The Notebook paths.nb

In this notebook we arrive at the result in Eq. (11), which is the generalized entanglement measure for the intermediate case of path superposition with non-negligible gaussian width. The calculation proceeds as follows: (1) defining the non-relativistic action, (2) finding the classical solutions of the system, (3) computing the gaussian integrals in Eq. (9), (4) calculating for this wavefunction the generalized entanglement measure [Swain et al, Phys. Rev. A 105, 052441 (2022)] defined in Eq. (28), to get Eq. (11).

```
<< VariationalMethods`

$Assumptions = {m > 0, d > 0, ω > 0, ξ > 0, t > 0, ϕ > 0 , ϵ > 0 , Ω > 0 ,
   ti > 0, y1 ∈ Reals, y2 ∈ Reals, y1p ∈ Reals, y2p ∈ Reals, 4 ϵ^2 ϕ < 1,
   trp ≥ 0, ξ1 ∈ Reals, ξ2 ∈ Reals, s1i ∈ Reals, s2i ∈ Reals, s1j ∈ Reals,
   s2j ∈ Reals, s1k ∈ Reals, s2k ∈ Reals, s1l ∈ Reals, s2l ∈ Reals};

(*defining the dimensionless quantities ϵ,
ϕ and Ω which fully define the problem.*)
ℏ = ϵ^2 d^2 m ω;
(*ϵ = α/d is a measure of the "quantumness" of the particles*)
G = ϕ ℏ d ω / (m^2) ;
(*ϕ = Gm²/ℏωd is a measure of the effect of gravity on the system*)
c = d ω / (Ω);
(*Ω = ωd/c is a measure of the effect of retardation in the system*)

α = Sqrt[ℏ / (m ω)]; (*the width of the gaussian*)

(*a function calculating an integral of the form fPre Exp[fExp],
where fPre is a polynomial and fExp a 2nd order polynomial. Taken
  from https://mathematica.stackexchange.com/a/6846.*)
gaussMoment[fPre_, fExp_, vars_] := Module[{coeff, dist, ai, μ, norm},
  coeff = CoefficientArrays[fExp, vars, "Symmetric" → True];
  ai = Inverse[2 coeff[[3]]];
  μ = -ai.coeff[[2]];
  dist = MultinormalDistribution[μ, -ai];
  norm = 1 / PDF[dist, vars] /. Thread[vars → μ];
  norm Exp[1 / 2 coeff[[2]].μ + coeff[[1]]] ×
    Distribute@Expectation[fPre, vars ≈ dist]]

(*functions replacing coefficients of given polynomials with
 single symbols. This makes mathematica work much faster.*)
myMatrix[symb_, d1_, d2_, d3_, d4_] :=
  Table[Subscript[symb, i1, i2, i3, i4], {i1, d1}, {i2, d2}, {i3, d3}, {i4, d4}];
symbolize[poly_, vars2_, symb_] :=
```

```
  Module[{lst, flst, symbolized, dims, symbCoeffs},
   lst = CoefficientList[poly, vars2];
   dims = Dimensions[lst];
   symbCoeffs = myMatrix[symb, dims⟦1⟧, dims⟦2⟧, dims⟦3⟧, dims⟦4⟧];
   Do[
    If[lst⟦i1, i2, i3, i4⟧ == 0, symbCoeffs⟦i1, i2, i3, i4⟧ = 0];
    , {i1, 1, dims⟦1⟧}, {i2, 1, dims⟦2⟧}, {i3, 1, dims⟦3⟧}, {i4, 1, dims⟦4⟧}];
   symbolized = Internal`FromCoefficientList[symbCoeffs, vars2];
   symbolized
  ];

(*a function wrapping gaussMoment,
replacing coefficients with symbols before integrating.*)
myGauss[fPre_, fExp_, vars1_] :=
 Module[{a0exp, a0pre, aexp, apre, sympre, symexp, res},
  a0exp = CoefficientList[fExp, vars];
  symexp = symbolize[fExp, vars, aexp];
  a0pre = CoefficientList[fPre, vars];
  sympre = symbolize[fPre, vars, apre];
  res = gaussMoment[ sympre , symexp, vars1] /.
    {aexp → a0exp, apre → a0pre, Subscript → Part};
  res
 ]

(*operations on complex numbers done in a
 custom way which for some reason works faster.*)
myRe[var_] := Module[{var1, var1C, re, im},
  var1 = var // ComplexExpand // Evaluate;
  var1C = var1 // Conjugate // Refine;
  re = (var1 + var1C) / 2 // Simplify;
  re
 ]

myIm[var_] := Module[{var1, var1C, re, im},
  var1 = var // ComplexExpand // Evaluate;
  var1C = var1 // Conjugate // Refine;
  im = -ⅈ (var1 - var1C) / 2 // Simplify;
  im
 ]

myConj[var_] := Module[{var1, var1C, re, im},
  var1 = var // ComplexExpand // Evaluate;
  var1C = var1 // Conjugate // Refine;
  var1C
 ]

(*the series expansion to second order in ϵ and
```

```
 zeroth order in Ω. The second function is for quantities
 which will be taken with a square root later.*)
mySeries[expr_] := Series[expr, {Ω, 0, 0}, {ϵ, 0, 2}] // Normal;
mySeriesSq[expr_] := Series[expr, {Ω, 0, 0}, {ϵ, 0, 4}] // Normal;
```

Action

We define action of the gravitational interaction: SGhb = $S_G / \hbar$. This is the Newtonian potential, as we work in the non-relativistic limit in this calculation. The functions q1, q2 are the variables for the lagrangian and action.

In[◦]:=
```
LG12 = (G m^2 / 2) / (d + α q1[ti] + α q2[ti]) / ℏ   // mySeries // Simplify;
LGhb = LG12 + (LG12 /. {q1 → q2, q2 → q1}) // mySeries // Simplify
SGhb = Integrate[LGhb, {ti, 0, t}];
```

Out[◦]=

$$\phi\,\omega\left(1-\epsilon\,(q1[ti]+q2[ti])+\epsilon^2\,(q1[ti]+q2[ti])^2\right)$$

The free, uncoupled action: Sunc = $\Sigma_{a=1,2}\, S_a / \hbar$:

In[◦]:=
```
Lunc = (m (α q1'[ti])^2 / 2 + m (α q2'[ti])^2 / 2) / ℏ // mySeries // Simplify
Sunc = Integrate[Lunc, {ti, 0, t}];
```

Out[◦]=

$$\frac{q1'[ti]^2+q2'[ti]^2}{2\,\omega}$$

Now that we have defined the action, we proceed to finding the solution to the classical equations of motion, which we will use for the stationary-phase approximation in Eq. (9).

Classical Solutions

We find the classical trajectories of the particles for initial locations y1p, y2p = $y'_1/\alpha,\ y'_2/\alpha$ and final locations y1, y2 = $y_1/\alpha,\ y_2/\alpha$. Here, the y's are in units of α, the gaussian's width. We do it by solving the system under the second order approximation in ϵ. The problem becomes two harmonic oscillators with some frequency trp$\times\omega$, which are coupled by another spring, which is gravity. The variable trp is just a bookkeeping variable which will be taken to zero to achieve the trajectories of the two otherwise free particles coupled by gravity.

In[◦]:=
```
L[ti] := (LGhb + Lunc);
L[ti] // Simplify
```

Out[◦]=

$$\phi\,\omega\left(1-\epsilon\,(q1[ti]+q2[ti])+\epsilon^2\,(q1[ti]+q2[ti])^2\right)+\frac{q1'[ti]^2+q2'[ti]^2}{2\,\omega}$$

In[∘]:=
```
eqs = EulerEquations[L[ti], {q1[ti], q2[ti]}, ti] //
  Expand (*the classical equations of motion*)
```

Out[∘]=

$$\left\{-\epsilon\,\phi\,\omega + 2\,\epsilon^2\,\phi\,\omega\,\text{q1}[\text{ti}] + 2\,\epsilon^2\,\phi\,\omega\,\text{q2}[\text{ti}] - \frac{\text{q1}''[\text{ti}]}{\omega} == 0,\right.$$
$$\left.-\epsilon\,\phi\,\omega + 2\,\epsilon^2\,\phi\,\omega\,\text{q1}[\text{ti}] + 2\,\epsilon^2\,\phi\,\omega\,\text{q2}[\text{ti}] - \frac{\text{q2}''[\text{ti}]}{\omega} == 0\right\}$$

In[∘]:=
```
sol = DSolve[{eqs⟦1⟧, eqs⟦2⟧, q1[0] == y1p, q2[0] == y2p, q1[t] == y1, q2[t] == y2},
   {q1[ti], q2[ti]}, {ti}] // Simplify;(*their solution*)
```

In[∘]:=
```
x1[time_] := q1[ti] /. sol⟦1⟧ /. ti → time;
x2[time_] := q2[ti] /. sol⟦1⟧ /. ti → time;
x1[ti]
x2[ti]
```

Out[∘]=

$$\frac{1}{4\left(-1+e^{4\,t\,\epsilon\,\sqrt{\phi}\,\omega}\right)t\,\epsilon}\,e^{-2\,\text{ti}\,\epsilon\,\sqrt{\phi}\,\omega}\Big(-e^{2\,t\,\epsilon\,\sqrt{\phi}\,\omega}\,t\,(-1+2\,\text{y1}\,\epsilon+2\,\text{y2}\,\epsilon)+e^{2\,(t+2\,\text{ti})\,\epsilon\,\sqrt{\phi}\,\omega}\,t\,(-1+2\,\text{y1}\,\epsilon+2\,\text{y2}\,\epsilon)+$$
$$e^{4\,t\,\epsilon\,\sqrt{\phi}\,\omega}\,t\,(-1+2\,\text{y1p}\,\epsilon+2\,\text{y2p}\,\epsilon)-e^{4\,\text{ti}\,\epsilon\,\sqrt{\phi}\,\omega}\,t\,(-1+2\,\text{y1p}\,\epsilon+2\,\text{y2p}\,\epsilon)-$$
$$e^{2\,\text{ti}\,\epsilon\,\sqrt{\phi}\,\omega}\,(2\,\text{ti}\,(\text{y1}-\text{y1p}-\text{y2}+\text{y2p})\,\epsilon+t\,(1+2\,\text{y1p}\,\epsilon-2\,\text{y2p}\,\epsilon))+$$
$$e^{2\,(2\,t+\text{ti})\,\epsilon\,\sqrt{\phi}\,\omega}\,(2\,\text{ti}\,(\text{y1}-\text{y1p}-\text{y2}+\text{y2p})\,\epsilon+t\,(1+2\,\text{y1p}\,\epsilon-2\,\text{y2p}\,\epsilon))\Big)$$

Out[∘]=

$$\frac{1}{4\left(-1+e^{4\,t\,\epsilon\,\sqrt{\phi}\,\omega}\right)t\,\epsilon}\,e^{-2\,\text{ti}\,\epsilon\,\sqrt{\phi}\,\omega}\Big(-e^{2\,t\,\epsilon\,\sqrt{\phi}\,\omega}\,t\,(-1+2\,\text{y1}\,\epsilon+2\,\text{y2}\,\epsilon)+e^{2\,(t+2\,\text{ti})\,\epsilon\,\sqrt{\phi}\,\omega}\,t\,(-1+2\,\text{y1}\,\epsilon+2\,\text{y2}\,\epsilon)+$$
$$e^{4\,t\,\epsilon\,\sqrt{\phi}\,\omega}\,t\,(-1+2\,\text{y1p}\,\epsilon+2\,\text{y2p}\,\epsilon)-e^{4\,\text{ti}\,\epsilon\,\sqrt{\phi}\,\omega}\,t\,(-1+2\,\text{y1p}\,\epsilon+2\,\text{y2p}\,\epsilon)+$$
$$e^{2\,\text{ti}\,\epsilon\,\sqrt{\phi}\,\omega}\,(2\,\text{ti}\,(\text{y1}-\text{y1p}-\text{y2}+\text{y2p})\,\epsilon+t\,(-1+2\,\text{y1p}\,\epsilon-2\,\text{y2p}\,\epsilon))+$$
$$e^{2\,(2\,t+\text{ti})\,\epsilon\,\sqrt{\phi}\,\omega}\,(2\,\text{ti}\,(-\text{y1}+\text{y1p}+\text{y2}-\text{y2p})\,\epsilon+t\,(1-2\,\text{y1p}\,\epsilon+2\,\text{y2p}\,\epsilon))\Big)$$

Sanity check: initial and final locations

In[∘]:=
```
x1[0] // mySeries // Simplify
x2[0] // mySeries // Simplify
x1[t] // mySeries // Simplify
x2[t] // mySeries // Simplify
```

Out[∘]=

y1p

Out[∘]=

y2p

Out[∘]=

y1

Out[∘]=

y2

sanity check: check that the solution actually solves the classical equation

In[ ]:=
```
L[ti] := LGhb + Lunc;
EulerEquations[L[ti], {q1[ti], q2[ti]}, ti] /. {q1 → x1, q2 → x2} //
  mySeries // Simplify
```
Out[ ]=
```
{True, True}
```

Wavefunction

We would now like to compute the wavefunction $\psi^{\sim\,\mathrm{fi}}(\mathrm{y1},\ \mathrm{y2})$ as given in Eq. (9). We start with achieving the expression for the on-shell (= stationary-phase approximated) action $S^{\sim}_{\alpha} + S^{\sim}_{G}$, here Shb.

In[ ]:=
```
Lhb =  LGhb + Lunc /. {q1 → x1, q2 → x2} // mySeries // Simplify;
Shb1 = Integrate[Lhb , {ti, 0, t}] ;
Shb =
 Shb1 - (Shb1 /. {y1 → 0, y2 → 0, y1p → 0, y2p → 0}) // Expand // Refine // Simplify
```
Out[ ]=

$$\frac{1}{6\,t\,\omega}\Big(3\,y2^2 - 6\,y2\,y2p + 3\,y2p^2 - 3\,t^2\,y2\,\epsilon\,\phi\,\omega^2 - 3\,t^2\,y2p\,\epsilon\,\phi\,\omega^2 + 2\,t^2\,y2^2\,\epsilon^2\,\phi\,\omega^2 + 2\,t^2\,y2\,y2p\,\epsilon^2\,\phi\,\omega^2 + 2\,t^2\,y2p^2\,\epsilon^2\,\phi\,\omega^2 + t^2\,y1\,\epsilon\,(-3 + 4\,y2\,\epsilon + 2\,y2p\,\epsilon)\,\phi\,\omega^2 + t^2\,y1p\,\epsilon\,(-3 + 2\,y2\,\epsilon + 4\,y2p\,\epsilon)\,\phi\,\omega^2 + 2\,y1\,y1p\,(-3 + t^2\,\epsilon^2\,\phi\,\omega^2) + y1^2\,(3 + 2\,t^2\,\epsilon^2\,\phi\,\omega^2) + y1p^2\,(3 + 2\,t^2\,\epsilon^2\,\phi\,\omega^2)\Big)$$

We now solve the y1p and y2p integrals while also performing the approximations. We denote for any function f the parts fExp and fPre such that $f(x) = \mathrm{fPre}(x) \times e^{\mathrm{fExp}(x)}$.
The initial state is a sum of four gaussians with $\xi 1, \xi 2 = \pm\,\beta/\alpha$. We therefore perform one calculation (the variable summand) and then use it four times with the appropriate replacements of $\xi 1$, $\xi 2$.

In[ ]:=
```
vars = {y1, y2, y1p, y2p};
summand  =  Exp[ - (y1p - ξ1) ^2 / 2 - (y2p - ξ2) ^2 / 2] *
   (ⅈ / ((-ⅈ + ω t) (3 + 3 ⅈ ω t + 4 ϵ^2 ϕ (ω t)^2))) ^ (-1 / 2);
(*four of these make up the initial state. prefactor
 added for a simpler expression later*)

wf4vars = summand Exp[ⅈ Shb] // mySeriesSq // Simplify;
(*the integrand in Eq. (9).*)
wf4varsExp  =  Exponent[wf4vars, ⅇ] // mySeries // Simplify;
wf4varsPre  =  wf4vars Exp[-wf4varsExp]  // mySeriesSq // Simplify;
wf  = myGauss[  wf4varsPre , wf4varsExp, {y1p, y2p}] // mySeriesSq // Simplify;
(*This is ψ~ fi (y1, y2)*)
wfExp =  Exponent[wf, ⅇ] // mySeries // Simplify;
wfPre =  wf Exp[-wfExp]  // mySeriesSq //  Simplify;
wfExpC  =  wfExp // myConj  // Simplify; (*complex conjugate*)
wfPreC  = wfPre // myConj // Simplify;
```

calculate the norm squared normsq of the state, integrating each separate exponent separately using our myGauss function:

```
wfExp0 = {wfExp /. {ξ1 → ξ, ξ2 → ξ}, wfExp /. {ξ1 → -ξ, ξ2 → ξ},
    wfExp /. {ξ1 → ξ, ξ2 → -ξ}, wfExp /. {ξ1 → -ξ, ξ2 → -ξ}};
wfExpC0 = {wfExpC /. {ξ1 → ξ, ξ2 → ξ}, wfExpC /. {ξ1 → -ξ, ξ2 → ξ},
    wfExpC /. {ξ1 → ξ, ξ2 → -ξ}, wfExpC /. {ξ1 → -ξ, ξ2 → -ξ}};
wfPre0 = {wfPre /. {ξ1 → ξ, ξ2 → ξ}, wfPre /. {ξ1 → -ξ, ξ2 → ξ},
    wfPre /. {ξ1 → ξ, ξ2 → -ξ}, wfPre /. {ξ1 → -ξ, ξ2 → -ξ}};
wfPreC0 = {wfPreC /. {ξ1 → ξ, ξ2 → ξ}, wfPreC /. {ξ1 → -ξ, ξ2 → ξ},
    wfPreC /. {ξ1 → ξ, ξ2 → -ξ}, wfPreC /. {ξ1 → -ξ, ξ2 → -ξ}};

normsq = 0;
Do[
 preee = wfPreC0[[i]] × wfPre0[[j]] // mySeriesSq;
 preee = preee // Simplify;
 res = myGauss[preee, wfExpC0[[i]] + wfExp0[[j]], {y1, y2}];
 res = res // mySeriesSq;
 res = res // Simplify;
 If[i ≠ j, res = 2 myRe[res];];
 normsq += res;
 , {i, 1, Length[wfExp0]}, {j, i, Length[wfExp0]}]
normsq = normsq  // Simplify;
```

Generalized Entanglement Measure

we now calculate the entanglement measure in Eq. (28) after replacing the norm square in the formula by multiplication with the conjugate:

$|\int \psi(y1, y2)\, \psi^*(y'1, y2)\, dy2|^2 = \int \psi^*(y1, y2)\, \psi(y'1, y2)\, \psi(y1, y'2)\, \psi^*(y'1, y'2)\, dy2\, dy'2$

each ψ contains 4 elements, so we have 16 elements in the integrand. We calculate only once (variable summand2), and then sum over the 16 possible choices of the signs in the ξ's.

```
(*each of the four multipicants inside the integral above is
 slightly different in where is the ' and whether it is conjugate*)
wfPre1p = wfPre /. y1 → y1p;
wfExp1p = wfExp /. y1 → y1p;
wfPre2p = wfPre /. y2 → y2p;
wfExp2p = wfExp /. y2 → y2p;
wfPreC12p = wfPreC /. {y1 → y1p, y2 → y2p};
wfExpC12p = wfExpC /. {y1 → y1p, y2 → y2p};

(*we again get to the form f(x)=
 fPre(x)×e^fExp(x) before we calculate the integral using myGauss*)
thisPre = (wfPre1p /. {ξ1 → s1i ξ, ξ2 → s2i ξ})
      (wfPreC /. {ξ1 → s1j ξ, ξ2 → s2j ξ}) (wfPreC12p /. {ξ1 → s1k ξ, ξ2 → s2k ξ})
      (wfPre2p /. {ξ1 → s1l ξ, ξ2 → s2l ξ}) // mySeriesSq // Simplify;
Print["pre series"];
thisExp = (wfExp1p /. {ξ1 → s1i ξ, ξ2 → s2i ξ}) +
     (wfExpC /. {ξ1 → s1j ξ, ξ2 → s2j ξ}) + (wfExpC12p /. {ξ1 → s1k ξ, ξ2 → s2k ξ}) +
     (wfExp2p /. {ξ1 → s1l ξ, ξ2 → s2l ξ}) // Simplify;
Print["exp simp"];
summand2 = myGauss[thisPre, thisExp, {y1, y2, y1p, y2p}];
Print["int"];
summand2 = summand2 / normsq^2 // mySeriesSq // Simplify; (*normalize*)
Print["int ser"];
summand2 = summand2 // Simplify;
Print["int simp"];
```

```
pre series
exp simp
int
int ser
int simp
```

now sum over the 16 elements:

```
In[ ]:= sum = Sum[ summand2, {s1i, {-1, 1}}, {s2i, {-1, 1}}, {s1j, {-1, 1}}, {s2j, {-1, 1}},
     {s1k, {-1, 1}}, {s2k, {-1, 1}}, {s1l, {-1, 1}}, {s2l, {-1, 1}}] // Simplify;
```

finally, the generalized entanglement measure (Eq. 28) is:

```
In[ ]:= gem = Sqrt[2 (1 - sum)] // Expand // Simplify
Out[ ]=
```

$$\left(1 \Big/ \left(3\left(1+e^{\xi^2}\right)\right)\right) 2\, t\, \epsilon^2\, \phi\, \omega \sqrt{\left(9+3\, t^2\left(1-3\,\xi^2\right)\omega^2+t^4\left(1-2\,\xi^2\right)^2\omega^4+e^{2\,\xi^2}\left(9+36\,\xi^4+3\,t^2\,\omega^2+t^4\,\omega^4+9\,\xi^2\left(4+t^2\,\omega^2\right)\right)+2\,e^{\xi^2}\left(9+3\,t^2\,\omega^2-9\,t^2\,\xi^4\,\omega^2+t^4\,\omega^4-2\,\xi^2\left(-9+t^4\,\omega^4\right)\right)\right)}$$

find a nicer representation (Eq. 11) with order 1 functions (Eq. 29):

```
In[ ]:= coefflist = (gem / (2 t ϵ^2 ϕ ω))^2 /. {ξ → x, ω → 1} // CoefficientList[#, t] & ;
```

In[ ]:=
```
f0 = coefflist[[1]] - 4 x^2 (1 + x^2) // Simplify
```
Out[ ]=

$$\left(1+e^{2x^2}-4x^2-4x^4+e^{x^2}\left(2-4x^2-8x^4\right)\right)\Big/\left(1+e^{x^2}\right)^2$$

In[ ]:=
```
f2 = 3 coefflist[[3]] - 3 x^2 // Simplify
```
Out[ ]=

$$\left(1+e^{2x^2}-6x^2+e^{x^2}\left(2-6x^2-6x^4\right)\right)\Big/\left(1+e^{x^2}\right)^2$$

In[ ]:=
```
f4 = 9 coefflist[[5]] // Simplify
```
Out[ ]=

$$\left(1+e^{x^2}-2x^2\right)^2\Big/\left(1+e^{x^2}\right)^2$$

```
gem^2 -
   (2 t ϵ^2 ϕ ω Sqrt[f0 + 4 x^2 (1 + x^2) + f2 (ω t)^2 / 3 + x^2 (ω t)^2 + f4 (ω t)^4 / 9])^
    2 /. ξ → x // FullSimplify
 (*a sanity check: this should be zero if Eq. (11) really
    equals to our result from gem above.*)
```
Out[ ]=

0

Plot the functions:

```
Plot[{(1 + e^(2 x^2) - 4 x^2 - 4 x^4 + e^(x^2) (2 - 4 x^2 - 8 x^4)) / (1 + e^(x^2))^2 /. x → xx / 2,
   (1 + e^(2 x^2) - 6 x^2 + e^(x^2) (2 - 6 x^2 - 6 x^4)) / (1 + e^(x^2))^2 /. x → xx / 2,
   (1 + e^(x^2) - 2 x^2)^2 / (1 + e^(x^2))^2 /. x → xx / 2}, {xx, 0, 8},
 PlotLegends → Placed[{"f0(x)", "f2(x)", "f4(x)"}, {Right, Bottom}],
 PlotTheme → "Monochrome", AxesLabel → {"x"}]
(*the x is divided by two because in the paper the distance
 between the paths is β and in this notebook it is 2β.*)
```
Out[ ]=