-Lobatto quadrature points and weights will be used for integration over one element

```
In[8]:= getGaussLobattoPointsAndWeights[n_, a_, b_] :=
Module[{x, w, p},
  (* roots of the derivative of the (n-1)st Legendre polynomial are inner points
    of the Gauss-Lobatto quadrature on [-1,1]*)
  p[z_] = LegendreP[n - 1, z];
  If[n == 2,
    x = {-1.0, 1.0},
    x = N[Flatten[{-1.0, Sort[Re[z /. N[Solve[D[p[z], z] == 0, z], 20]]], 1.0}]]
  ];
  (* to get weights we need values of this polynomial *)
  w = 2.0
  Flatten[{1.0, Table[1.0 / (N[p[x[[i]]], 20) ^ 2, {i, 2, n - 1}], 1.0}] / (n (n - 1));
  (* shifting and scaling to the interval [a,b] *)
  x = (b - a) x / 2 + (b + a) / 2;
  w = (b - a) w / 2;
  Return[{x, w}]
]
getGaussLobattoPointsAndWeights[5, 0, 1]
Out[9]= {{0., 0.1726731646, 0.5, 0.8273268354, 1.},
{0.05, 0.2722222222, 0.3555555556, 0.2722222222, 0.05}}
```

Full grid and weights

```
In[10]:= getFEMPointsAndWeights[nGL_, endPoints_] :=
Module[{nEl, nPoints, xGL, wGL, x, w},
  nEl = Length[endPoints] - 1;
  nPoints = nEl * (nGL - 1) + 1;
  (* Print["Number of all points/basis functions is ", nPoints]; *)
  x = ConstantArray[0.0, nPoints];
  w = ConstantArray[0.0, nPoints];
  Do[
    {xGL, wGL} =
      getGaussLobattoPointsAndWeights[nGL, endPoints[[i]], endPoints[[i + 1]]];
    x[[ (i - 1) * (nGL - 1) + 1 ;; i * (nGL - 1) + 1]] = xGL;
    (* weights at points which are common to two elements are added up *)
    w[[ (i - 1) * (nGL - 1) + 1 ;; i * (nGL - 1) + 1]] += wGL,
    {i, 1, nEl}
  ];
  Return[{x, w}]
]
getFEMPointsAndWeights[4, {0, 1, 3, 6}]
Out[11]= {{0., 0.2763932023, 0.7236067977, 1., 1.552786405, 2.447213595, 3.,
3.829179607, 5.170820393, 6.}, {0.08333333333, 0.4166666667, 0.4166666667,
0.25, 0.8333333333, 0.8333333333, 0.4166666667, 1.25, 1.25, 0.25}}
```

Derivatives of the Lagrange polynomials at GL points on [-1,1] - result is a matrix nGL x nGL of $D[l_i(x), x = x_k]$

```

In[12]:= derivativesLagPol[nGL_] :=
Module[{xGL, wGL, dLP, hlp},
  dLP = ConstantArray[0.0, {nGL, nGL}];
  {xGL, wGL} = getGaussLobattoPointsAndWeights[nGL, -1.0, 1.0];
  Do[
    (* Diagonal terms *)
    dLP[[i, i]] = 0.0;
    Do[
      If[i ≠ s, dLP[[i, i]] = dLP[[i, i]] + 1.0 / (xGL[[i]] - xGL[[s]]),
      {s, 1, nGL}
    ];
    (* Off-diagonal terms *)
    Do[
      hlp = 1.0;
      Do[
        If[(j ≠ i) && (j ≠ k), hlp = hlp * (xGL[[k]] - xGL[[j]]) / (xGL[[i]] - xGL[[j]]),
        {j, 1, nGL}
      ];
      dLP[[i, k]] = hlp / (xGL[[i]] - xGL[[k]]);
      dLP[[k, i]] = 1.0 / (hlp * (xGL[[k]] - xGL[[i]])),
      {k, i + 1, nGL}
    ],
    {i, 1, nGL}
  ];
  Return[dLP];
];
derivativesLagPol[4]

Out[13]= {{-3., -0.8090169944, 0.3090169944, -0.5},
{4.045084972, -3.330669074 × 10-16, -1.118033989, 1.545084972},
{-1.545084972, 1.118033989, 2.220446049 × 10-16, -4.045084972},
{0.5, -0.3090169944, 0.8090169944, 3.}}

```

Construction of the stiffness matrix (ϕ'_i, ϕ'_j)

```

In[14]:= constructStiffnessMatrix[nGL_, endPoints_] :=
Module[{nEl, nPoints, xFEM, wFEM, xGL, wGL, dLP, dBF, k1, ii, jj, oldCorner, A},
  nEl = Length[endPoints] - 1;
  nPoints = nEl * (nGL - 1) + 1;
  (* get weights for all points *)
  {xFEM, wFEM} = getFEMPointsAndWeights[nGL, endPoints];
  (* calculate derivatives of the Lagrange
  interpolating polynomials at GL points on [-1,1] *)
  dLP = derivativesLagPol[nGL];
  (* build the stiffness matrix *)
  A = ConstantArray[0.0, {nPoints, nPoints}];
  oldCorner = 0.0;
  Do[
    {xGL, wGL} =
      getGaussLobattoPointsAndWeights[nGL, endPoints[[k]], endPoints[[k + 1]]];
    (* dilatation of derivatives of LP to be the derivatives
    of the basis functions on the k-th element *)
    dBF = 2.0 * dLP / (endPoints[[k + 1]] - endPoints[[k]]);
    k1 = (k - 1) * (nGL - 1) + 1;
    (* index of the first point of the k-th element in x *)
    Do[
      (* normalization factor of basis functions *)
      dBF[[i, All]] = dBF[[i, All]] / Sqrt[wFEM[[k1 + i - 1]]],
      {i, 1, nGL}
    ];
    Do[
      ii = k1 + i - 1; (* current row in the A matrix *)
      Do[
        jj = k1 + j - 1; (* current column in the A matrix *)
        A[[ii, jj]] = Sum[wGL[[s]] * dBF[[i, s]] * dBF[[j, s]], {s, 1, nGL}];
        A[[jj, ii]] = A[[ii, jj]],
        {j, i, nGL}
      ],
      {i, 1, nGL}
    ];
    A[[k1, k1]] += oldCorner;
    oldCorner = A[[k1 + nGL - 1, k1 + nGL - 1]],
    {k, 1, nEl}
  ];
  Return[A]
]
constructStiffnessMatrix[2, {0, 1, 2, 3, 4}] // MatrixForm

```

Out[15]//MatrixForm=

$$\begin{pmatrix} 2. & -1.414213562 & 0. & 0. & 0. \\ -1.414213562 & 2. & -1. & 0. & 0. \\ 0. & -1. & 2. & -1. & 0. \\ 0. & 0. & -1. & 2. & -1.414213562 \\ 0. & 0. & 0. & -1.414213562 & 2. \end{pmatrix}$$

Time evolution using the Crank-Nicolson implicit

Parameters of numerical solution:

```
In[16]:= pini = 3.0; mass = 1.0; xini = -7.0; sigma = 1.0;
{xmin, xmax} = {-20.0, 10.0};
{tmin, tmax} = {0.0, 1.0};
(* check that the interval is large enough *)
N[psiExact[xmin, tmin, xini, sigma, pini, mass], 20]
N[psiExact[xmax, tmax, xini, sigma, pini, mass], 20]
```

```
Out[19]=  $-2.693633337 \times 10^{-19} + 8.620714619 \times 10^{-20} i$ 
```

```
Out[20]=  $3.572886099 \times 10^{-18} + 4.374105074 \times 10^{-18} i$ 
```

Set equidistant elements and calculate initial state and Hamiltonian matrix on the FEM-DVR grid:

```
In[21]:= nGL = 14;
nEl = 30;
endPoints = Table[N[xmin + i * (xmax - xmin) / nEl], {i, 0, nEl}];
{xFEM, wFEM} = getFEMPointsAndWeights[nGL, endPoints];
Nb = Length[xFEM];
Print["Number of points/basis functions: ", Nb];

(* coefficients of the initial wave packet  $\psi(x)$  in the FEM basis *)
psiini = N[psi0[xFEM, xini, sigma, pini]] * Sqrt[wFEM];
(* stiffness matrix which is used to construct the Hamiltonian matrix *)
A = constructStiffnessMatrix[nGL, endPoints];
(* Hamiltonian matrix *)
H = A[[2 ;; Nb - 1, 2 ;; Nb - 1]] / (2.0 * mass);
```

Number of points/basis functions: 391

Time evolution:

```
In[30]:= {nx, nt} = {Nb - 2, 21}
dt = N[(tmax - tmin) / (nt - 1)]
T = N[Range[tmin, tmax, dt]];

(* Initialization of the array with zeroes - Dirichlet's boundary conditions *)
psi = ConstantArray[0.0, {nx, nt}];
error = ConstantArray[0.0, nt];

(* Initial state *)
psi[[All, 1]] = psiini[[2 ;; Nb - 1]];

(* generalized Crank-Nicolson method -
exp(-i H dt) approximated by a Pade [n/n] approximant *)
nCN = 5;
roots = N[x /. Solve[PadeApproximant[Exp[x], {x, 0, {nCN, nCN}}] == 0, x]];
Do[
  tmppsi = psi[[All, n]];
  Do[
    tmppsi = (IdentityMatrix[nx] + i * dt * H / roots[[i]]).tmppsi;
    tmppsi =
      LinearSolve[IdentityMatrix[nx] - i * dt * H / Conjugate[roots[[i]]], tmppsi],
    {i, 1, nCN}
  ];
  psi[[All, n + 1]] = tmppsi,
  {n, 1, nt - 1}
];
```

```

(* to get the functional values of the solution at grid
points we have to multiply the coefficients by Sqrt[w] *)
Do[
  psi[[All, n]] = psi[[All, n]] / Sqrt[wFEM[[2 ;; Nb - 1]]],
  {n, 1, nt}
];

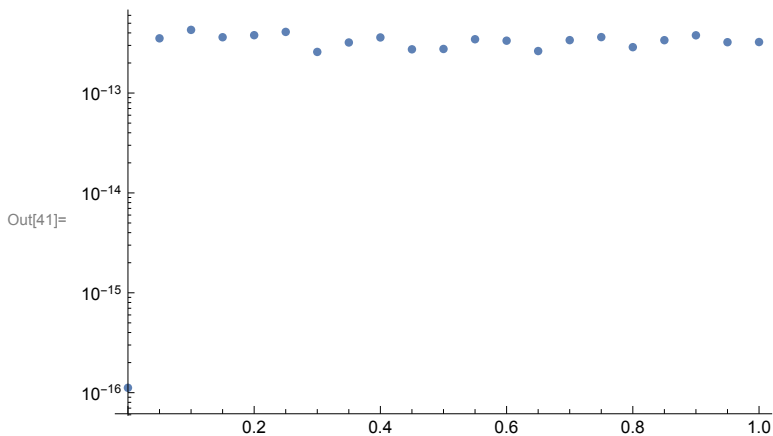
(* compare with the exact solution *)
Do[
  error[[n]] = 0.0;
  Do[
    error[[n]] = Max[error[[n]],
      Abs[psi[[j, n]] - psiExact[xFEM[[j + 1]], T[[n]], xini, sigmaini, pini, mass]]],
    {j, 1, nx}
  ],
  {n, 1, nt}
];
ListLogPlot[Table[{T[[n]], error[[n]]}, {n, 1, nt}]],
PlotRange -> All]
Print["Maximal error: ", Max[error]]

(* fancy plotting *)
Manipulate[
  n = Round[t / dt] + 1;
  ListLinePlot[Table[{xFEM[[j + 1]], Abs[psi[[j, n]]^2}], {j, 1, nx}],
  PlotRange -> {-0.5, 1.5}],
  {t, tmin, tmax, dt}
]

```

Out[30]= {389, 21}

Out[31]= 0.05



Maximal error: $4.290731481 \times 10^{-13}$

Out[43]=

