Задача 1

Уравнение Шреденгера для атома водорода имеет вид:

$$-\frac{h^2}{2mr^2}\left(r^2\psi'\right)' - \frac{e^2}{r}\psi = E\,\psi[x]$$

$$-r^2\psi'' - 2r\psi' - r\psi = r^2 E\,\psi[x]$$

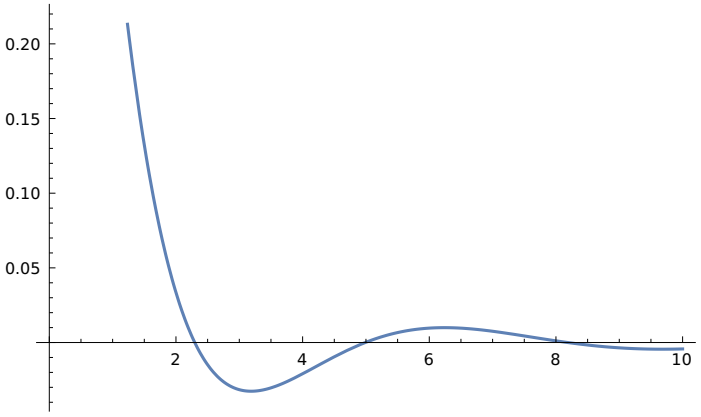
In[20]:=
```
m = 1;
ħ = 1;
e = 1;
l = 0;
```

$$\frac{-1}{2m}\psi''[r] - \frac{2}{r}\psi'[r] + \frac{2m}{\hbar^2}\left(-\frac{e^2}{r} - EE\right)\psi[r] + \frac{l(l+1)}{2mr^2}\psi[r]$$

Out[24]=
$$2\left(-0.1 - \frac{1}{r}\right)\psi[r] - \frac{2\psi'[r]}{r} - \frac{\psi''[r]}{2}$$

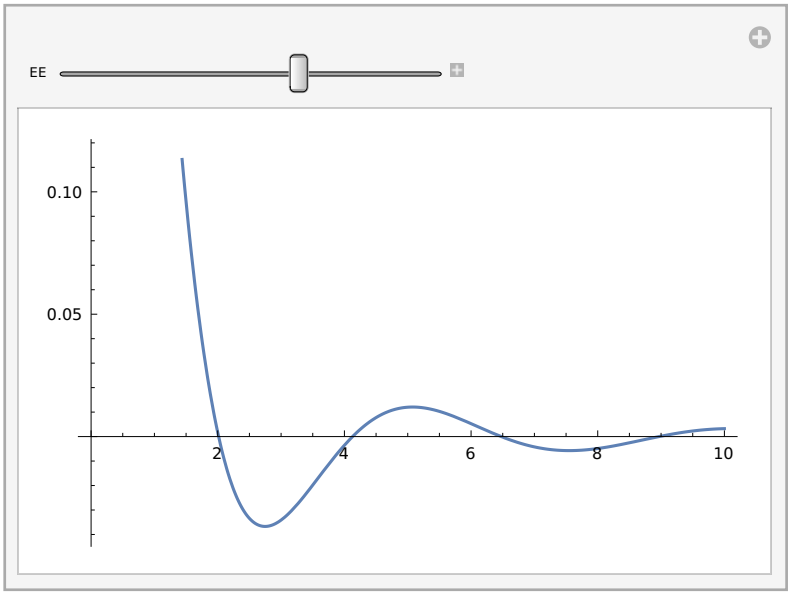
In[28]:=
```
EE = 0.1;
solution = NDSolve[{(-1/(2 m)) ψ''[r] - (2/r) ψ'[r] + (2 m/ħ^2) (-(e^2/r) - EE) ψ[r] + (l (l + 1))/(2 m r^2) ψ[r] == 0,
    ψ[10^(-8)] == 1, ψ'[10^(-8)] == 0}, ψ, {r, 10^(-8), 10}][[1]];
Plot[ψ[r] /. solution, {r, 10^(-8), 10}]
```

Out[30]=



In[31]:=
```
Manipulate[
 solution = NDSolve[{(-1/(2 m)) ψ''[r] - (2/r) ψ'[r] + (2 m/ħ^2) (-(e^2/r) - EE) ψ[r] + (l (l + 1))/(2 m r^2) ψ[r] == 0,
    ψ[10^(-8)] == 1, ψ'[10^(-8)] == 0},
   ψ, {r, 10^(-8), 10}][[1]];
 Plot[ψ[r] /. solution, {r, 10^(-8), 10}],
 {EE, -1, 1}
]
```

Out[31]=




```
solution = NDSolve[{(-1/(2 m)) ψ''[r] - (2/r) ψ'[r] + (2 m/ħ^2) (-(e^2/r) - EE) ψ[r] + (l (l + 1))/(2 m r^2) ψ[r] == 0,
    ψ[10^(-8)] == 1, ψ'[10^(-8)] == 0},
   ψ, {r, 10^(-8), 10}][[1]];
Plot[ψ[r] /. solution, {r, 10^(-8), 10}]
```

Задача 2

In[32]:=
```
x /: x^m_ := -x^(m-2) /; (m ≥ 2)
```

In[33]:=
```
p[x_] := x^5 - 6 x^4 + 5 x^3 + 10 x^2 - x + 1
```

In[34]:=
```
p[x]
```

```
-15 - 5 x
```

Задача 3

In[35]:=
```
i /:
 i^2 := -1
j /:
 j^2 := -1
k /:
 k^2 := -1
i j ^:= k
j k ^:= i
k i ^:= j
```

In[41]:=
```
L1 = 5 + 6 i + 7 j + 10 k;
L2 = 15 + 3 i + 31 j + 4 k;
L1 + L2
```

Out[43]=
$$20 + 9\,i + 38\,j + 14\,k$$

In[45]:=
```
Expand[L1 * L2]
```

Out[45]=
$$-200 + 443\,i + 314\,j + 377\,k$$

Задача 4

In[46]:=
```
HamEq[H_, coord_] := Module[{n, i, equations},
  n = Length[coord];
  equations = Table[0, {i1, n}, {j1, 2}];
  For[i = 1, i ≤ n, i++,
   equations[[i, 1]] = - D[H, coord[[i, 1]][t]];
   equations[[i, 2]] = D[H, coord[[i, 2]][t]]
  ];
  equations
 ];
```

In[52]:=
```
H0 = p1[t]^2/(2 m1) + p2[t]^2/(2 m2) + c0/2 [q1[t]^2 + q2[t]^2];
HamEq[H0, {{q1, p1}, {q2, p2}}]
```

Out[53]=
$$\left\{\left\{-2\,q1[t]\left(\frac{c0}{2}\right)'[q1[t]^2 + q2[t]^2],\ \frac{p1[t]}{m1}\right\},\ \left\{-2\,q2[t]\left(\frac{c0}{2}\right)'[q1[t]^2 + q2[t]^2],\ \frac{p2[t]}{m2}\right\}\right\}$$

Задача 5

In[54]:=
```
HamJacEq[H_, coord_] :=
 Module[{n, i, equation , newc , rule0 , rule1 , rule2 , SS},
  n = Length[coord];
  newc = StringRiffle [Table[coord[[i, 1]], {i, 1, n}], ","];
  SS = ToExpression ["S[" <> newc <> ",t]"];
  rule1 = Table[coord[[i, 2]][t] → D[SS, coord[[i, 1]]], {i, 1, n}];
  rule0 = Table[coord[[i, 1]][t] → coord[[i, 1]], {i, 1, n}];
  rule2 = Table[coord[[i, 1]] → coord[[i, 1]][t], {i, 1, n}];
  equation = H /. rule0 /. rule1 ;
  equation = equation + D[SS, t];
  Return[equation /. rule2]
 ];
```

In[55]:=
```
HamJacEq[H0, {{q1, p1}, {q2, p2}}]
```

Out[55]=
$$\frac{c0}{2}\left[q1[t]^2 + q2[t]^2\right] + S^{(0,0,1)}[q1[t],\ q2[t],\ t] + \frac{S^{(0,1,0)}[q1[t],\ q2[t],\ t]^2}{2\ m2} + \frac{S^{(1,0,0)}[q1[t],\ q2[t],\ t]^2}{2\ m1}$$