# Exact solution for two-particle system

The Schrodinger Equation for two particles is

$$\left(-\frac{\partial^2}{\partial s_1{}^2}-\frac{\partial^2}{\partial s_2{}^2}+s_1{}^2+s_2{}^2-\frac{1}{2}\beta\,(s_1-s_2)^2\right)\psi[s_1,\ s_2]=E\psi[s_1,\ s_2]$$

The wavefunction solution to this equation is

$$\psi(x_1,\,x_2)=(x_1-x_2)\,\mathrm{Exp}\left[-\frac{1}{2}\left(\gamma\left(x_1{}^2+x_2{}^2\right)+\alpha\,x_1\,x_2\right)\right]$$

with

$$\gamma=\frac{1}{2}\left(1+\sqrt{1-\beta}\right)\qquad\text{and}\qquad\alpha=1-\sqrt{1-\beta}\qquad\text{with}\qquad E=1+3\sqrt{1-\beta}$$

Note that $\gamma+\frac{1}{2}\alpha=1\;\to\;\alpha=2\,(1-\gamma)$. This is not a general result (for $N\neq 2$). Note also that $\frac{1}{2}<\gamma\leq 1$

## Basic Definitions

Use the result that $\alpha=2\,(1-\gamma)$ to eliminate $\alpha$ in the expression for the wavefunction

```
ψ[x1_, x2_] = (x1 - x2) Exp[-1/2 (γ (x1^2 + x2^2) + α x1 x2)] /. {α → 2 (1 - γ)} // FullSimplify
```

$$e^{-x1\,x2-\frac{1}{2}(x1-x2)^2\gamma}\,(x1-x2)$$

```
γExact = 1/2 (1 + Sqrt[1 - β]);
αExact = 1 - Sqrt[1 - β];
ψExact[x1_, x2_] = ψ[x1, x2] /. {γ → γExact} // FullSimplify
```

$$e^{-x1\,x2-\frac{1}{4}(x1-x2)^2\left(1+\sqrt{1-\beta}\right)}\,(x1-x2)$$

## Check that this is indeed the solution to the Schrodinger equation:

Evaluate $\hat{H}\,\psi$:

```
LHS = Simplify[(-∂x1,x1 ψExact[x1, x2]) + (-∂x2,x2 ψExact[x1, x2]) +
   (x1^2 + x2^2) ψExact[x1, x2] - 1/2 β (x1 - x2)^2 ψExact[x1, x2], Assumptions → β < 1]
```

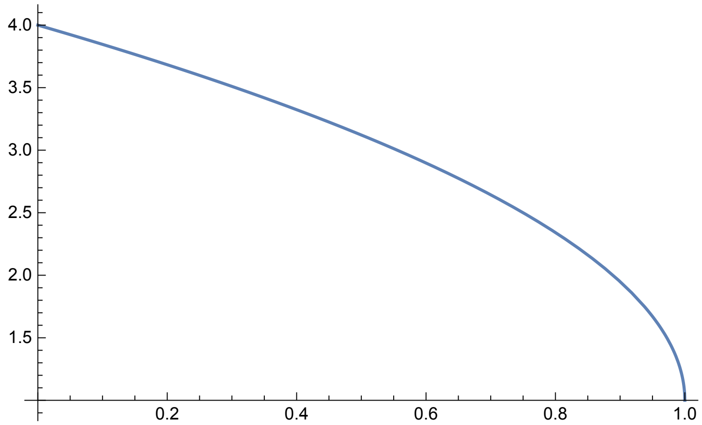
$$e^{-x1\,x2-\frac{1}{4}(x1-x2)^2\left(1+\sqrt{1-\beta}\right)}\,(x1-x2)\left(1+3\sqrt{1-\beta}\right)$$

This is equal to a contant times $\psi$. Divide by $\psi$ to show this.

```
eExact = FullSimplify[LHS / ψExact[x1, x2], Assumptions → β < 1]
```

$$1+3\sqrt{1-\beta}$$

```
Plot[eExact, {β, 0, 1}]
```




## Determine density and kinetic energy density for arbitrary γ

Integrate to find the normalization constant. This integral now is evaluated relatively quickly, but evaluation is “turned off” by using :=. Also, the result is a bit ugly, so we will not bother to normalize the wavefunction.

```
ans := Integrate[ψ[x1, x2]^2, {x1, -∞, ∞}, {x2, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}]
```

$$\text{normConst} = \frac{\sqrt{(-1+2\gamma)^{3/2}}}{\sqrt{\pi}};$$

Check that this works (again, this takes some time, so evaluation is turned off)

```
ans := Integrate[normConst^2 ψ[x1, x2]^2,
  {x1, -∞, ∞}, {x2, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}]
```

Find the one- and two-particle density matrices

```
ρ12[x1_, x2_] = ψ[x1, x2]^2
```

$$e^{-2\,x1\,x2-(x1-x2)^2\gamma}\,(x1-x2)^2$$

```
ρ[x_] =
 Integrate[ρ12[x, x2], {x2, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}] // FullSimplify
```

$$\frac{e^{\frac{x^2(1-2\gamma)}{\gamma}}\sqrt{\pi}\,(2\,x^2+\gamma)}{2\,\gamma^{5/2}}$$

Find the one- and two-particle kinetic energy expressions. Note that the “a” versions use the $(\partial_{x1}\psi[x1,\ x2])^2$ expressions and the “b” version use $\psi[x1,\ x2]\,\partial_{x1,x1}\psi[x1,\ x2]$. the “a” version ensures $k[x] \geq 0$. Both give the same result for the total kinetic energy

```
k12a[x1_, x2_] = (∂x1 ψ[x1, x2])^2 + (∂x2 ψ[x1, x2])^2 // FullSimplify
```

$$e^{-2\,x1\,x2-(x1-x2)^2\gamma}\left(2+(x1-x2)^2\left(2+x1^2+x2^2-2\left(2+(x1-x2)^2\right)\gamma+2\,(x1-x2)^2\gamma^2\right)\right)$$

```
k1a[x_] =
 Integrate[k12a[x, x2], {x2, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}] // FullSimplify
```

$$\frac{1}{4\,\gamma^{9/2}}\,e^{\frac{x^2(1-2\gamma)}{\gamma}}\sqrt{\pi}\,\left(4\,x^4\,(1-2\,\gamma)^2+\gamma^2\,\left(3-2\,\gamma+6\,\gamma^2\right)+4\,x^2\,\gamma\,(3+\gamma\,(-7+3\,\gamma))\right)$$

This looks a bit ugly, but it is just equal to $\left(a + b\,x^2 + c\,x^4\right)e^{-d\,x^2}$

```
k12b[x1_, x2_] =
 (-ψ[x1, x2] ∂x1,x1 ψ[x1, x2]) + (-ψ[x1, x2] ∂x2,x2 ψ[x1, x2]) // FullSimplify
```

$$e^{-2\,x1\,x2-(x1-x2)^2\,\gamma}\,(x1-x2)^2\,\left(-2-x1^2-x2^2+2\,\left(3+(x1-x2)^2\right)\gamma-2\,(x1-x2)^2\,\gamma^2\right)$$

```
k1b[x_] =
 Integrate[k12b[x, x2], {x2, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}] // FullSimplify
```

$$\frac{1}{4\,\gamma^{9/2}}\,e^{\frac{x^2(1-2\gamma)}{\gamma}}\sqrt{\pi}\,\left(-4\,x^4\,(1-2\,\gamma)^2-4\,x^2\,\gamma\,(3+(-7+\gamma)\,\gamma)+\gamma^2\,\left(-3+2\,\gamma+6\,\gamma^2\right)\right)$$

Show that both versions give the same total kinetic energy

```
kTota = Integrate[k1a[x], {x, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}] // FullSimplify
```

$$\frac{\pi\,(-1+3\,\gamma)}{(-1+2\,\gamma)^{3/2}}$$

```
kTotb = Integrate[k1b[x], {x, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}] // FullSimplify
```

$$\frac{\pi\,(-1+3\,\gamma)}{(-1+2\,\gamma)^{3/2}}$$

## Divide out prefactor and Gaussian to write kinetic energy, density and derivatives as polynomials

```
ρ[x]
```

$$\frac{e^{\frac{x^2(1-2\gamma)}{\gamma}}\sqrt{\pi}\,\left(2\,x^2+\gamma\right)}{2\,\gamma^{5/2}}$$

```
preFact = ρ[x] / (2 x^2 + γ) // FullSimplify
```

$$\frac{e^{\frac{x^2(1-2\gamma)}{\gamma}}\sqrt{\pi}}{2\,\gamma^{5/2}}$$

```
ρ0 = ρ[x] / preFact // FullSimplify
```

$$2\,x^2+\gamma$$

```
kina = k1a[x] / preFact
```

$$\frac{1}{2\,\gamma^2}\left(4\,x^4\,(1-2\,\gamma)^2+\gamma^2\,\left(3-2\,\gamma+6\,\gamma^2\right)+4\,x^2\,\gamma\,(3+\gamma\,(-7+3\,\gamma))\right)$$

**ρP = Collect[(∂x ρ[x]) / preFact // FullSimplify, x]**

$$4\,x^3\left(-2+\frac{1}{\gamma}\right)+x\,(6-4\,\gamma)$$

**ρPP = Collect[(∂x,x ρ[x]) / preFact // FullSimplify, x]**

$$2\,(3-2\,\gamma)+\frac{8\,x^4\,(1-2\,\gamma)^2}{\gamma^2}+\frac{8\,x^2\,(-3+\gamma)\,(-1+2\,\gamma)}{\gamma}$$

**ρPPP = Collect[(∂x,x,x ρ[x]) / preFact // FullSimplify, x]**

$$-\frac{16\,x^5\,(1-2\,\gamma)^2\,(-1+2\,\gamma)}{\gamma^3}-\frac{12\,x\,(5-2\,\gamma)\,(-1+2\,\gamma)}{\gamma}-\frac{16\,x^3\,(-5+\gamma)\,(-1+2\,\gamma)^2}{\gamma^2}$$

**ρPPPP = Collect[(∂x,x,x,x ρ[x]) / preFact // FullSimplify, x]**

$$\frac{16\,x^4\,(1-2\,\gamma)^2\,(-15+2\,\gamma)\,(-1+2\,\gamma)}{\gamma^3}+\frac{12\,(-5+2\,\gamma)\,(-1+2\,\gamma)}{\gamma}+\frac{32\,x^6\,(-1+2\,\gamma)^4}{\gamma^4}-\frac{24\,x^2\,(-1+2\,\gamma)\,\left(15-34\,\gamma+8\,\gamma^2\right)}{\gamma^2}$$

Consider these when $\gamma = 1$. This corresponds to $\beta = 0$ so they should give the same results we found earlier i

**Collect[{kina, ρ0, ρP, ρPP, ρPPP, ρPPPP} /. γ → 1 // FullSimplify, x] // TableForm**

$\frac{7}{2}-2\,x^2+2\,x^4$
$1+2\,x^2$
$2\,x-4\,x^3$
$2-16\,x^2+8\,x^4$
$-36\,x+64\,x^3-16\,x^5$
$-36+264\,x^2-208\,x^4+32\,x^6$

We had found a combination of rho and its derivatives that generate a fourth order polynomial:

$$\mathbf{f\rho = \frac{1}{4}\,\frac{\rho PP^2-\rho P\,\rho PPP}{\rho 0}\ /.\ \gamma\to 1\ //\ FullSimplify}$$

$$1+4\,x^4$$

Which then allowed us to write the kinetic energy density as a function of $\rho$, $\rho$PP and f$\rho$

$$\mathbf{3\,\rho 0+\frac{1}{2}\,\rho PP-\frac{1}{2}\,f\rho\ /.\ \gamma\to 1\ //\ FullSimplify}$$

$$\frac{7}{2}-2\,x^2+2\,x^4$$

Can we do the same thing when $\gamma \neq 1$(i.e. $\beta \neq 0$)? Consider the density and derivatives when $\gamma = 3/4$.

```
Collect[{kina, ρ0, ρP, ρPP, ρPPP, ρPPPP} /. γ → 3/4 // FullSimplify, x] // TableForm
```

$\frac{39}{16} - \frac{3 x^2}{2} + \frac{8 x^4}{9}$

$\frac{3}{4} + 2 x^2$

$3 x - \frac{8 x^3}{3}$

$3 - 12 x^2 + \frac{32 x^4}{9}$

$-28 x + \frac{272 x^3}{9} - \frac{128 x^5}{27}$

$-28 + 128 x^2 - 64 x^4 + \frac{512 x^6}{81}$

These are just polynomials like we had for the non-interacting case, so we can probably find combinations of rho and its derivatives that generate the kinetic energy density.

## Determine a combination of the density and derivatives that gives a 4th order equation for $\gamma = 3/4$.

```
kin = Collect[kina /. γ → 3/4 // FullSimplify, x]
rho = Collect[ρ0 /. γ → 3/4 // FullSimplify, x]
rp = Collect[ρP /. γ → 3/4 // FullSimplify, x]
rpp = Collect[ρPP /. γ → 3/4 // FullSimplify, x]
rppp = Collect[ρPPP /. γ → 3/4 // FullSimplify, x]
rpppp = Collect[ρPPPP /. γ → 3/4 // FullSimplify, x]
```

$$\frac{39}{16} - \frac{3 x^2}{2} + \frac{8 x^4}{9}$$

$$\frac{3}{4} + 2 x^2$$

$$3 x - \frac{8 x^3}{3}$$

$$3 - 12 x^2 + \frac{32 x^4}{9}$$

$$-28 x + \frac{272 x^3}{9} - \frac{128 x^5}{27}$$

$$-28 + 128 x^2 - 64 x^4 + \frac{512 x^6}{81}$$

First consider only terms up to rppp.

We find $\frac{rp^2 + \frac{3}{2}\left(rpp^2 - rp\ rppp\right)}{rho} = 18 - 12 x^2 + \frac{32 x^4}{3}$

But this turns out to be a linear combination of rho and rpp.

Who would have known?

## Consider all terms including rpppp.

$$\text{poly} = \text{Collect}\left[a\, rp^2 + b\, rpp^2 + c\, rppp^2 + d\, rpppp^2 + e\, rp\, rpp + f\, rp\, rppp + g\, rp\, rpppp + h\, rpp\, rppp + i\, rpp\, rpppp + j\, rppp\, rpppp,\ x\right]$$

$$9 b + 784 d - 84 i + (9 e - 84 g - 84 h + 784 j)\, x + (9 a - 72 b + 784 c - 7168 d - 84 f + 720 i)\, x^2 + \left(-44 e + \frac{1376 g}{3} + \frac{1280 h}{3} - \frac{39872 j}{9}\right) x^3 + \left(-16 a + \frac{496 b}{3} - \frac{15232 c}{9} + 19968 d + \frac{496 f}{3} - \frac{16448 i}{9}\right) x^4 + \left(\frac{128 e}{3} - \frac{1600 g}{3} - \frac{4288 h}{9} + \frac{156416 j}{27}\right) x^5 + \left(\frac{64 a}{9} - \frac{256 b}{3} + \frac{95488 c}{81} - \frac{1355776 d}{81} - \frac{2560 f}{27} + \frac{33536 i}{27}\right) x^6 + \left(-\frac{256 e}{27} + \frac{5120 g}{27} + \frac{13312 h}{81} - \frac{220160 j}{81}\right) x^7 + \left(\frac{1024 b}{81} - \frac{69632 c}{243} + \frac{462848 d}{81} + \frac{1024 f}{81} - \frac{8192 i}{27}\right) x^8 + \left(-\frac{4096 g}{243} - \frac{4096 h}{243} + \frac{360448 j}{729}\right) x^9 + \left(\frac{16384 c}{729} - \frac{65536 d}{81} + \frac{16384 i}{729}\right) x^{10} - \frac{65536 j\, x^{11}}{2187} + \frac{262144 d\, x^{12}}{6561}$$

$$\text{ans} = \text{Collect}\left[\text{FullSimplify}\left[\text{poly} - \text{rho}\left(k + m x + n x^2 + o x^3 + p x^4 + q x^5 + r x^6 + s x^7 + t x^8 + u x^9 + v x^{10}\right)\right],\ x\right]$$

$$9 b + 784 d - 84 i - \frac{3 k}{4} + \left(9 e - 84 (g + h) + 784 j - \frac{3 m}{4}\right) x + \left(9 a - 72 b + 784 c - 7168 d - 84 f + 720 i - 2 k - \frac{3 n}{4}\right) x^2 + \left(-\frac{4}{9} (99 e - 1032 g - 960 h + 9968 j) - 2 m - \frac{3 o}{4}\right) x^3 + \left(-\frac{16}{9} (9 a - 93 b + 952 c - 11232 d - 93 f + 1028 i) - 2 n - \frac{3 p}{4}\right) x^4 + \left(\frac{64}{27} (18 e - 225 g - 201 h + 2444 j) - 2 o - \frac{3 q}{4}\right) x^5 + \left(\frac{64}{81} (9 a - 4 (27 b - 373 c + 5296 d + 30 f - 393 i)) - 2 p - \frac{3 r}{4}\right) x^6 + \left(-\frac{256}{81} (3 e - 60 g - 52 h + 860 j) - 2 q - \frac{3 s}{4}\right) x^7 + \left(\frac{1024}{243} (3 b - 68 c + 3 (452 d + f - 24 i)) - 2 r - \frac{3 t}{4}\right) x^8 + \left(-\frac{4096}{729} (3 (g + h) - 88 j) - 2 s - \frac{3 u}{4}\right) x^9 + \left(\frac{16384}{729} (c - 36 d + i) - 2 t - \frac{3 v}{4}\right) x^{10} + \left(-\frac{65536 j}{2187} - 2 u\right) x^{11} + \left(\frac{262144 d}{6561} - 2 v\right) x^{12}$$

```
ans = Collect[
  FullSimplify[poly - rho (k + m x + n x^2 + o x^3 + p x^4 + q x^5 + r x^6 + s x^7 + t x^8 + u x^9 + v x^10),
   Assumptions → {a > 0, b > 0, c > 0, d > 0, e > 0, f > 0, g > 0, h > 0,
     i > 0, j > 0, k > 0, n > 0, q > 0, r > 0, s > 0, t > 0, u > 0, v > 0}], x]
```

$$9 b + 784 d - 84 i - \frac{3 k}{4} + \left(9 e - 84 (g + h) + 784 j - \frac{3 m}{4}\right) x + \left(9 a - 72 b + 784 c - 7168 d - 84 f + 720 i - 2 k - \frac{3 n}{4}\right) x^2 + \left(-\frac{4}{9} (99 e - 1032 g - 960 h + 9968 j) - 2 m - \frac{3 o}{4}\right) x^3 + \left(-\frac{16}{9} (9 a - 93 b + 952 c - 11232 d - 93 f + 1028 i) - 2 n - \frac{3 p}{4}\right) x^4 + \left(\frac{64}{27} (18 e - 225 g - 201 h + 2444 j) - 2 o - \frac{3 q}{4}\right) x^5 + \left(\frac{64}{81} (9 a - 4 (27 b - 373 c + 5296 d + 30 f - 393 i)) - 2 p - \frac{3 r}{4}\right) x^6 + \left(-\frac{256}{81} (3 e - 60 g - 52 h + 860 j) - 2 q - \frac{3 s}{4}\right) x^7 + \left(\frac{1024}{243} (3 b - 68 c + 3 (452 d + f - 24 i)) - 2 r - \frac{3 t}{4}\right) x^8 + \left(-\frac{4096}{729} (3 (g + h) - 88 j) - 2 s - \frac{3 u}{4}\right) x^9 + \left(\frac{16384}{729} (c - 36 d + i) - 2 t - \frac{3 v}{4}\right) x^{10} + \left(-\frac{65536 j}{2187} - 2 u\right) x^{11} + \left(\frac{262144 d}{6561} - 2 v\right) x^{12}$$

```
Collect[FullSimplify[ans /. {v → d 262144 / (2 * 6561), u → -j 65536 / (2 * 2187)}], x]
```

$$9 b + 784 d - 84 i - \frac{3 k}{4} + \left(9 e - 84 (g + h) + 784 j - \frac{3 m}{4}\right) x + \left(9 a - 72 b + 784 c - 7168 d - 84 f + 720 i - 2 k - \frac{3 n}{4}\right) x^2 + \left(-44 e + \frac{32}{9} (129 g + 120 h - 1246 j) - 2 m - \frac{3 o}{4}\right) x^3 + \left(-16 a + \frac{16}{9} (93 b - 952 c + 11232 d + 93 f - 1028 i) - 2 n - \frac{3 p}{4}\right) x^4 + \left(\frac{64}{27} (18 e - 225 g - 201 h + 2444 j) - 2 o - \frac{3 q}{4}\right) x^5 + \left(\frac{64}{81} (9 a - 4 (27 b - 373 c + 5296 d + 30 f - 393 i)) - 2 p - \frac{3 r}{4}\right) x^6 + \left(-\frac{256}{81} (3 e - 60 g - 52 h + 860 j) - 2 q - \frac{3 s}{4}\right) x^7 + \left(\frac{1024}{243} (3 b - 68 c + 3 (452 d + f - 24 i)) - 2 r - \frac{3 t}{4}\right) x^8 - \frac{2}{243} (2048 (g + h - 30 j) + 243 s) x^9 + \frac{2 (8192 (3 c - 110 d + 3 i) - 2187 t) x^{10}}{2187}$$

```
Collect[FullSimplify[ans /. {v → d 262144 / (2 * 6561), u → -j 65536 / (2 * 2187)} /.
    {t -> 8192 (3 c - 110 d + 3 i) / 2187, s → -2048 (g + h - 30 j) / 243}], x]
```

$$9 b + 784 d - 84 i - \frac{3 k}{4} + \left(9 e - 84 (g + h) + 784 j - \frac{3 m}{4}\right) x + \left(9 a - 72 b + 784 c - 7168 d - 84 f + 720 i - 2 k - \frac{3 n}{4}\right) x^2 + \left(-44 e + \frac{32}{9} (129 g + 120 h - 1246 j) - 2 m - \frac{3 o}{4}\right) x^3 + \left(-16 a + \frac{16}{9} (93 b - 952 c + 11232 d + 93 f - 1028 i) - 2 n - \frac{3 p}{4}\right) x^4 + \left(\frac{64}{27} (18 e - 225 g - 201 h + 2444 j) - 2 o - \frac{3 q}{4}\right) x^5 + \left(\frac{64}{81} (9 a - 4 (27 b - 373 c + 5296 d + 30 f - 393 i)) - 2 p - \frac{3 r}{4}\right) x^6 - \frac{2}{81} (128 (3 e - 62 g - 54 h + 920 j) + 81 q) x^7 + \frac{2}{729} (512 (9 b - 210 c + 4288 d + 9 f - 222 i) - 729 r) x^8$$

```
Collect[FullSimplify[ans /. {v → d 262144 / (2 * 6561), u → -j 65536 / (2 * 2187)} /.
     {t -> 8192 (3 c - 110 d + 3 i) / 2187, s → -2048 (g + h - 30 j) / 243} /.
    {r -> 512 (9 b - 210 c + 4288 d + 9 f - 222 i) / 729,
     q → -128 (3 e - 62 g - 54 h + 920 j) / 81}], x]
```

$$\frac{1}{4} (36 b + 3136 d - 3 (112 i + k)) + \frac{1}{4} (36 e - 336 (g + h) + 3136 j - 3 m) x - \frac{1}{4} (-36 a + 8 (36 b - 392 c + 3584 d + 42 f - 360 i + k) + 3 n) x^2 - \frac{1}{36} (8 (198 e - 2064 g - 1920 h + 19936 j + 9 m) + 27 o) x^3 - \frac{1}{36} (64 (9 a - 93 b + 952 c - 11232 d - 93 f + 1028 i) + 72 n + 27 p) x^4 + \frac{2}{27} (624 e - 128 (64 g + 57 h - 726 j) - 27 o) x^5 + \frac{2}{243} (32 (27 a - 342 b + 4896 c - 72128 d - 378 f + 5160 i) - 243 p) x^6$$

```
Collect[FullSimplify[ans /. {v → d 262 144 / (2 * 6561), u → -j 65 536 / (2 * 2187)} /.
     {t -> 8192 (3 c - 110 d + 3 i) / 2187, s → -2048 (g + h - 30 j) / 243} /. {r ->
      512 (9 b - 210 c + 4288 d + 9 f - 222 i) / 729, q → -128 (3 e - 62 g - 54 h + 920 j) / 81} /.
   {p -> 32 (27 a - 342 b + 4896 c - 72 128 d - 378 f + 5160 i) / 243,
    o → (624 e - 128 (64 g + 57 h - 726 j)) / 27}], x]
```

$$\frac{1}{4}(36\,b+3136\,d-3\,(112\,i+k))+\frac{1}{4}(36\,e-336\,(g+h)+3136\,j-3\,m)\,x-\frac{1}{4}(-36\,a+8\,(36\,b-392\,c+3584\,d+42\,f-360\,i+k)+3\,n)\,x^2-\frac{2}{9}(4\,(69\,e-772\,g-708\,h+7888\,j)+9\,m)\,x^3-\frac{2}{81}(756\,a-16\,(504\,b-5508\,c+68\,576\,d+513\,f-5916\,i)+81\,n)\,x^4$$

```
Collect[FullSimplify[ans /. {v → d 262 144 / (2 * 6561), u → -j 65 536 / (2 * 2187)} /.
      {t -> 8192 (3 c - 110 d + 3 i) / 2187, s → -2048 (g + h - 30 j) / 243} /. {r ->
        512 (9 b - 210 c + 4288 d + 9 f - 222 i) / 729, q → -128 (3 e - 62 g - 54 h + 920 j) / 81} /.
    {p -> 32 (27 a - 342 b + 4896 c - 72 128 d - 378 f + 5160 i) / 243,
     o → (624 e - 128 (64 g + 57 h - 726 j)) / 27} /.
   {n → -(756 a - 16 (504 b - 5508 c + 68 576 d + 513 f - 5916 i)) / 81,
    m → -4 (69 e - 772 g - 708 h + 7888 j) / 9}], x]
```

$$9\,b+784\,d-84\,i-\frac{3\,k}{4}+\left(32\,e-\frac{1024\,g}{3}-320\,h+\frac{10\,240\,j}{3}\right)x+\left(16\,a-\frac{2}{27}(4\,(495\,b-5400\,c+58\,480\,d+540\,f-5388\,i)+27\,k)\right)x^2$$

```
Collect[FullSimplify[ans /. {v → d 262 144 / (2 * 6561), u → -j 65 536 / (2 * 2187)} /.
        {t -> 8192 (3 c - 110 d + 3 i) / 2187, s → -2048 (g + h - 30 j) / 243} /.
      {r -> 512 (9 b - 210 c + 4288 d + 9 f - 222 i) / 729,
       q → -128 (3 e - 62 g - 54 h + 920 j) / 81} /.
     {p -> 32 (27 a - 342 b + 4896 c - 72 128 d - 378 f + 5160 i) / 243,
      o → (624 e - 128 (64 g + 57 h - 726 j)) / 27} /.
    {n → -(756 a - 16 (504 b - 5508 c + 68 576 d + 513 f - 5916 i)) / 81,
     m → -4 (69 e - 772 g - 708 h + 7888 j) / 9} /. {k → (9 b + 784 d - 84 i) 4 / 3}], x]
```

$$\frac{16}{27}(54\,e-576\,g-540\,h+5760\,j)\,x+\frac{16}{27}(27\,a-288\,b+2700\,c-32\,768\,d-270\,f+3072\,i)\,x^2$$

```
Collect[FullSimplify[ans /. {v → d 262 144 / (2 * 6561), u → -j 65 536 / (2 * 2187)} /.
        {t -> 8192 (3 c - 110 d + 3 i) / 2187, s → -2048 (g + h - 30 j) / 243} /.
       {r -> 512 (9 b - 210 c + 4288 d + 9 f - 222 i) / 729,
        q → -128 (3 e - 62 g - 54 h + 920 j) / 81} /.
      {p -> 32 (27 a - 342 b + 4896 c - 72 128 d - 378 f + 5160 i) / 243,
       o → (624 e - 128 (64 g + 57 h - 726 j)) / 27} /.
     {n → -(756 a - 16 (504 b - 5508 c + 68 576 d + 513 f - 5916 i)) / 81,
      m → -4 (69 e - 772 g - 708 h + 7888 j) / 9} /. {k → (9 b + 784 d - 84 i) 4 / 3} /.
   {i → -(27 a - 288 b + 2700 c - 32 768 d - 270 f) / 3072,
    j → -(54 e - 576 g - 540 h) / 5760}], x]
```

0

Now put all these substitutions into the product expression divided by rho. It should be a simple polynomial

```
ans = Collect[
  FullSimplify[(poly / rho) /. {v → d 262 144 / (2 * 6561), u → -j 65 536 / (2 * 2187)} /.
        {t -> 8192 (3 c - 110 d + 3 i) / 2187, s → -2048 (g + h - 30 j) / 243} /. {r -> 512
          (9 b - 210 c + 4288 d + 9 f - 222 i) / 729, q → -128 (3 e - 62 g - 54 h + 920 j) / 81} /.
      {p -> 32 (27 a - 342 b + 4896 c - 72 128 d - 378 f + 5160 i) / 243,
       o → (624 e - 128 (64 g + 57 h - 726 j)) / 27} /.
     {n → -(756 a - 16 (504 b - 5508 c + 68 576 d + 513 f - 5916 i)) / 81,
      m → -4 (69 e - 772 g - 708 h + 7888 j) / 9} /. {k → (9 b + 784 d - 84 i) 4 / 3} /.
   {i → -(27 a - 288 b + 2700 c - 32 768 d - 270 f) / 3072,
    j → -(54 e - 576 g - 540 h) / 5760}], x]
```

$$\frac{1}{192}(189\,a + 288\,b + 18\,900\,c - 28\,672\,d - 1890\,f) + \frac{1}{15}(33\,e - 14\,(8\,g + 15\,h))\,x + \frac{1}{144}(135\,a - 2\,(720\,b + 4386\,c - 77\,824\,d + 99\,f))\,x^2 + \frac{4}{135}(-309\,e + 1376\,g + 1770\,h)\,x^3 + \frac{1}{324}(-783\,a + 6048\,b + 15\,396\,c - 729\,088\,d + 3222\,f)\,x^4 + \frac{16}{27}(15\,e - 80\,g - 86\,h)\,x^5 + \frac{1}{243}(333\,a - 2016\,b - 2540\,c + 327\,680\,d - 1794\,f)\,x^6 - \frac{64}{243}(9\,e - 64\,g - 58\,h)\,x^7 + \frac{8}{729}(-9\,a + 96\,b + 124\,c - 26\,624\,d + 90\,f)\,x^8 + \frac{512\,(3\,e - 32\,g - 30\,h)\,x^9}{10\,935} + \frac{131\,072\,d\,x^{10}}{6561}$$

Can we eliminate the higher powers of x (and the odd powers) without making the entire expression disappear?

```
Collect[FullSimplify[ans /. {d → 0, h -> (3 e - 32 g) / 30}], x]
```

$$\frac{3}{64}(21 a + 32 b + 2100 c - 210 f) + \frac{4}{15}(3 e + 28 g) x + \frac{1}{48}(45 a - 480 b - 2924 c - 66 f) x^2 - \frac{16}{135}(33 e + 128 g) x^3 + \frac{1}{108}(-261 a + 2016 b + 5132 c + 1074 f) x^4 + \frac{256}{405}(6 e + 11 g) x^5 + \frac{1}{243}(333 a - 2 (1008 b + 1270 c + 897 f)) x^6 - \frac{1024 (3 e - 2 g) x^7}{3645} + \frac{8}{729}(-9 a + 96 b + 124 c + 90 f) x^8$$

```
Collect[FullSimplify[
  ans /. {d → 0, h -> (3 e - 32 g) / 30} /. {f → -(-9 a + 96 b + 124 c) / 90, g → 3 e / 2}], x]
```

$$\frac{4 (10935 b + 102060 c)}{3645} + 12 e x + \frac{4 (729 a - 7776 b - 53784 c) x^2}{3645} - \frac{80 e x^3}{3} + \frac{4 (-1296 a + 7344 b + 30816 c) x^4}{3645} + \frac{128 e x^5}{9} + \frac{4 (576 a - 384 b - 256 c) x^6}{3645}$$

```
Collect[FullSimplify[
  ans /. {d → 0, h -> (3 e - 32 g) / 30} /. {f → -(-9 a + 96 b + 124 c) / 90, g → 3 e / 2} /.
   {e → 0, c -> (576 a - 384 b) / 256}], x]
```

$$\frac{4}{3}(189 a - 117 b) + \frac{4}{3}(-99 a + 60 b) x^2 + \frac{4}{3}(56 a - 32 b) x^4$$

Determine the values of the coefficients that accomplish this.

```
{a, b, c, d, e, f, g, h, i, j} /. {v → d 262144 / (2 * 6561), u → -j 65536 / (2 * 2187)} /.
          {t -> 8192 (3 c - 110 d + 3 i) / 2187, s → -2048 (g + h - 30 j) / 243} /.
         {r -> 512 (9 b - 210 c + 4288 d + 9 f - 222 i) / 729,
          q → -128 (3 e - 62 g - 54 h + 920 j) / 81} /.
        {p -> 32 (27 a - 342 b + 4896 c - 72128 d - 378 f + 5160 i) / 243,
         o → (624 e - 128 (64 g + 57 h - 726 j)) / 27} /.
       {n → -(756 a - 16 (504 b - 5508 c + 68576 d + 513 f - 5916 i)) / 81,
        m → -4 (69 e - 772 g - 708 h + 7888 j) / 9} /. {k → (9 b + 784 d - 84 i) 4 / 3} /.
     {i → -(27 a - 288 b + 2700 c - 32768 d - 270 f) / 3072,
      j → -(54 e - 576 g - 540 h) / 5760} /.
    {d → 0, h -> (3 e - 32 g) / 30} /. {f → -(-9 a + 96 b + 124 c) / 90,
    g → 3 e / 2} /.
   {e → 0, c -> (576 a - 384 b) / 256} //
 FullSimplify
```

$$\left\{a, b, \frac{3}{4}(3 a - 2 b), 0, 0, -3 a + b, 0, 0, -\frac{9 a}{4} + \frac{3 b}{2}, 0\right\}$$

So we can choose any values for a and b to generate a 4th order polynomial.
The general form is

$$a\, rp^2 + b\, rpp^2 + c\, rppp^2 + d\, rpppp^2 + e\, rp\, rpp + f\, rp\, rppp + g\, rp\, rpppp + h\, rpp\, rppp + i\, rpp\, rpppp + j\, rppp\, rpppp$$

If we choose $a = 1$ and $b = 3/2$ we get the same result we had when we considered only third derivatives of rho. This was a linear combination of rho and rPP, so we know we do not want that.

Choose $a = 0$ and $b = 1$. Note that we could use any values of a and b except for $b = \frac{3}{2} a$.

$$\mathbf{fp} = \frac{\mathbf{rpp}^2 - \frac{3}{2}\,\mathbf{rppp}^2 + \mathbf{rp\ rppp} + \frac{3}{2}\,\mathbf{rpp\ rpppp}}{\mathbf{rho}} \mathbin{//} \mathbf{FullSimplify}$$

$$-156 + 80\,x^2 - \frac{128\,x^4}{3}$$

This expression is, at least, not inconsistent with the result for $\beta = 0$: $\mathrm{fp} = \frac{\mathrm{rpp}^2 - \mathrm{rp\ rppp}}{\mathrm{rho}}$. Presumably the result for general $\beta$ reduces to this form when $\beta \to 0$.

Find the values of the coefficients that give the kinetic energy:

**kin**

$$\frac{39}{16} - \frac{3\,x^2}{2} + \frac{8\,x^4}{9}$$

**Collect[a rho + b rpp + c fp , x]**

$$\frac{3\,a}{4} + 3\,b - 156\,c + (2\,a - 12\,b + 80\,c)\,x^2 + \left(\frac{32\,b}{9} - \frac{128\,c}{3}\right)x^4$$

**rules =**

$$\mathbf{Solve}\left[\left\{\left(\frac{3\,a}{4} + 3\,b - 156\,c\right),\ (2\,a - 12\,b + 80\,c)\ ,\ \left(\frac{32\,b}{9} - \frac{128\,c}{3}\right)\right\} == \left\{\frac{39}{16},\ -\frac{3}{2},\ \frac{8}{9}\right\},\ \{a,\ b,\ c\}\right]$$

$$\left\{\left\{a \to \frac{3}{8},\ b \to \frac{7}{64},\ c \to -\frac{3}{256}\right\}\right\}$$

**a rho + b rpp + c fp /. rules // FullSimplify**

$$\left\{\frac{39}{16} - \frac{3\,x^2}{2} + \frac{8\,x^4}{9}\right\}$$