Quantum analog of Ulam's conjecture can guide molecules, reactions

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Like navigating spacecraft through the solar system by means of gravity and small propulsive bursts, researchers can guide atoms, molecules and chemical reactions by utilizing the forces that bind nuclei and electrons into molecules (analogous to gravity) and by using light for propulsion. But, knowing the minimal amount of light required, and how that amount changes with the complexity of the molecule, has been a problem.

Now, by creating a quantum mechanical analog of Ulam's conjecture, researchers at the University of Illinois and the University of California have expanded the flexibility and controllability of quantum mechanical systems.

"Using photons, we can harness chaotic motion to control chemical reactions and to move quantum objects, such as nanoclusters, molecules and buckyballs," said Martin Gruebele, a William H. and Janet Lycan Professor of Chemistry, and the director of the Center for Biophysics and Computational Biology at Illinois.

Gruebele and co-author Peter Wolynes, a professor of chemistry and biochemistry at the University of California, describe their work in a paper accepted for publication in Physical Review Letters and posted on the journal's Web site.

Given sufficient time, classical chaotic motion will spontaneously connect two points in phase space with arbitrary precision. In 1956, American mathematician Stanislaw Ulam conjectured that owing to this phase space-filling aspect of chaotic trajectories, a minimal series of energy expenditures would suffice to transfer a body from one point to another much more rapidly than by spontaneous motion.

Ulam's conjecture is now routinely used to steer spacecraft around the solar system with minimal energy expenditure.

"The idea is that a complex system like our solar system has lots of planets, moons, and asteroids that can fling spacecraft gravitationally anywhere you want," said Gruebele, who is also a professor of physics and biophysics, and a researcher at the Beckman Institute. "Rather than powering a rocket on a brute force, direct route, you can shoot your spacecraft near some moon, and let the moon do most of the work."

Using photons as an energy source, electrons within molecules can move in much the same way as spacecraft in the solar system. But, there is a hitch: Quantum mechanics, not Newtonian dynamics, must be used to describe the motions. In quantum mechanics, the system is described by a wave function, or quantum state.

In their quantum mechanical analog of Ulam's conjecture, Gruebele and Wolynes show there are limits on how efficiently an external force can nudge a system from a given initial state to a target state. They use the concept of a "state space" to describe all the possible quantum states of the system.

"We can calculate where this initial state will most likely go, and we can calculate where the target state will most likely come from," Gruebele said. "We can then identify places in state space where the two are closest to one another."

Those locations are where energy is most efficiently applied to perform the desired quantum transformation from initial state to target state. The researchers' equations also tell them how many photons are needed, and set fundamental limits on the time required.

“We can wait for the best possible moment to use the least amount of energy,” Gruebele said. “What we have is a fast and accurate method for computing the most efficient way of steering a quantum system between two specified states.”

Source: University of Illinois at Urbana-Champaign

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