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

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

with

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

Note that $\gamma+\frac{1}{2}\alpha=1\rightarrow\alpha=2\,(1-\gamma)$. This is not a general result (for $N\neq2$). Note also that $\frac{1}{2}<\gamma\leq1$

Basic Definitions

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

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

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

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

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

```
In[4]:= 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]
```

This is equal to a contant times ψ. Divide by ψ to show this.

```
In[5]:= eExact = FullSimplify[LHS / ψExact[x1, x2], Assumptions → β < 1]

In[6]:= 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.

```
In[7]:= ans := Integrate[ψ[x1, x2]^2, {x1, -∞, ∞}, {x2, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}]
```

In[8]:=
```
normConst = Sqrt[(-1 + 2 γ)^(3/2)] / Sqrt[π];
```
$$\text{normConst} = \frac{\sqrt{(-1+2\gamma)^{3/2}}}{\sqrt{\pi}};$$

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

In[9]:=
```
ans := Integrate[normConst^2 ψ[x1, x2]^2,
   {x1, -∞, ∞}, {x2, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}]
```

Find the one- and two-particle density matrices

In[10]:=
```
ρ12[x1_, x2_] = ψ[x1, x2]^2
```

In[11]:=
```
ρ[x_] =
  Integrate[ρ12[x, x2], {x2, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}] // FullSimplify
```

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

In[12]:=
```
k12a[x1_, x2_] = (∂x1 ψ[x1, x2])^2 + (∂x2 ψ[x1, x2])^2 // FullSimplify
```

In[13]:=
```
k1a[x_] =
  Integrate[k12a[x, x2], {x2, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}] // FullSimplify
```

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

In[14]:=
```
k12b[x1_, x2_] =
  (-ψ[x1, x2] ∂x1,x1 ψ[x1, x2]) + (-ψ[x1, x2] ∂x2,x2 ψ[x1, x2]) // FullSimplify
```

In[15]:=
```
k1b[x_] =
  Integrate[k12b[x, x2], {x2, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}] // FullSimplify
```

Show that both versions give the same total kinetic energy

In[16]:=
```
kTota = Integrate[k1a[x], {x, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}] // FullSimplify
```

In[17]:=
```
kTotb = Integrate[k1b[x], {x, -∞, ∞}, Assumptions → {γ > 1/2, γ ≤ 1}] // FullSimplify
```

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

In[18]:=
```
ρ[x]
```

In[19]:=
```
preFact = ρ[x] / (2 x^2 + γ) // FullSimplify
```

In[20]:=
```
ρ0 = ρ[x] / preFact // FullSimplify
```

In[21]:=
```
kina = k1a[x] / preFact
```

In[22]:=
```
ρP = Collect[(∂x ρ[x]) / preFact // FullSimplify, x]
```

In[23]:=
```
ρPP = Collect[(∂x,x ρ[x]) / preFact // FullSimplify, x]
```

In[24]:=
```
ρPPP = Collect[(∂x,x,x ρ[x]) / preFact // FullSimplify, x]
```

In[25]:=
```
ρPPPP = Collect[(∂x,x,x,x ρ[x]) / preFact // FullSimplify, x]
```

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

In[26]:=
```
Collect[{kina, ρ0, ρP, ρPP, ρPPP, ρPPPP} /. γ → 1 // FullSimplify, x] // TableForm
```

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

In[27]:=
$$\text{f}\rho = \frac{1}{4}\,\frac{\rho\text{PP}^2 - \rho\text{P}\,\rho\text{PPP}}{\rho 0}\ \text{/. } \gamma \to 1\ \text{// FullSimplify}$$

Which then allowed us to write the kinetic energy density as a function of ρ, ρPP and fρ

In[28]:=
$$3\,\rho 0 + \frac{1}{2}\,\rho\text{PP} - \frac{1}{2}\,\text{f}\rho\ \text{/. } \gamma \to 1\ \text{// FullSimplify}$$

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

In[29]:=
```
Collect[{kina, ρ0, ρP, ρPP, ρPPP, ρPPPP} /. γ → 3/4 // FullSimplify, x] // TableForm
```

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 $\gamma = 3/4$.

In[30]:=
```
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]
```

First consider only terms up to rppp.

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

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

Who would have known?

Consider all terms including rpppp.

In[57]:=
```
poly = Collect[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]
```

In[58]:=
```
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)], x]
```

```
In[59]:= 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]

In[60]:= Collect[FullSimplify[ans /. {v → d 262 144 / (2 * 6561), u → -j 65 536 / (2 * 2187)}], x]

In[61]:= 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}], x]

In[62]:= 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}], x]

In[63]:= 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]

In[64]:= 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]

In[65]:= 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]
```

```
In[66]:= 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]
```

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]
```

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]
```

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

```
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]
```

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
```

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 $b = \frac{3}{2} a$.

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

This expression is, at least, not inconsistent with the result for $\beta = 0$: $fp = \frac{rpp^2 - rp\,rppp}{rho}$. Presumably the result for general β reduces to this form when $\beta \to 0$.
Find the values of the coefficients that give the kinetic energy:

```
kin
```

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

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

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