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Studying magnetic molecules with quantum Monte Carlo simulations LARRY ENGELHARDT — The term "magnetic molecules" refers to materials that contain a huge number ($\sim 10^{22}$) of identical molecules that do not interact with one another, and which each exhibit magnetic properties of a distinctly quantum character. While the theory to describe such systems has been established for many decades, the computational complexity of the subsequent calculations still provides a significant challenge today. The typical computational approach involves diagonalizing matrices, whose sizes grow *exponentially* with the size of the corresponding molecules. Because these matrices become extremely large, this approach cannot be applied to large molecules, even using the most advanced computers. We have avoided this obstacle by instead implementing a quantum Monte Carlo technique. We have used this technique to successfully model many recently synthesized magnetic molecules, even though, in some cases, the associated matrices would have been larger than 10^{18} rows by 10^{18} columns! Both the computational method and the subsequent analysis of physical systems will be summarized.

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