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Delineation of relative merits of SO2 and SO3 split-operator methods in solving the time-dependent Schrodinger equation for a perturbed harmonic oscillator

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Solution of the time dependent Schrodinger equation (TDSE) has been of considerable interest since the inception of quantum mechanics. In standard notation, the 1–D TDSE is given by, $i\hbar\partial\psi(x,t)/\partial t = \hat{H}(x,t)\psi(x,t)$. Often, the solution for this equation is written as $\psi(x,t) = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}(x,t')dt'\right]\psi(x,t_0)$, where $\psi(x,t_0)$ is the known wave function of the system at an initial time t_0. Various numerical schemes are implemented in calculating $\psi(x,t)$. From a spectrum of such methods the split operator (SO) methods have gained a wide recognition due to its accuracy at economical computer requirements. The popularity has been further fueled by some modifications to the original SO method, namely, the SO2 and SO3 methods. It appears that at present, the research community is carrying out calculations assuming that SO3 is always significantly more accurate than SO2.

We have proven recently that the approximation of the wave function by the form described above, introduces an error into the wave function in systems where the potential has an inseparable term in x and t.. This fact seems to limit the accuracy of both the SO2 and SO3 methods.

We have studied the relative merits of SO2 and SO3 methods in solving the Schrodinger equation for a perturbed harmonic oscillator (which has an inseparable term in x and t): viz. $i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + \frac{1}{2}\omega^2 x^2\psi(x,t) - \alpha x\sin(\gamma t)\,\psi(x,t)$ where α, γ, and ω are constant parameters and m is the mass. The calculations have been performed using both SO2 and SO3 methods for a spectrum of values (α,γ,ω). Accuracy of the methods has been estimated by comparing the numerical results with the known analytical results.

The accuracy of both methods increased with decreasing time step size in calculations. However, both methods became unstable near resonance, i.e. $\gamma \approx \omega$. Contrary to the popular belief, we have found that for some sets of parameters (α,γ,ω) the accuracies of SO2 and SO3 methods are comparable.

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