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Quantum simulation of thermodynamic and transport properties of the quark gluon plasma

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For quantum simulations of thermodynamic and transport properties of the quark-gluon plasma (QGP) within a unified approach, we combine Path Integral and Wigner (phase space) formulations of quantum mechanics. Thermodynamic properties of a strongly coupled QGP of constituent quasi-particles are studied by means of color path integral Monte-Carlo simulations (CPIMC). For the purpose of simulations we have presented the QGP partition function in the form of a color path integral with a new relativistic measure instead of the usual Gaussian one used in Feynman and Wiener path integrals. For the integration over the color degree of freedom we have developed a sampling procedure according to the SU(3) Haar measure. It is shown that this method is able to reproduce the available Lattice Quantum Chromodynamics (LQCD) data describing the deconfined phase of QGP. Canonically averaged two-time quantum operator correlation functions and related kinetic coefficients have been calculated according to the quantum Kubo formulas. In this approach, CPIMC is used not only for the calculation of thermodynamic functions, but also to provide equilibrium initial conditions (i.e. specific coordinates, momenta, spin, flavor and color of quasi-particle configurations) in order to accomplish generation of the color-phase-space trajectories as solutions of related dynamic differential equations. Correlation functions and kinetic coefficients are calculated as averages of related Weyl's symbols of dynamic operators along these trajectories. Using this approach we have calculated the diffusion coefficient and the shear viscosity in a good agreement with experimental data.

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Accurate first-principle calculations of the spectra of diatomic molecules in planetary atmospheres

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A summary will be given of various approaches that can be used to perform numerical Hartree-Fock method and many-body calculations on atoms and molecules. The theoretical approaches considered include the multi-configuration Hartree-Fock method and many-body perturbation theory. For light atoms and molecules, more than 98 percent of the correlation energy is due to pair excitations. Because molecules lack spherical symmetry, Schrodinger-like equations for molecules typically involve many more independent variables. While, the Hartree-Fock equations for atoms involve a single radial variable and the two-electron pair equation for atoms involve two radial variables, the Hartree-Fock equations for diatomic molecules involves two independent variables and the pair equation for diatomic molecules involve five independent variables. To deal with these problems of higher-dimensionality, my mathematical collaborators and I have developed numerical methods for dividing the variable space into smaller sub-regions in which the equations can be solved independently. This domain decomposition theory is described and numerical results are given for Hartree-Fock calculations for diatomic molecules and for numerical solutions of the first-order pair equations which can be used to evaluate the Goldstone diagrams that arise in many-body calculations of molecular spectra. The goal of our calculations is to describe the energy of two helium atoms approaching each other in a cold atomic collision and to obtain the spectral fingerprints of CO and OH molecules in planetary atmospheres.

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