The Phase-Amplitude method revisited

Professor George Rawitscher may have officially retired, but that has not stopped him striving for innovation. Free from the constraints of chasing grants and the fear of missteps, he is hunting for a better way to compute wave functions.

Your recent paper offers a computationally simpler technique for determining wave functions out to large distances. For the uninitiated, can you explain what a wave function is and how the wave of a wave function differs from a wave in physical space?

The wave in physical space (such as a sound wave in air) describes the location of tangible air molecules as they vibrate around their equilibrium positions, while a quantum-mechanical wave in space describes the probability amplitude of finding the particle in a certain point in space and time. However, although the interpretations in terms of their physical meaning are quite different, both wave manifestations obey similar wave equations.

Why has the 1962 paper by Seaton and Peach, which constitutes a foundation for your work, been relatively ignored until now?

There are several reasons. First, the amplitude equation is a nonlinear wave equation, and hence more difficult to solve. Furthermore, the advent of more modern spectral methods has greatly improved the economy of the solution of this nonlinear wave equation, but had not been applied to this particular case until now, and the solution is not yet applicable to more general situations. And finally, innovation is always more reluctantly accepted in the face of the inertia of well-established conventional methods.

Why is your method less prone to accumulating errors over large distances than finite elements, finite differences or integral equation methods?

Due to the non-oscillatory behaviour of both the amplitude and phase of a wave function, the overall distance domain does not have to be divided into partitions, and the accumulated computational error arising from joining one partition to the next is avoided. Because of the spectral nature of the computational algorithm and the non-oscillatory nature of the results, the number of computational support points in the whole radial domain can be small, avoiding the accumulation of rounding errors. Additionally, an approximate solution can be reduced to the algebraic solution of a cubic equation, which is computationally fast, can be done point by point, and does not lead to an accumulation of errors.

In which situations are conventional solutions to Schrödinger’s equation inadequate and thus call for the use of your Phase-Amplitude method?

In atomic systems at low temperatures, if the molecules present have an electric dipole moment, then the interaction between them is of very long range. Since the molecules have internal excitations, they can lead to resonances at very large distances that can be observed experimentally. However, the corresponding coupled equations are difficult to solve by conventional means. Other applications must exist for digital signals to be transmitted over long distances in optical fibres, but I am unfamiliar with the actual wave equations and their related problems for this case.

Waves from the past

Research from the University of Connecticut has uncovered and enhanced a largely overlooked method of describing waves dating back to the 1930s that promises more accurate models in various real-world applications.

WAVES EXIST IN many forms in our experience of the world: from electromagnetic waves that bring light and energy from the Sun to the sound waves that bring music to our ears or the waves that crash against the shores of our oceans. In quantum mechanics, waves are also used to describe the probability amplitude of finding a particle in a particular place and time. The square of the absolute value of this number gives the actual probability of finding the particle at a certain place and time. Although the waves are very different in terms of our physical experience of them, the wave functions used to describe them are actually mathematically very similar.

At the University of Connecticut in the US, Professor George Rawitscher is working to find a less computationally intensive, more accurate method of solving wave equations. Traditionally, waves are described through every point of their oscillation. This requires a huge number of computations to account for the rise and fall of the wave as it propagates. However, it is also possible to describe a wave using its phase and amplitude (Ph-A) – first suggested by W E Milne in the 1930s. Using this method, a sine function provides the oscillatory nature of the wave, but the phase and amplitude are non-oscillatory and increasing in nature, requiring fewer points to accurately define. This means that their calculation and storage are more efficient than those of the wave function itself.

SEATON AND PEACH

Rawitscher’s work was inspired by a paper from 1962 by Seaton and Peach that had been largely ignored by the community. The method’s biggest advantage is how it performs at large distances: the errors in conventional methods compound exponentially as they propagate, but the Ph-A method’s errors do not accumulate in...
the same way, and thus it remains accurate at the tail end of propagation.

While in the case of a simple sine wave this would not have great significance, as the nature of the phase and amplitude of the wave is well known ahead of time, in the case of interactions with a slow decrease with distance such as the electric force which decays as $1/(\text{distance})^2$ or the force between atomic molecules with electric dipoles which decays as $1/(\text{distance})^4$, the phase and amplitude increase as the wave propagates. Furthermore, the computational time using the method is approximately 10 times faster (G. Rawitscher, 2015, Computer Physics Communications, 191, 33-42).

### CALCULATING WAVES

Rawitscher has explored several methods in an attempt to improve upon the solution of wave equations. One was the spectral integral equation method (S-IEM). Although more stable than finite difference methods, S-IEM becomes more computationally intensive than iterative methods at high computational complexity ($N_1$) because it scales as $N_1^2$ instead of $N_1^3$. Another method evaluated by Rawitscher is the hybrid finite-element discrete variable representation (FE-DVR) technique. It is advantageous because the integrals can easily be performed using the Gauss-Lobatto integration algorithm, the matrix elements for the kinetic energy operator need not be recalculated for each partition and the convergence of the expansion is exponential. However, if there is a large number of partitions as with long-ranged potentials, then rounding and algorithm errors can become unacceptably large.

Hence, Rawitscher’s revised spectral Ph-A solution can become the method of choice in certain situations. For the $1/(\text{distance})^3$ case, an accuracy of five to six significant digits has been obtained.

### AMPLIFYING THE RESULT

Learning from these different techniques and attempting to best the Ph-A method, Rawitscher developed an iterative approach that would also avoid many of the drawbacks of the previous methods, particularly the large numerical errors that can occur using conventional finite-difference or finite-element methods.

His technique is applicable to collisions of atoms at very low temperatures, and potentially to the compression of digital signals transmitted over long distances. It could in principle be applied to numerous situations in order to calculate a wave function out to large distances reliably and economically. Now, Rawitscher and a number of collaborative experts are in the process of compiling a book that describes the basics of the spectral method, as well as its applications. Through this and other modes of communication, he hopes that other researchers will take up the method and develop it for the applications they are interested in.