Error with the Generalized Crank-Nicolson Method

Elijan Jakob Mastnak
Student ID: 28181157

A quick case study in how the values of r and M (which determine the order of the time and position derivative approximation, respectively) used in the Crank-Nicolson method used to solve the 10th MFP report affect the accuracy of the numerical solution (see also Ref. [1]). The error plotted in Figures 1 and 2 (below) is found according to

$$\mathcal{E} = \int_{x_0}^{x_j} \left|\psi(x, t_N) - \psi_{\text{analytic}}(x, t_N)\right|^2 \mathrm{d}x \tag{1}$$

where ψ and ψ_{analytic} are the numerical and analytic wavefunction solutions, respectively, at the simulation end time t_N.

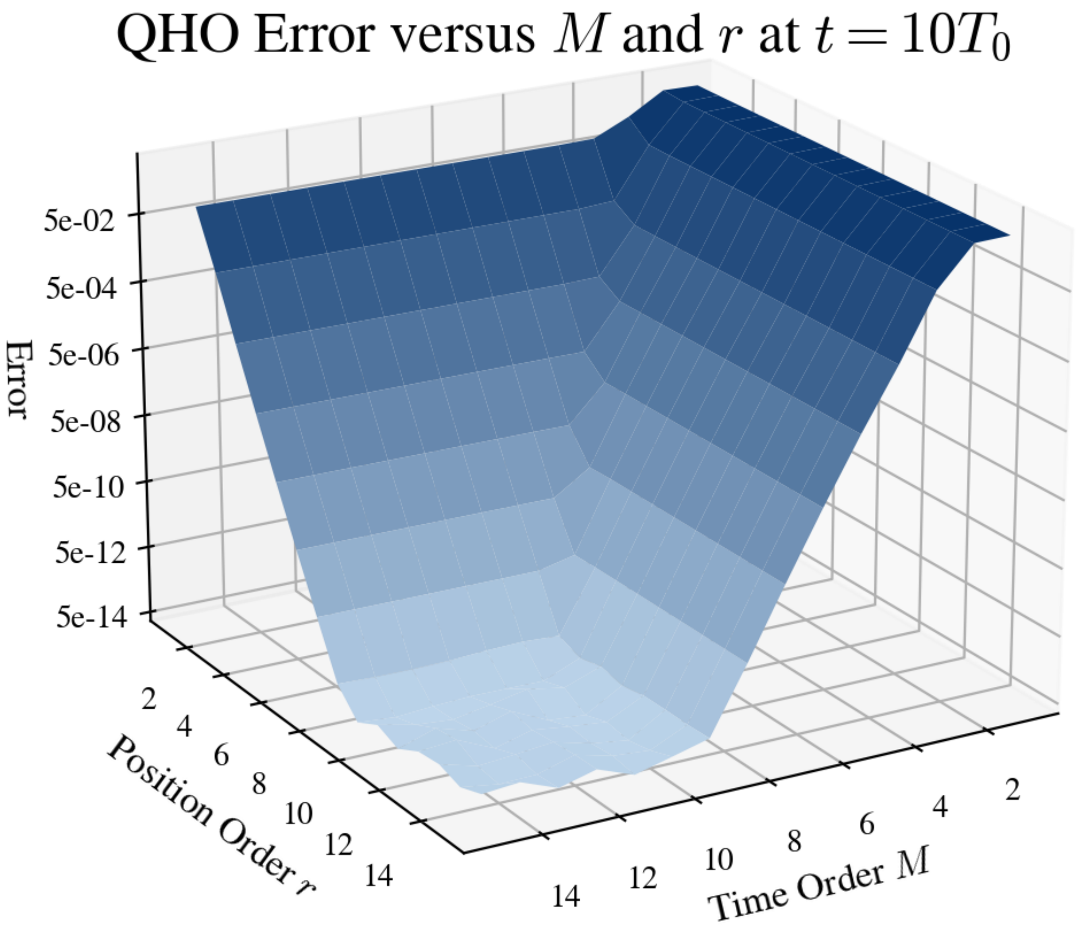

Figure 1: Error in the coherent state solution after a ten-period simulation as a function of r and M—note the logarithmic scale. High M improves the solution more than high r (compare the curves at $r \equiv 1$ and $M \equiv 1$. Found with $\Delta t = 0.2\pi$; error is calculated according to Equation 1. Note also the onset of a plateau at $r \gtrsim 7$ and $M \gtrsim 8$ beyond which the error does not improve—this evidently corresponds to the regime of non-negligible floating point error, as investigated more thoroughly in the Airy function report.

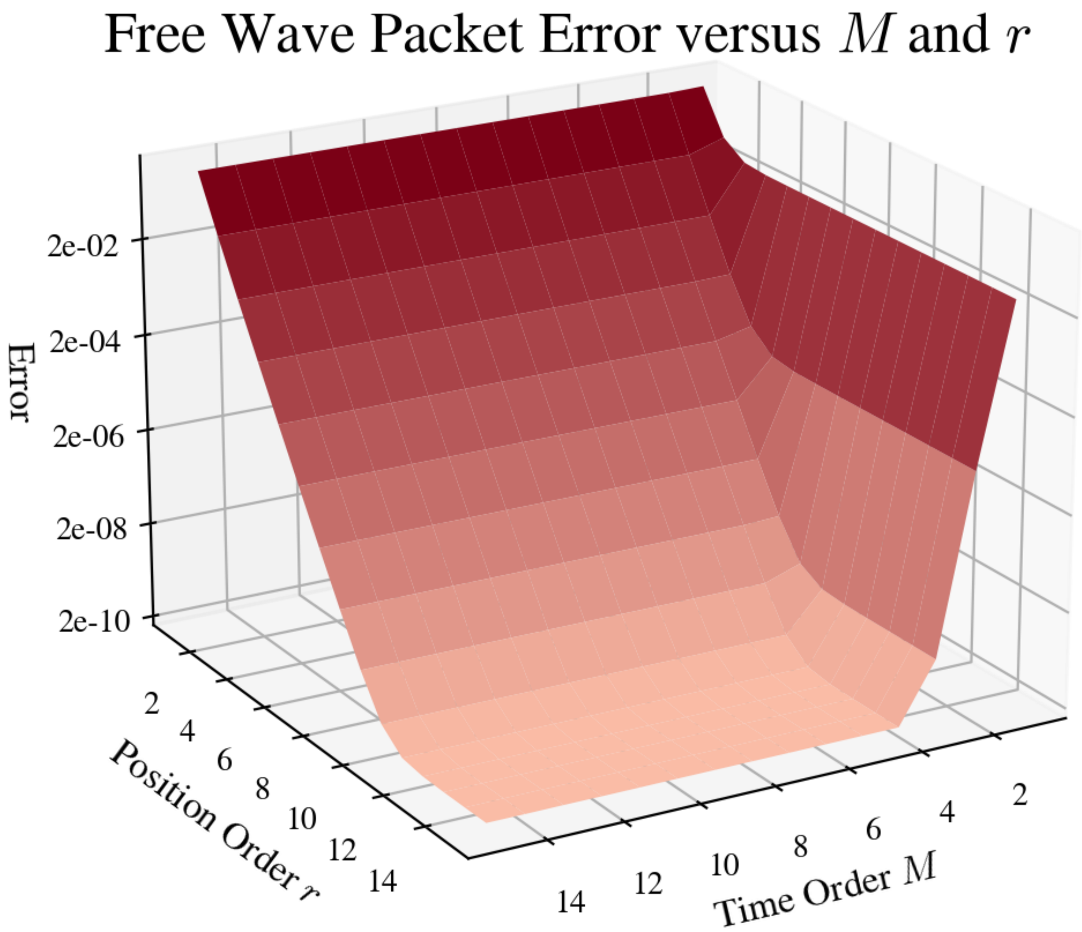

Figure 2: Error in the numerical solution for the wave packet at $a \approx 1.0$ as a function of r and M—note the logarithmic scale. Higher r improves the solution more than high M (compare the curves at $r \equiv 1$ and $M \equiv 1$. Found with $N = 500$. Note that the solution does not improve for $r \gtrsim 10$ and $M \gtrsim 4$, corresponding to the regime of non-negligible floating point error.

References

[1] W. van Dijk and F. M. Toyama. "Accurate numerical solutions of the time-dependent Schrödinger equation." Phys. Rev. E **75**, 036707 (2007). https://arxiv.org/pdf/physics/0701150.pdf