

Why are JLP and FD so different?

JLP uses a QuFoTr to provide an accurate momentum space representation, meaning it is almost exact for smooth functions, however it relies on the assumption that the wavefunction is periodic and the $-\phi_{\max}$ and $+\phi_{\max}$ connect smoothly. If that assumption holds then JLP is accurate but if ϕ_{\max} is too small the wavefunction wraps around the boundary and interferes with themselves and if ϕ_{\max} is too large the spacing between grid points is coarse and the wavefunction is undersampled and so error rises

FD approximates derivatives locally between neighbouring points which doesn't rely on periodicity, it is only second order accurate so the convergence is slower but steady and predictable.

The reason we see such a large dip for JLP is because of how sensitive it is to the boundaries of ϕ , at these sweet spots, which is where the NS sampling condition is perfectly balanced, the accuracy rapidly increases. For FD we don't see this because it purely depends on the resolution we choose.

Test of FD resolution:

I expected the error of the FD method to decrease as n_q increased however as you increase n_q another error increases that is it extends the available momentum range which means you get unphysical results, you get higher momentum modes which give large k