51 Computational quantum mechanics

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Description

This project is part of an ongoing (over the last 18 years) large basic research program in quantum-mechanical calculations of systems with many interacting particles. The systems we study include properties of nuclei and neutron stars, atomic physics systems such as Bose-Einstein condensation of dilute atomic gases and systems of interest for solid state and nanotechnology. To study these systems, we have used several calculational methods and have developed large codes which all are highly parallelized and run easily on the national infrastructure. The methods we have specialized in are so-called Monte Carlo approaches (diffusion and variational Monte Carlo for quantum mechanical systems), large-scale diagonalization methods, solution of time-dependent partial differential equations and so-called coupled cluster methods.

The CPU-time that we apply for is devoted to production calculations and basic developments of our algorithms. The project, with continuous support from NOTUR over many years, has resulted in almost 100 scientific publications in international journals with peer-review. The scientific output is not expected to diminish.

Results

The complex nature of the nuclear forces among protons and neutrons generates a broad range and diversity of nuclear phenomena. Developing a comprehensive description of nuclei and their reactions represents one of the great intellectual opportunities for physics. As nuclear physicists have seen during the past 10 years, success will require theoretical and experimental investigations of isotopes with unusual neutron-to-proton ratios. Such nuclei, which are typically not found on Earth, are called exotic or rare.

The collaboration between the Oslo group and CMA, Oak Ridge National Laboratory, USA, and Michigan State University, USA, has resulted in several papers on ab initio studies of nuclei. A main emphasis is put on the coupled cluster method and recent results now allow us to perform ab initio calculations of both stable and unstable nuclei. We have developed a formalism which allows for a complex single-particle basis that includes bound, resonant and non-resonant continuum states. Our present codes can treat a single-basis which includes almost 3000 single-particle states. Furthermore, ORNLs and CMAs Gaute Hagen, together with David Dean, ORNL and adjunct professor at CMA, and Thomas Papenbrock at ORNL, have included the calculation of triples correlations and three-body forces in the coupled-cluster formalism. These calculations reproduce other benchmark calculations of few-body systems. This represents a major breakthrough

for ab initio calculations of systems with many interacting particles in nuclear physics, in particular since the experimental programs are pushing the limits of stability for nuclear matter. and hold great promise for ab initio calculations of heavier nuclei. The inclusion of three-body forces and pertinent effective interactions with a complex single-particle basis will allow us to address several important questions in nuclear many-body theory.

Publications

Scientific journals with peer review only 2006-2007 (approx. last 24 months):

[1] Gorska, M.; Grawe, H.; Banu, A.; Burger, A.; Doornenbal, P.; Gerl, J,; Hjorth-Jensen, Morten; Hübel, H.; Nowacki, F.; Otsuka, Takahuro; et al.. Nuclear structure far off stability - New results from RISING. Journal of Physics: Conference Series 2006;49:59-64

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[4] Hagen, G; Hjorth-Jensen, Morten; Vaagen, JS. State-dependent interactions for the Gamow shell model. Journal of Physics G. Nuclear and Particle Physics 2005;31:S1337-S1348

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[8] Leske, J; Speidel, KH; Schielke, S; Gerber, J; Maier-Komor, P; Engeland, Torgeir; Hjorth-Jensen, Morten. Experimental g factor and B(E2) value of the 4(1)(+) state in Coulomb-excited Zn-66 compared to shell-model predictions. Physical Review C, Nuclear Physics 2006;73

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[11] M.P. Kartamyshev, T. Engeland, M. Hjorth-Jensen, and E.Osnes, Physical Review C 76, 024313 (2007)

[12] S. Kvaal, M. Hjorth-Jensen, and H. Møll Nilsen, Physical Review B 76, References_55: 085421 (2007)

[13] Algin, E; Schiller, A; Voinov, A; Agvaanluvsan, U; Belgya, T; Bernstein, LA; Brune, CR; Chankova, Rosita; Garrett, PE; Grimes, SM; Guttormsen, Magne Sveen; Hjorth-Jensen, Morten; Hornish, MJ; Johnson, CW; Massey, T; Mitchell, GE; Rekstad, John Bernhard; Siem, Sunniva; Younes, W., Physics of Atomic Nuclei 70, 1634 (2007)

[14] Hagen, Gaute; Dean, David J.; Hjorth-Jensen, Morten; Papenbrock, Thomas. Complex coupled-cluster approach to an ab-initio description of open quantum systems. Physics Letters B 656, 169-173 (2007)

[15] Hagen, Gaute Dean, David J., Hjorth-Jensen, Morten, Papenbrock, Thomas, Schwenk, Achim, Physical Review C 76 (2007)

[16] Vaman, C.; Andreoiu, C.; Bazin, D.; Becerril, A.; Brown, B.A.; Campbell, C. M.; Chester, A.; Cook, J.M.; Dinca, D.C.; Gade, A.; Galaviz, D.; Glasmacher, T.; Hjorth-Jensen, Morten; Horoi, M.; Miller, D.; Moeller, V.; Mueller, W.F.; Schiller, A.; Starosta, K.; Stolz, A.; Terry, J.R.; Volya, A.; Zelevinsky, V.; Zwahlen, H., Physical Review Letters 99, 162501 (2007)

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Ph.D. dissertation:

[18] Eirik Ovrum. *Geometry of Entanglement and Quantum Simulators*. Supervisors Morten Hjorth-Jensen and Jon Magne Leinaas. 1 June 2007

Master degree theses:

[19] Espen-Flage Larsen. *Numerical studies of quantum dots*. Supervisor Morten Hjorth-Jensen. June 2006

[20] Joachim Berdahl Haga. *Bose-Einstein Condensates: Numerical solution of the Gross-Pitaevskii equation using finite elements*. Supervisor Morten Hjorth-Jensen. June 2006

[21] Jon Thonstad. *Modified URCA processes in neutron stars*. Supervisor Morten Hjorth-Jensen. June 2007

[22] Sutharsan Amurgiam. *Neutrino bremsstrahlung processes in neutron stars*. Supervisor Morten Hjorth-Jensen. June 2007

[23] Gustav Ragnar Jansen. *Studies of Hypernuclei*. Supervisor Morten Hjorth-Jensen. June 2008

[24] Ole Petter Harbitz. *Nuclear structure around* $A = 16$. Supervisors Torgeir Engeland and Morten Hjorth-Jensen. June 2008

Popular science papers:

[25] Hjorth-Jensen, Morten, META 1/2007, 18-19 (2007)

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