I suggest to change title, as time-dependent quantum systems to me implies that the potential is time-dependent: Time-dependent Quantum Wave Packet Dynamics Actioned

P1, first paragraph: remove "and linear combinations of such solutions to form wave packets"

Actioned.

P1, 2nd paragraph: "Theory and computations are key for rationalising experimental observations..."

"The concept of a wave packet, i.e. a time-dependent and non-stationary wavefunction, is particularly..."

Actioned

"Wave packets can be exploited...." , maybe add "..., and appear naturally whenever a system is excited by coherent light such as a laser." Could provide a reference to the Nobel Prize lecture by Ahmed Zewail (1999). Actioned

et al should be written as et al. ie "\it{et al}.\" Actioned

can elucidate - here I would say "can yield key insights" Actioned

beyond those that are structural -> beyond the evolution of molecular geometry as a function of time by studying the..... Actioned

P2, 2nd paragraph: "This combines the computational scaling...." Maybe just continue the previous sentence, saying "...products,8,9, and provides high accuracy and comparatively effective scaling properties. Wave packets can also be formed from solutions of the TISE by multiplying the wavefunctions with a phase factor exp(), where...." At end of paragraph add a reference to early paper by Eric Heller (~1980). All actioned (assuming Heller’s paper is on frozen Gaussians)

P3: not sure, maybe ask Mark Wilson. I guess you could generate a tinyURL which would not immediately give away your identity? Or actually add all the contents of the github as a giant appendix? There are nice latex scripts for formatting (Matlab) code available. Asked Mark, he said it’s ok to include the link

P5

Eq 2.4 define alpha and beta functions. Actioned

P10

Below eq 2.39, do you mean "Like g(k),"? Yes, I was just naming the function, *g*, but I have included the full *g*(*k*) now.

P11

Sentence wrong? Don't you mean: "This is primarily because the TDSE is analytically soluble only for the most simple of systems,..."? Yes, my bad!

Maybe say "Two numerical methods will be discussed" Actioned

P12

Did you define the abbreviation SO (for split operator)? It was defined in the short intro, but I will redefine SO and CN in the introduction since I have now taken it out of the short intro of Chapter 3.

Do you have a reference for pseudo-spectral methods? Need to visit the library to find a book

Typo: "Once can show" Actioned

P14

I am not sure about the statement that "This allows for the critical role of wave packets.... without the complication of quantum effects, such as....". These wps are definitely quantum! Isn't it better to just say that it provides an opportunity to explore the behaviour in simple and well-understood model systems, or something along those lines? Agreed; changes made.

P25

Yes, add the calculation of <x2>. Actioned

P32-33

Comment on dk: physically we do not expect the composition of the wp in momentum space to change in the absence of external force (which is the case for a constant potential V(x)=a). You do nicely point out this in the Conclusion where you reference the conservation of momentum (in the absence of a force). Noted

P45-46

First paragraph is in presence tense, while second paragraph shifts over to past sense. Stick to present! Actioned – present tense used throughout the conclusions section

P45, line -4 from bottom typo " ,relative" Actioned

P46 "Chirping provides a useful framework by which the ....." rewrite as "Chirping of the wavepacket, for instance via shaped optical excitation fields, can be exploited for more accurate or specific measurements of photochemical dynamics. For example,....." You could even add a suitable reference to nonadiabatic dynamics (some review) here! Change to wording made, and three references for reviews added.