Higher-order Quantum Euler-Lagrange Equations

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```
%typeset_mode True
```

1 Bohmian Trajectories in 1-D for the Time-Independent Schrodinger Equation

Schiff-Poirier, eqs. (1-4)

Notation

```
hbar = var('hbar',latex_name='\hbar'); hbar
m = var('m'); m
t = var('t'); t
x = function('x'); x(t)
x0t = var('x0t',latex_name='x')
V = function('V'); V(x0t)
```

$\hbar$
m
t
$x(t)$
$V(x)$

Derivatives

```
x1t = var('x1t',latex_name='\dot{x}')
x2t = var('x2t',latex_name='\ddot{x}')
x3t = var('x3t',latex_name='\dddot{x}')
x4t = var('x4t',latex_name='x^{(4)}')
x5t = var('x5t',latex_name='x^{(5)}')
x6t = var('x6t',latex_name='x^{(6)}')
xt = {x0t:x(t),x1t:diff(x(t),t),x2t:diff(x(t),[t,t]),
      x3t:diff(x(t),[t,t,t]),x4t:diff(x(t),t,4),
```

```
      x5t:diff(x(t),t,5),x6t:diff(x(t),t,6)}
tx = dict([v,k] for k,v in xt.items())
```

Variables

```
X = [x0t,x1t,x2t,x3t]; X
```

$[x, \dot{x}, \ddot{x}, \dddot{x}]$

Quantum Potential

```
def Q(x0t,x1t,x2t,x3t):
    return hbar^2/4/m * (x3t/x1t^3 - 5/2 * x2t^2/x1t^4)
Q(*X)
```

$$-\frac{\hbar^2 \left(\frac{5\,\ddot{x}^2}{\dot{x}^4} - \frac{2\,\dddot{x}}{\dot{x}^3}\right)}{8\,m}$$

Lagrangian

```
function('L')(*X)
```

$L(x, \dot{x}, \ddot{x}, \dddot{x})$

```
def L(x0t,x1t,x2t,x3t):
    return 1/2 * m*x1t^2 - Q(x0t,x1t,x2t,x3t)  - V(x0t)
L(*X)
```

$$\frac{1}{2}\,m\dot{x}^2 + \frac{\hbar^2 \left(\frac{5\,\ddot{x}^2}{\dot{x}^4} - \frac{2\,\dddot{x}}{\dot{x}^3}\right)}{8\,m} - V(x)$$

The Lagrangian is singular in the sense of Ostrogradsky.

```
diff(L(*X),[x3t,x3t])
```

0

1.1 Higher-order Euler-Lagrange Equation for a function of one variable

$$\frac{\partial \mathcal{L}}{\partial f} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial \mathcal{L}}{\partial f'}\right) + \frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\frac{\partial \mathcal{L}}{\partial f''}\right) - \ldots + (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(\frac{\partial \mathcal{L}}{\partial f^{(n)}}\right) = 0$$

where $f = x(t)$, $x = t$, $f' = \dot{x}$, etc.

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{\partial}{\partial t}\left(\frac{\mathcal{L}}{\dot{x}}\right) + \frac{\partial^2}{\partial t^2}\left(\frac{\mathcal{L}}{\ddot{x}}\right) - \ldots + (-1)^n \frac{\partial^n}{\partial t^n}\left(\frac{\mathcal{L}}{x^{(n)}}\right) = 0$$

```
def EL(L):
    return (diff(L(*X),X[0]) -
             diff(diff(L(*X),X[1]).subs(xt),t) +
             diff(diff(L(*X),X[2]).subs(xt),t,2) -
```

```
            diff(diff(L(*X),X[3]).subs(xt),t,3))
EL(L).subs(tx).expand()
```

$$-m\ddot{x} - \frac{5\,\hbar^2\dddot{x}^3}{2\,m\dot{x}^6} + \frac{2\,\hbar^2\ddot{x}\dddot{x}}{m\dot{x}^5} - \frac{\hbar^2 x^{(4)}}{4\,m\dot{x}^4} - D[0]\,(V)\,(x)$$

1.2 Ostrogradsky momenta

```
P = list(range(4))
P[1] = (diff(L(*X),X[1]) - diff(diff(L(*X),X[2]).subs(xt),t) +
        diff(diff(L(*X),X[3]).subs(xt),t,2))
P[2] = diff(L(*X),X[2]) - diff(diff(L(*X),X[3]).subs(xt),t)
P[3] = diff(L(*X),X[3])
```

```
P[1].subs(tx).expand()
P[2].subs(tx).expand()
P[3].subs(tx).expand()
```

$$m\dot{x} - \frac{\hbar^2\ddot{x}^2}{2\,m\dot{x}^5} + \frac{\hbar^2\dddot{x}}{4\,m\dot{x}^4}$$

$$\frac{\hbar^2\ddot{x}}{2\,m\dot{x}^4}$$

$$-\frac{\hbar^2}{4\,m\dot{x}^3}$$

```
H = P[1] * X[1] + P[2] * X[2] + P[3] * X[3] - L(*X)
H.subs(tx).expand()
```

$$\frac{1}{2}\,m\dot{x}^2 - \frac{5\,\hbar^2\ddot{x}^2}{8\,m\dot{x}^4} + \frac{\hbar^2\dddot{x}}{4\,m\dot{x}^3} + V\,(x)$$

```
bool( H.subs(tx) == 1/2*m*x1t^2+V(x0t)+Q(*X) )
```

True

Schiff-Poirier eqs. (5-8)

```
p,r,s = var('p,r,s')
(s*(2*p-s)/2/m+V(X[0])-2*r^2*s^4/m/hbar^2).subs({
        s:m*X[1], r:hbar^2*X[2]/4/m^2/X[1]^4,
        p:m*X[1]+hbar^2/4/m*(X[3]/X[1]^4-2*X[2]^2/X[1]^5)}
).expand()
```

$$\frac{1}{2}\,m\dot{x}^2 - \frac{5\,\hbar^2\ddot{x}^2}{8\,m\dot{x}^4} + \frac{\hbar^2\dddot{x}}{4\,m\dot{x}^3} + V\,(x)$$

2 Bohmian Trajectories in 1-D for the Time-Dependent Schrodinger Equation

Schiff-Poirier eqs. (10,11).

Notation

```
C=var('C')
```

Derivatives

```
x1c = var('x1c',latex_name="x'")
x2c = var('x2c',latex_name="x''")
x3c = var('x3t',latex_name="x'''")
x4c = var('x4t',latex_name="x''''")
xc = {x0t:x(t,C),x1t:diff(x(t,C),t),x1c:diff(x(t,C),C),
      x2c:diff(x(t,C),C,2),x3c:diff(x(t,C),C,3),x4c:diff(x(t,C),C,4)\
   }
cx = dict([v,k] for k,v in xc.items())
```

Variables

```
XC = [x0t,x1t,x1c,x2c,x3c];XC
```

$[x, \dot{x}, x', x'', x''']$

Quantum Potential

```
def QC(x0t,x1t,x1c,x2c,x3c):
    return hbar^2/4/m * (x3c/x1c^3 - 5/2 * x2c^2/x1c^4)
QC(*XC)
```

$$-\frac{\hbar^2\left(\frac{5\,x''^2}{x'^4}-\frac{2\,x'''}{x'^3}\right)}{8\,m}$$

Lagrangian

```
function('L')(*XC)
```

$L\left(x, \dot{x}, x', x'', x'''\right)$

```
def LC(x0t,x1t,x1c,x2c,x3c):
    return 1/2 * m*x1t^2 - QC(x0t,x1t,x1c,x2c,x3c)  - V(x0t)
LC(*XC)
```

$$\frac{1}{2}\,m\dot{x}^2+\frac{\hbar^2\left(\frac{5\,x''^2}{x'^4}-\frac{2\,x'''}{x'^3}\right)}{8\,m}-V\left(x\right)$$

2.1 Euler-Lagrange equation for a single function of two variables with higher-order derivatives

$$\frac{\partial\mathcal{L}}{\partial f}-\frac{\partial}{\partial x_1}\left(\frac{\partial\mathcal{L}}{\partial f_{,1}}\right)-\frac{\partial}{\partial x_2}\left(\frac{\partial\mathcal{L}}{\partial f_{,2}}\right)+\frac{\partial^2}{\partial x_1^2}\left(\frac{\partial\mathcal{L}}{\partial f_{,11}}\right)+\frac{\partial^2}{\partial x_1\partial x_2}\left(\frac{\partial\mathcal{L}}{\partial f_{,12}}\right)+\frac{\partial^2}{\partial x_2^2}\left(\frac{\partial\mathcal{L}}{\partial f_{,22}}\right)$$
$$-\ldots+(-1)^n\frac{\partial^n}{\partial x_2^n}\left(\frac{\partial\mathcal{L}}{\partial f_{,22\ldots2}}\right)=0$$

where $f = x(t, C)$, $x_1 = t$, $x_2 = C$, $f_{,1} = \dot{x}, f_{,2} = x'$, etc.

$$\frac{\partial \mathcal{L}}{x} - \frac{\partial}{\partial t}\left(\frac{\mathcal{L}}{\dot{x}}\right) - \frac{\partial}{\partial C}\left(\frac{\mathcal{L}}{x'}\right) + \frac{\partial^2}{\partial C^2}\left(\frac{\mathcal{L}}{x''}\right) - \frac{\partial^3}{\partial C^3}\left(\frac{\mathcal{L}}{x'''}\right)$$

```
def ELC(LC):
    return (diff(LC(*XC),XC[0]) -
            diff(diff(LC(*XC),XC[1]).subs(xc),t) -
            diff(diff(LC(*XC),XC[2]).subs(xc),C) +
            diff(diff(LC(*XC),XC[3]).subs(xc),C,2) -
            diff(diff(LC(*XC),XC[4]).subs(xc),C,3))
ELC(LC).subs(cx).expand()
```

$$-mD[0,0]\left(x\right)\left(t,C\right) - \frac{5\,\hbar^2 x''^3}{2\,mx'^6} + \frac{2\,\hbar^2 x'' x'''}{mx'^5} - \frac{\hbar^2 x''''}{4\,mx'^4} - D[0]\left(V\right)\left(x\right)$$