

anything else could have produced mass concentrations of this magnitude.

At this meeting, however, the controversy was notably absent. Two of the original Seven Samurai, Alan Dressler of the Mount Wilson and Las Campanas Observatories, and Sandra Faber of Lick Observatory presented a survey showing that galaxies on the far side of the purported Great Attractor are falling back inwards, thus demonstrating that there really is a mass concentration there. At the same session, moreover, Robert A. Schommer of Rutgers University presented the results of an independent survey that showed the same thing.

In short, the Great Attractor is real. Now, where did it come from?

■ **The Great Wall(s).** Just last fall, Margaret J. Geller and John P. Huchra of the Harvard-Smithsonian Center for Astrophysics announced their discovery of "the Great Wall"—a system of thousands of galaxies arrayed across the cosmos in the form of a vast, crumpled membrane (*Science*, 17 November 1989, pp. 885 and 897). With a width of at least 500 million light-years, it seemed to be the largest coherent structure ever seen in the universe. The question was whether it was anything more than a statistical fluke, a chance superposition of smaller structures. If so, then the Great Wall would be at least as hard to understand as the Great Attractor.

Now the answer is in, and it seems to be "Yes." At the meeting, Alex S. Szalay of Johns Hopkins University and David C. Koo of Lick Observatory presented a compilation of four galaxy surveys at the north and south galactic poles—the two opposing points on the sky where the interference from stars and dust in our own galaxy is least. Each survey covers a very narrow patch of sky, but compensates by including galaxies that are very faint and very distant. In effect, the combined survey yields a core sample through the universe. And when Szalay and company plot the number of galaxies as a function of redshift, it becomes very apparent that the Great Wall is not alone: other concentrations of galaxies occur with a nearly periodic spacing of about 400 million light-years.

Whatever this repeating structure means, says Szalay—he prefers to call it a "characteristic distance" rather than a periodicity—it is telling us something profound about how the large-scale structure of the universe came into being. The question is what?

It is also telling us what many other astronomers at the meeting were saying: the cold dark matter model is dead. The question is what will replace it? No one yet seems to have an answer.

■ **M. MITCHELL WALDROP**

Understanding the Simplest Reaction

Sixty years after its initial development, quantum mechanics has finally succeeded in completely describing the simplest possible chemical reaction. A team headed by Richard Zare at Stanford University has shown that the reaction $\text{H} + \text{H}_2 \rightarrow \text{H}_2 + \text{H}$ proceeds almost exactly as predicted by two separate groups of theoreticians, one led by William Miller at the University of California at Berkeley and the other by Donald Truhlar at the University of Minnesota in Minneapolis.

Although this might seem like a small step to those outside the field of chemical dynamics, Miller says, "We're all jumping up and down." Long ago, the equations of quantum mechanics were solved to give the precise behavior of individual atoms, but the dynamics of chemical reactions—interactions involving at least three atoms and the exchange of one or more atoms—had defied exact description.

The transfer of a single hydrogen atom in $\text{H} + \text{H}_2 \rightarrow \text{H}_2 + \text{H}$ may look simple, but it was not easy for either theorists or experimental scientists to get a good look at it. For experimentalists, Zare says, the problems include producing hydrogen atoms that move fast enough to overcome the electrical repulsion from H_2 molecules and measuring how many product molecules are in a given quantum state.

In his work, Zare actually performed the reaction $\text{D} + \text{H}_2 \rightarrow \text{HD} + \text{H}$, where D is deuterium, a heavy isotope of hydrogen with one proton and one neutron. The theoretical calculations for this reaction are almost identical to the ones involving only hydrogen atoms, and the substitution of deuterium makes it easier to identify the end products. Zare used a laser to split DBr molecules, creating D atoms with enough energy to react with molecules of H_2 . After the reaction, the same laser ionized the HD molecules so that they could be detected and analyzed by a mass spectrometer.

Zare measured how many HD molecules were produced in the reaction with a given rotation, or spin, and compared this distribution with those predicted by Miller and Truhlar. Within experimental error, "there is nearly perfect agreement between theory and experiment," Zare says. He also compared his results with calculations made using the quasi-classical trajectory approximation—a technique that omits some of the quantum effects—and found its estimates to be slightly but consistently off.

For theorists, the problems in calculating the reaction arise from the need to solve quantum mechanical equations for three atoms—with six or more individual particles—with the atoms moving relative to each other. Just a few years ago, theorists first computed the total reaction rate of $\text{H} + \text{H}_2 \rightarrow \text{H}_2 + \text{H}$ as a function of how energetically the H atom and H_2 molecule come together. At the time, however, they still were unable to calculate the fine details, such as the probability that the product H_2 molecule would be in a given vibrational and rotational quantum state.

The technical difficulties, Truhlar says, centered on the boundary conditions—the mathematical descriptions of the system before and after the reaction. The exchange of atoms makes it difficult to match up the before and after boundary conditions. Truhlar sidestepped the difficulty by transforming the problem of solving differential equations with boundary conditions into a problem in linear algebra.

Miller says he and John Zhang discovered a subtlety about the boundary conditions that had hampered calculations. "Once we realized this subtlety, there were lots of simplifications that were obvious," he says. Those simplifications made computing the reaction's dynamics "straightforward, although not trivial," he says.

Earlier experiments by Richard Bersohn at Columbia University showed that the total reaction rate of $\text{H} + \text{D}_2 \rightarrow \text{HD} + \text{D}$, where the initial and final quantum states were not taken into account, was predicted quite well by the quasi-classical trajectory method. Now Zare's work shows that although quasi-classical methods may be good enough to predict the broad outlines of the reaction, quantum mechanics is needed to provide the details. "The world really is quantum mechanical on the molecular level, not classical," Zare says.

■ **ROBERT POOL**

ADDITIONAL READING

N. C. Blais, M. Zhao, D. G. Truhlar, D. W. Schwenke, D. J. Kouri, "Quantum mechanical calculations and quasi-classical trajectories for comparison to stimulated Raman pumping measurements of the high-energy state-to-state reaction dynamics of $\text{D} + \text{H}_2 \rightarrow \text{HD} + \text{H}$," *Chem. Phys. Lett.*, in press.

D. A. V. Kliner, K.-D. Rinnen, R. N. Zare, "The $\text{D} + \text{H}_2$ reaction: Comparison of experiment with quantum-mechanical and quasi-classical calculations," *ibid.*, in press.

J. Z. H. Zhang and W. H. Miller, "Quantum reactive scattering via the Kohn Variational Principle; differential and integral cross sections for $\text{D} + \text{H}_2 \rightarrow \text{HD} + \text{H}$," *J. Chem. Phys.* **91**, 1528 (1989).