path integral, summing over all possible paths, the paths leading to the desired result interfere constructively and add up. Those leading to undesired states cancel out. All this is achieved by adjusting phases."

Extensions

A similar process can be carried out in a continuous, or analog, fashion. Edward Farhi (MIT) and Sam Gutmann (Northeastern University) describe this "analog analogue" of Grover's algorithm.[6] In their model, they consider an N-dimensional Hilbert space with a Hamiltonian that has only one nonzero eigenvalue, E. The task is to find the corresponding eigenvector, $|E\rangle$. They show that if one starts with an arbitrary normalized vector and adds an appropriate driving term to the Hamiltonian, after a time of order $\hbar\sqrt{N}/E$ the system will typically have a substantial amplitude in state $|E\rangle$.

Other extensions of Grover's algorithm apply it to more general problems. Boyer, Brassard, Høyer and Tapp consider the case in which the database holds c items that satisfy the desired condition.[4] If the number c is known in advance, one of the c items can be found with near certainty after $\pi\sqrt{N}/4\sqrt{c}$ iterations. (It is assumed that c is small compared to N.) For the case in which c is not known in advance, they provide a modified algorithm that achieves success, on average, after about $4\sqrt{N/c}$ iterations.

Brassard and coworkers[4] have also developed a quantum algorithm that can estimate the number of items c, using a combination of Grover's algorithm and techniques borrowed from Shor's factorization algorithm. The number of steps required is proportional to $\sqrt{N}$, with the details depending on the accuracy required and the value of c itself.

Christoph Dürr (University of Paris–South) and Høyer have devised a fast quantum algorithm for finding the smallest number in an unsorted table of numbers.[7] Brassard, Høyer and Tapp have devised a quantum algorithm that solves the "collision problem" faster than any possible classical algorithm.[8] The collision problem for a function F is to find two distinct integers m_0 and m_1 such that $F(m_0) = F(m_1)$. The speedup, for F acting on integers up to N, is from $N^{1/2}$ to $N^{1/3}$. This may seem like a small advance for an arcane problem, but the security of cryptographic protocols that use hashing functions depends on the difficulty of solving the collision problem.

Quantum telecomputation

Grover has used techniques similar to those of his search algorithm to develop fast algorithms for estimating the median and mean of populations of numbers to a specified accuracy. He has also shown how to further speed up the mean calculation by a constant factor by "quantum telecomputation," in which a number of quantum processors are run in parallel and linked by quantum entanglement (as occurs in Einstein–Podolsky–Rosen pairs of particles).[9]

Grover and—independently—Barbara M. Terhal (University of Amsterdam) and John A. Smolin (IBM Thomas J. Watson Research Center) have devised fast quantum algorithms for retrieving information from a database in a single quantum query of the database.[10] (The result was also implicit, but not emphasized, in a 1993 paper by Bernstein and Vazirani.) In Grover's search algorithm, each database query returns one bit of information relating to whether the sought item is present in a particular location. The single-query algorithms return one bit of information that answers a complicated question about many of the database's records. (For example: "Is the sought item present in the specified sequence of records?") These algorithms are of interest because classical algorithms must take at least $\log N$ database queries to perform what can be done in a single quantum query. The quantum algorithms do not provide faster searches because about N or more other quantum steps are needed before or after the database query, and large numbers of registers are needed. Nevertheless, they are of importance for showing another way in which quantum operations can outperform classical systems.

The variety of these applications suggests that, in Grover's search algorithm, quantum computer programmers may have the "killer app" that will drive demand for working devices.

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From Ethane to Benzene through a Supersonic Nozzle

> By exploiting a nonequilibrium reaction, Harvard chemists have found they can readily produce a high yield of unsaturated hydrocarbons starting with a hydrocarbon that is normally rather unreactive.

Organic chemists have long been challenged to find an easy way to break apart, or activate, the single bonds in methane so that they could use this very abundant compound as a building block to synthesize organic compounds. But methane is stubbornly unreactive. Recently, Dudley Herschbach and his colleagues at Harvard University found that they could use a catalytic supersonic nozzle to produce high yields of more reactive intermediaries starting with ethane—a cousin of methane.[1] The new method is tantalizing, although it has not yet worked with methane—and even if it were to, it would have to be scaled up from producing thimblefuls to churning out millions of barrels of hydrocarbons before it would be of interest to the petroleum industry. Short of that, the catalytic supersonic nozzle is of interest as a way to do nonequilibrium chemistry.

Methane (CH_4) and ethane (C_2H_6) are members of the alkane family (C_nH_{2n+2}). All family members feature single bonds between the carbon and hydrogen atoms that are relatively hard to break. The Harvard chemists start with a chamber of ethane gas at pressures around 85 torr and temperatures of about 1000 °C. The gas flows out of the chamber through a supersonic nozzle (essentially a pinhole) made from either nickel or molybdenum, elements known to catalyze the breakdown of ethane into radicals and hydrogen atoms. Mass spectroscopy done on the gases emerging from the nozzle indicates that 40% of the molecules in the ethane beam are converted to unsaturated higher hydrocarbons—that is, compounds with more carbon and relatively fewer hydrogen atoms and hence more double bonds.

From a number of indicators, the Harvard researchers attribute about 15% of the output to benzene—C_6H_6 in a configuration with alternating single and double bonds—although they do not have definitive proof that some other forms of C_6H_6 are not also being produced.

Herschbach feels that the supersonic nozzle gives greater yields of higher hydrocarbons than static techniques because the catalytic reaction in the nozzle is occurring far from equilibrium and thus is not constrained by equilibrium. He speculates that, during their 10 ms contact with the catalytic surface at the nozzle, the ethane molecules are transformed into radicals (C_2H_5 and CH_3) plus hydrogen atoms. If this decomposition were to occur in equilibrium, the products would react further to form just the thermodynamically most stable species: graphite on the surface and almost solely hydrogen molecules in the gas phase, with only traces of higher hydrocarbons. In the nozzle, however, the radical gets whisked away as soon as it is produced, becoming free to undergo reactions and form the higher hydrocarbons.

In the mass spectrum of the hydrocarbons C_nH_m produced in the supersonic nozzle, most of the peaks correspond to masses of molecules with equal numbers of carbon and hydrogen atoms, at least for low n; at higher n, the product molecules tend to have fewer hydrogens than carbons. Peaks for even numbers of carbons are higher than those for odd numbers of carbons. These results are so far unexplained.

Also unexplained is exactly what is going on within the nozzle: Do the hydrocarbons stem from the catalytic reaction at the nozzle? By exactly what reactions? Much work remains to be done—to explore, for example, the dependence of the products on the temperature, and on the material and size of the nozzle. The Harvard group is beginning to study the impact of the contact time of the gas with the nozzle.

Chemists have used long supersonic nozzles as a versatile tool for both collision and spectroscopic experiments. Richard Zare of Stanford University is now excited about this new application. "It allows the gas to have a really short residence time on a catalytic surface followed by a rapid quenching of the reaction, or isolation of its products." Several groups are pursuing such short-contact-time surface reactions using different approaches.[2]

Herschbach and his colleagues suggest in their paper that some researchers may want to make use of the molecular beam emerging from the supersonic nozzle, which contains high fluxes of such species as C_3H_3, C_4H_2 and C_4H_4. Some of the hydrocarbon radicals produced in their nozzle may also be of interest to astrophysicists who are trying to identify such molecules in the interstellar medium.[3]

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