Physics 880.05: PS#1 Solutions

1. MATLAB Sandbox.
   - Starting on the next page is a printout of a MATLAB session with sample results for parts (a) through (e).
   - Most of these are self-explanatory, but let's look at (e) more closely.

   Wikipedia says that the Zassenhauss formula is

$$e^{t(X+Y)} = e^{tX}\, e^{tY}\, e^{-\frac{t^2}{2}[X,Y]}\, e^{\frac{t^3}{6}(2[Y,[X,Y]]+[X,[X,Y]])}\cdots$$

so we expect naively that approximating $e^{-\epsilon(T+V)}$ by $e^{-\epsilon T}e^{-\epsilon V}$ should make an error of order $t^2 \to \epsilon^2$, and multiplying N of them together could have an error $N\epsilon^2 \sim O(\epsilon)$. In fact, the trace $\mathrm{Tr}[(e^{-\epsilon(T+V)})^N]$ differs from $\mathrm{Tr}[(e^{-\epsilon T}e^{-\epsilon V})^N]$ by $O(\epsilon^2)$:

Check the formula:

$$e^{t(X+Y)} = 1 + t(X+Y) + \tfrac{1}{2}t^2(X+Y)(X+Y) + \ldots = 1 + t(X+Y) + \tfrac{t^2}{2}(X^2+XY+YX+Y^2) + \ldots$$

$$e^{tX}e^{tY} = (1+tX+\tfrac{t^2}{2}X^2+\ldots)(1+tY+\tfrac{t^2}{2}Y^2+\ldots) = 1 + tX + tY + \tfrac{1}{2}t^2X^2 + t^2XY + \tfrac{1}{2}t^2Y^2 + \ldots$$

$$\Rightarrow e^{t(X+Y)} - e^{tX}e^{tY} = \tfrac{1}{2}t^2[XY+YX-2XY] = -\tfrac{1}{2}t^2[X,Y] \checkmark$$

But note that $e^{-\epsilon T}e^{-\epsilon V}e^{-\epsilon T}e^{-\epsilon V} = e^{-\epsilon T/2}\left[e^{-\epsilon T/2}e^{-\epsilon V}e^{-\epsilon T/2}\right]e^{-\epsilon T/2}$

and the error is given by the terms in [ ]'s:

$$e^{+\frac{t}{2}X}e^{+tY}e^{+\frac{t}{2}X} = (1+\tfrac{t}{2}X+\tfrac{1}{8}t^2X^2)(1+tY+\tfrac{t^2}{2}Y^2)(1+\tfrac{t}{2}X+\tfrac{t^2}{8}X^2)\cdots$$

$$= 1 + \tfrac{t}{2}X + tY + \tfrac{t}{2}X + \tfrac{t^2}{2}XY + \tfrac{1}{8}t^2X^2 + \tfrac{t^2}{2}Y^2 + \tfrac{t^2}{2}YX + \tfrac{t^2}{4}X^2 + \tfrac{t^2}{8}X^2$$

$$= 1 + \tfrac{t}{2}(X+Y) + \tfrac{t^2}{2}(X^2+XY+YX+Y^2) + O(t^3)$$

so to this order it agrees with the exact result

$\Rightarrow$ the error is ϵ^3 rather than ϵ^2! [Note that the trace takes care of the terms at the end of the product].