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Strongly Correlated Systems “Lendület” research group:

Örs Legeza, Imre Hagymási, Gergely Barcza, Szilárd Szalay, Miklós Werner, Kornél Kapás, Ádám Ganyecz, Mihály Máté, András Olasz, Andor Menczer, Rohit Babar, Péter Nyári, Szabolcs Földes, Patrik Penc, Jenő Sólyom, Tamás Mosoni

In this year we have continued our research on various strongly correlated systems using the *Density Matrix Renormalization Group* (DMRG) method and *Matrix Product State* (MPS) based algorithms. We have wide range international collaborations with more than twenty institutes around the world, also together with industrial partners such as NVIDIA, SandboxAQ, RiverLane Ltd, and Furukawa Electric, resulting in fifteen research articles in high rank international journals, and six preprints. We have organized two international workshops, in the Insititute for Advanced Study at the Technische Universität München and AIME2024 in Budapest. We have given some thirtyfive talks on different conferences and seminars, and we have presented six posters. We have applied our scientific software (Budapest QC-DMRG program package) to various spin and electron systems, which have been used with great success in numerous research institutes and universities around the world, for, e.g., simulating material properties of solid state systems or molecules, or for the quantum simulation of the information technology itself. As will be presented below, among many others, we have examined strongly correlated electrons in magnetic materials in several quantum phases, identified exotic quantum phases of matter, investigated time dependent phenomena, studied entanglement in two-nucleon systems, and identified classical and quantum correlations in molecules, playing important role in chemical compounds. We have also presented detailed mathematical analysis of various concepts in quantum entanglement theory of qubits and fermions, and dynamics of open quantum systems. Here we summarize only selected results due to length restrictions.

Condensed matter theory. — We studied the phase diagram of the antiferromagnetic J_1-J_2 Heisenberg model on the pyrochlore lattice with S=1 spins at zero and finite temperatures. We used a combination of complementary state-of-the-art quantum many-body approaches such as DMRG, density-matrix purification and pseudo-Majorana functional renormalization group (PMFRG). We presented an efficient approach to preserve the applicability of the PMFRG for spin-1 systems at finite temperatures despite the inevitable presence of unphysical spin states. The good performance of our methods was first demonstrated for the nearest-neighbor pyrochlore Heisenberg model, where the finite temperature behavior of the specific heat and uniform susceptibility showed excellent agreement within PMFRG and density-matrix purification. Including an antiferromagnetic second neighbor coupling, we found that the non-magnetic ground-state phase of the nearest neighbor model extended up to $J_2/J_1 \sim 0.02$ within DMRG, beyond which magnetic k=0 long-range order sets in. Our PMFRG calculations found the phase transition in a similar regime $J_2/J_1 \sim 0.035(8)$ which, together with the DMRG result, provided a strong argument for the existence of a small but finite non-magnetic ground-state phase in the spin-1 pyrochlore Heisenberg model.

We also presented a hybrid numerical approach to simulate quantum many-body problems on two spatial dimensional quantum lattice models via the non-Abelian ab initio version of the DMRG method on state-of-the-art high-performance computing infrastructures. We

demonstrated that for the two-dimensional spinless fermion model and for the Hubbard model on torus geometry, altogether several orders of magnitude in computational time could be saved by performing calculations on an optimized basis and by utilizing hybrid CPU-multiGPU parallelization. At least an order of magnitude reduction in computational complexity resulted from mode optimization, while a further order of reduction in wall time was achieved by massive parallelization. Our results were measured directly in the number of floating point operations and seconds. A detailed scaling analysis of the obtained performance as a function of matrix ranks and as a function of system size up to 12x12 lattice topology was discussed. Our CPU-multiGPU model also tremendously accelerated the calculation of the one- and two-particle reduced density matrices, which could be used to construct various order parameters and trace quantum phase transitions with high fidelity.

The collective tunneling of a Wigner necklace—a crystal-like state of a small number of strongly interacting electrons confined to a suspended nanotube and subject to a double-well potential—was theoretically analyzed as well, and compared with experiments. Density matrix renormalization group computations, exact diagonalization, and instanton theory provided a consistent description of this very strongly interacting system, and showed good agreement with experiments. Experimentally extracted and theoretically computed tunneling amplitudes exhibited a scaling collapse. Collective quantum fluctuations renormalized the tunneling, and substantially enhanced it as the number of electrons increased.

We also studied the information propagation in the one-dimensional infinite temperature Hubbard model with a dissipative particle sink at the end of a semi-infinite chain. In the strongly interacting limit the two-site mutual information and the operator entanglement entropy exhibited a rich structure with two propagating information fronts and superimposed interference fringes. A classical reversible cellular automaton model quantitatively captured the transport and the slow, classical part of the correlations but failed to describe the rapidly propagating information jet. The fast quantum jet resembled coherent free particle propagation, with the accompanying long-ranged interference fringes that were exponentially damped by short-ranged spin correlations in the many-body background.

Parafermions are anyons with the potential for realizing nonlocal qubits that are resilient to local perturbations. Compared with Majorana zero modes, braiding of parafermions implements an extended set of topologically protected quantum gates. This, however, comes at the price that parafermionic zero modes cannot be realized in the absence of strong interactions, posing a challenge for their theoretical depiction. We constructed a simple lattice model for interacting spinful electrons with parafermionic zero-energy modes. By DMRG calculations we identified a broad range of parameters with well-localized zero modes, whose parafermionic nature is substantiated by their unique periodic Josephson spectrum.

Nuclear physics. — The recently proposed combination of the valence-space in-medium similarity renormalization group (VS-IMSRG) with the DMRG offers a scalable and flexible many-body approach for strongly correlated open-shell nuclei. We used the VS-DMRG to investigate the low-lying spectroscopy of N = 50 isotones, which are characteristic for their transition between single-particle and collective excitations. We also studied electromagnetic transitions and showed the advantage of the VS-DMRG to capture the underlying physics more efficiently, with significantly improved convergence compared to state-of-the-art shell-model truncations. Combined with an analysis of quantum information measures, this further established the VS-DMRG as a valuable method for ab initio calculations of nuclei.

We also explored the entanglement and correlation in two-nucleon systems using isospin formalism. With the help of Slater decomposition, we derived analytical expressions for various entanglement measures. Specifically, we analyzed the one- and two-mode entropies, mutual informations, and a basis-independent characteristic known as the one-body entanglement entropy. To understand the impact of pairing, we consider interactions involving isovector and isoscalar L=0 pairing terms. Our findings showed that certain pairing interactions can maximize one-body entanglement entropy of ground states when both total angular momentum and total isospin have zero projections. We provided numerical examples for the sd shell and explore the mutual informations in *LS* coupled and *jj* coupled single-particle bases. We found that the shell structure and angular momentum coupling significantly impact the measures of entanglement. We outlined the implications of conserving angular momentum and isospin on one-mode entropies, irrespective of particle number.

Quantum Chemistry. — We reported cutting edge performance results on a single node hybrid CPU-multi GPU implementation of the spin adapted ab initio DMRG method on current state-of-the-art NVIDIA DGX-H100 architectures. We evaluated the performance of the DMRG electronic structure calculations for the active compounds of the FeMoco and cytochrome P450 (CYP) enzymes with complete active space (CAS) sizes of up to 113 electrons in 76 orbitals [CAS(113, 76)] and 63 electrons in 58 orbitals [CAS(63, 58)], respectively. We achieved 246 teraFLOPS of sustained performance, an improvement of more than 2.5-times compared to the performance achieved on the DGX-A100 architectures and an 80-times acceleration compared to an OpenMP parallelized implementation on a 128-core CPU architecture. Our work highlighted the ability of tensor network algorithms to efficiently utilize high-performance GPU hardware and shows that the combination of tensor networks with modern large-scale GPU accelerators can pave the way towards solving some of the most challenging problems in quantum chemistry and beyond.

Heavy atom compounds represent a challenge for computational chemistry due to the need for simultaneous treatment of relativistic and correlation effects. Often such systems also exhibit strong correlation, which hampers the application of perturbation theory or single-reference coupled cluster (CC) methods. As a viable alternative, we have proposed externally correcting the CC method using the DMRG wave functions, yielding the DMRG-tailored CC method. Earlier we reported a first implementation of this method in the relativistic context, which was restricted to molecules with real double group symmetry. Now we presented a fully general implementation of the method, covering complex and quaternion double groups as well. The 4c-TCC method thus became applicable to polyatomic molecules, including heavy atoms. For the assessment of the method, we performed calculations of the chiral uranium compound NUHFI, which was previously studied in the context of the enhancement of parity violation effects. In particular, we performed calculations of a cut of the potential energy surface of this molecule along the stretching of the N–U bond, where the system exhibits strong multireference character. Since there were no experimental data for NUHFI, we performed also an analogous study of the (more symmetric) NUF_3 molecule, where the vibrational frequency of the N–U bond can be compared with spectroscopic data.

Material science. — Color centers in hexagonal boron nitride (hBN) have attracted considerable attention due to their remarkable optical properties enabling robust room temperature photonics and quantum optics applications in the visible spectral range. On the other hand, identification of the microscopic origin of color centers in hBN has turned out to

be a great challenge that hinders the in-depth theoretical characterization, on-demand fabrication, and development of integrated photonic devices. This is also true for the blue emitter, which is a result of irradiation damage in hBN, emitting at 436 nm wavelength with desirable properties. We proposed the negatively charged nitrogen split interstitial defect in hBN as a plausible microscopic model for the blue emitter. To this end, we carried out a comprehensive first-principles theoretical study of the nitrogen interstitial. We carefully analyzed the accuracy of first-principles methods and showed that the commonly used HSE hybrid exchange–correlation functional fails to describe the electronic structure of this defect. Using the generalized Koopman's theorem, we fine-tuned the functional and obtained a zero-phonon photoluminescence (ZPL) energy in the blue spectral range. We showed that the defect exhibits a high emission rate in the ZPL line and features a characteristic phonon side band that resembles the blue emitter's spectrum. Furthermore, we studied the electric field dependence of the ZPL and numerically showed that the defect exhibits a quadratic Stark shift that is perpendicular to plane electric fields, making the emitter insensitive to electric field fluctuations in the first order. We emphasized the need for assessing the accuracy of common first-principles methods in hBN and exemplified a workaround methodology. Furthermore, our work is a step towards understanding the structure of the blue emitter and utilizing it in photonics applications.

The recently discovered B centers in hBn show promise for integration in scalable quantum technologies thanks to site-specific defect generation and a reproducible wavelength. We employed spectral hole burning spectroscopy and resonant polarization measurements to observe nearly coherent hBN quantum emitters, both as singles and in ensembles, with three discrete polarization axes indicative of a C_{2v} symmetry defect. Our results constituted an important milestone toward the implementation of hBN quantum emitters in integrated quantum photonics.

Point defect qubits in semiconductors have demonstrated their outstanding capabilities for high spatial resolution sensing generating broad multidisciplinary interest. Hexagonal boron nitride hosting point defect qubits have recently opened up new horizons for quantum sensing by implementing sensing foils. The sensitivity of point defect sensors in hBN is currently limited by the linewidth of the magnetic resonance signal, which is broadened due to strong hyperfine couplings. We reported on a vacancy-related spin qubit with an inherently low symmetry configuration, the VB2 center, giving rise to a reduced magnetic resonance linewidth at zero magnetic fields. The VB2 center is also equipped with a classical memory that can be utilized for storing population information. Using scanning transmission electron microscopy imaging, we confirmed the existence of the VB2 configuration in free-standing monolayer hBN.

Algorithmic aspects. — Tensor network methods provide a powerful way to simulate quantum many-body wavefunctions, but for large systems it is essential to exploit the freedom to rotate the underlying single particle modes. Previous low-cost methods for doing so are limited to nearest-neighbour two-orbital rotations, and fail to produce a stationary point on the fixed-rank MPS manifold times the unitary group, instead exhibiting undesirable fluctuations. We presented a new approach that overcomes this deficiency and jointly optimizes over the MPS manifold and the full unitary group, via macro-steps consisting of a carefully constructed sequence of two-qubit operations including swap gates controlled permutations. The minimization of a global quantity, the block entropy area, guarantees that

the method fulfills all criteria with respect to partial derivatives. Large scale DMRG simulations of strongly correlated molecular systems and two-dimensional fermionic lattice models demonstrated monotone convergence with respect to macro-steps, simultaneously achieving low energy and low entanglement.

We theoretically derived and validated with large scale simulations a remarkably accurate power law scaling of errors for the restricted active space DMRG (DMRG-RAS) method in electronic structure calculations. This yields a new extrapolation method, DMRG-RAS-X, which reaches chemical accuracy for strongly correlated systems such as the chromium dimer, dicarbon up to a large cc-pVQZ basis and even a large chemical complex such as the FeMoco with significantly lower computational demands than those of previous methods. The method is free of empirical parameters, performed robustly and reliably in all examples we tested, and has the potential to become a vital alternative method for electronic structure calculations in quantum chemistry and more generally for the computation of strong correlations in nuclear and condensed matter physics.

We also introduced novel algorithmic solutions for hybrid CPU-multiGPU tensor network state algorithms utilizing non-Abelian symmetries building on AI-motivated state-of-the-art hardware and software technologies. Furthermore, benchmarks up to CAS(113, 76) on Hilbert space dimensions up to 2.88×10^{36} demonstrated the utilization of NVIDIA's highly specialized AI accelerators via NVIDIA Tensor Cores, leading to performance around 115 TFLOPS on a single node supplied with eight NVIDIA A100 devices. In comparison to strict U(1) implementations with matching accuracy, our solution had an estimated effective performance of 300-500 TFLOPS, which emphasized the mutual need for both algorithmic and technological developments to push current frontiers on classical computation.