Exchanging Insights on Quantum Behavior

Teller's Contributions to Condensed-Matter Physics

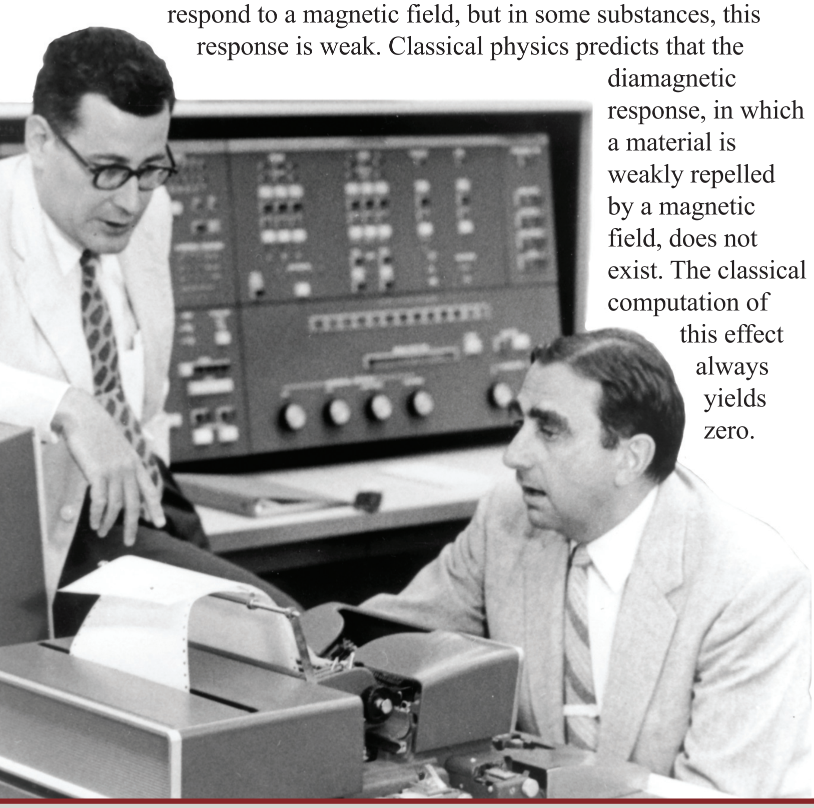
January 15, 2008, marks the 100th anniversary of Edward Teller's birth. This highlight is the third in a series of 10 honoring his life and contributions to science.

FOR Edward Teller, scientific research was a collaborative venture. He thrived on the exchange of ideas with other scientists. This approach allowed him to keep up to date on developments in many disciplines and helped him find connections between basic science research and potential applications.

Teller's work in condensed-matter physics shows the success of his collaborative style. Some of his research built on the ideas presented by his colleagues. In other projects, his insight led to a new understanding of atomic behavior in liquids, bulk solids, and material surfaces.

Solving a Quantum Puzzle

The discovery of quantum mechanics allowed scientists to unravel many of the paradoxes found in classical physics. One such paradox involved the magnetic properties of materials. All materials respond to a magnetic field, but in some substances, this response is weak. Classical physics predicts that the diamagnetic response, in which a material is weakly repelled by a magnetic field, does not exist. The classical computation of this effect always yields zero.



In 1930, Lev Landau, a physicist from Russia and friend of Teller's, applied quantum mechanics to address this paradox. Using the Schrödinger equation, Landau showed that an electron's orbit contributes to a material's diamagnetic susceptibility. He then computed this effect in a free-electron gas.

Werner Heisenberg, Teller's advisor from the University of Leipzig, suggested that Landau had not completely resolved the paradox and challenged Teller to explain the physical processes in the complex computations. The results, which appeared in the German journal *Zeitschrift für Physik* in 1931, presented a new way of looking at diamagnetism. In his study, Teller directly computed the electric current density induced by a magnetic field and showed how electron orbits at a material's outer edge contribute to Landau's solution. Physicists have since found this physical explanation to have several useful applications, for example, in determining the states of electrons in metals.

An Extended Model of Adsorption

Another important collaboration involved Stephen Brunauer, a fellow Hungarian and one of Teller's first students at George Washington University. Brunauer wanted to extend the Langmuir model—which describes the adsorption process for a layer of material one molecule thick—to multiple layers. An adsorbed material may change the overall behavior of an open surface, but it does not chemically react with the surface's molecular structure. For example, when condensation forms on glass, the water vapor molecules do not react with the glass, but rather form thin puddles of liquid phase. Understanding this adsorption process is important for applications involving catalysts.

Brunauer proposed that a surface's attractive force extends beyond the first layer of adsorbed material. Teller countered that the attraction would be too weak to hold multiple molecular layers. Instead, he proposed an adsorption model that accounts for the balance between an atom's simultaneous tendencies to attach and evaporate. To test Teller's hypothesis, Brunauer asked Paul Emmett, a physical chemist at the Department of Agriculture, to experimentally verify the model. The resulting Brunauer–Emmett–Teller equation of state, published in the *Journal of the American Chemical Society* in 1938, is still broadly applied in surface physics.

Harold Brown (left) and Edward Teller work on LARC, the Livermore Advanced Research Computer.

Teller and his wife, Mici, examine a model used to teach nuclear physics. In the background is the first page of the 1953 paper on the Metropolis algorithm.

How Polar Salts Respond to Light

In 1941, Teller led his colleagues Russell Lyddane and Robert Sachs to develop a rule describing the dielectric constant needed to explain how photons propagate in salts. Now called the Lyddane–Sachs–Teller relationship, this rule relates the very high and very low frequency-limiting values of a material's dielectric constant to the basic frequencies of salt's internal ion modes.

Published in *Physical Review*, the relationship can be used to explain insulating polar solids such as table salt, to determine the frequencies at which photons are reflected by the salt medium, and to study ferroelectric materials. The Lyddane–Sachs–Teller relationship is also analogous to nuclear vibrations—a connection that led Maurice Goldhaber and Teller to predict ubiquitous high-energy gamma-ray absorption resonances in nuclei.

Metropolis Accelerates Computational Science

Before Teller left Los Alamos National Laboratory to found Lawrence Livermore, he worked with Marshall Rosenbluth, his former student from the University of Chicago, to design the hydrogen bomb. The two physicists ran their equation-of-state calculations on the new Los Alamos computer being built by Nicholas Metropolis. At the time, scientists thought these calculations required an astronomical amount of effort, and a rigorous solution considering every possible microscopic state could not be computed for such a large system.

Teller and Rosenbluth realized that many points in phase space represent highly unlikely configurations, and random selection would thus be an ineffective sampling method. Instead, Teller imagined using a method that accepts or rejects a change in the system according to a probabilistic rule that mimics the system's dynamics.

Working with this idea, Rosenbluth designed an algorithm to select the samples. Teller's wife, Mici, began the computational work to encode the algorithm. Marshall's wife, Arianna, completed the code and carried out the calculations.

The result, now known as the Metropolis algorithm, has proven to be an extraordinary tool. Published in 1953 in *Journal of Chemical Physics*, this method has been used not only to calculate many properties of condensed matter but also to solve mathematical problems such as combinatorial optimization. In 2000, *Computing in Science and Engineering* chose Metropolis as one of the top 10 algorithms having the "greatest influence on the development and practice of science and engineering in the 20th century." The original 1953 paper has been referenced in more than 10,000 peer-reviewed articles, including a 1966 report on plasma equations of state by Livermore scientists Stephen Brush, Harry Sahlin, and Teller—their collaborator and mentor.

When Ernest O. Lawrence and Teller founded Lawrence Livermore in 1952, they encouraged Laboratory researchers to exchange ideas with their colleagues and those working in other disciplines. This tradition of collaborative, multidisciplinary science remains a hallmark of the research at Livermore.

—*Carolin Middleton*

Key Words: condensed-matter physics, Brunauer–Emmett–Teller equation of state, Edward Teller, Lyddane–Sachs–Teller relationship, Metropolis algorithm.

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