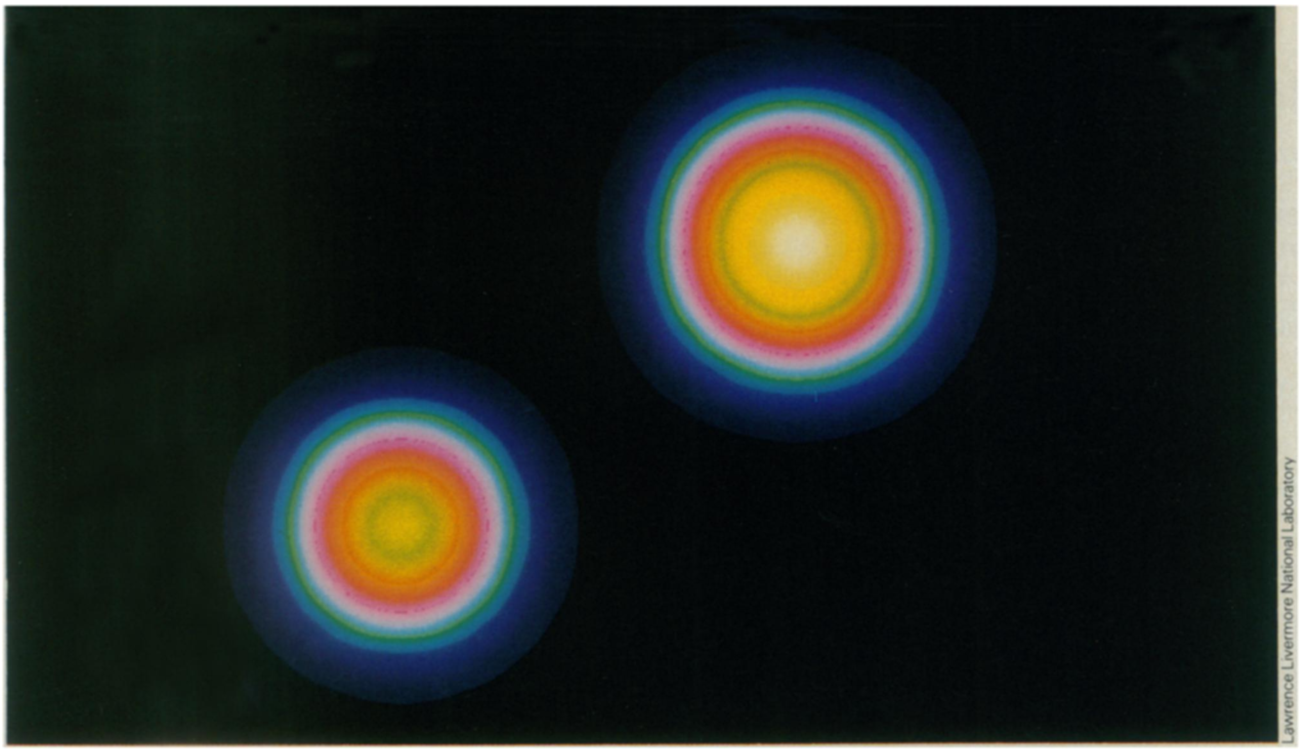
Lawrence Livermore National Laboratory

Quantum Mechanics by Computer

By making waves on a modern computer, scientists can calculate the theory of nuclear collisions

By DIETRICK E. THOMSEN

Wave equations — wave functions — are the mathematical way of describing the behavior of things in quantum mechanics. The physical basis of this is that on the microscopic level every object is at the same time both a particle and a bundle of waves. So the mathematics that describes dynamics on this level turns out to be the mathematics of wave functions.

Wave functions are far from being the easiest things in mathematics to solve and compute with. To calculate the behavior of an atomic nucleus, for instance, involves working with dozens or hundreds of wave functions (each proton and neutron has its own) that are related to one another in such a way that the solution to each one depends on all the others. They cannot be solved one by one; they have to be solved ensemble, dozens or hundreds of simultaneous equations, as mathematicians would describe it.

By hand the task is formidable, perhaps practically impossible. However, at the Lawrence Livermore National Laboratory, a Cray I, one of the latest, biggest and fastest of computers has now come to the rescue. Using it M. S. Weiss and co-workers have been able to calculate what happens in various kinds of collisions of a krypton nucleus with a lanthanum nucleus. Then, with the latest computer graphics they are able to display these processes in an animated film. The two nuclei approach each other, collide, in some cases fuse, in others come apart, and everything is decorated with bright false colors representing the density levels of matter inside the nuclei.

The pictures and the information in them represent the solution of 146 simultaneous wave functions, one for every two nucleons, every two particles in the two nuclei. There is one function for every two nucleons rather than every one because the mathematics contains one important approximation. Nucleons can come with two directions of spin, spin up or spin down. This theory does not distinguish between the two spin states, so each function actually represents the average of one of each.

The pictures show a dozen instances, starting from a head-on collision and proceeding to instances of greater and greater offset between the centers of the two nuclei until they arrive at a sideswipe in which the nuclei hardly touch each other. The collisions near head-on result in fusion. A little offset contributes an angular momentum: The fusion product rotates. More offset and the nuclei collide, losing a lot of energy, but retaining enough to come apart again. This is known as deep inelastic scattering. Finally, an instance where the two nuclei do not touch, but where distortions and vibrations are produced in them by the force between them when they are close.

Weiss says the film wakes physicists up when he shows it at the end of a talk. He mentions one experimentalist who came up and said how nice it was to be able to actually see these things. "At least four levels of abstraction," Weiss comments, "and he talks about seeing it." Yet viewing the film, one can understand what the experimentalist meant.

The calculations behind the film are quite accurate in predicting the main events of the collisions, and that is what is really important. According to Weiss, they predict accurately the conditions under which fusion is likely, the proper range of deep inelastic scattering and so forth.

In the pictures the behavior looks like that of a fluid, liquid drops coming together. Weiss stresses that it is actually the sum of discrete motions, those 146 individual wave functions. One of the purposes of the exercise was to see whether it was possible to derive a macroscopic theory — that is, one that would give a simpler mathematical expression for the over-all behavior of the nuclei, and that would yield the desired predictions without having to start from the 146 individual wave functions. It turns out, Weiss says, that a macroscopic theory is possible in some particular cases, but the microscopic one, starting from the individual wave functions, remains the general one.

Computation was the serious hindrance to doing it before now. As Weiss says, the theory itself was written down years ago by P. A. M. Dirac, one of the pioneer theorists of quantum mechanics. It took Weiss and co-workers a year to figure out how to feed the computation to the computer. Each of the dozen collisions — which takes about 10^{-21} seconds in real time, but is displayed in extreme slow motion in the film — took an hour of computation time using the core of the Cray I computer. That's expensive computing, but, says Weiss, "I would never try it on a lesser computer." □