Dynamical mean field solution of the Bose-Hubbard model

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Modifying the recently proposed bosonic dynamical mean field theory (B-DMFT) for bosonic lattice models to avoid double counting of kinetic energies we find stable solutions to the B-DMFT equations and remarkable agreement with exact results from lattice Monte Carlo calculations. To solve the B-DMFT equations we present a new continuous-time Monte Carlo method for bosonic impurity models based on a diagrammatic expansion in the hybridization and condensate coupling. Applying the method to the three-dimensional Bose Hubbard model we obtain phase boundaries with less than 2% deviation from the exact result, which makes B-DMFT an ideal method to study the phase diagram of bosonic optical lattice systems. The solver is readily generalized to bosonic mixtures, spinful bosons, and Bose-Fermi mixtures.
We have demonstrated that quantized Berry phases can be used as a new tool for exploring gapped systems which do not exhibit symmetry breaking. Such a new approach is an alternative to conventional correlation functions. We investigate two spin-gap phases of the orthogonal dimer model. When the ratio of the competing exchange couplings is varied, the plaquette-singlet phase was found by Koga and Kawakami, between the dimer and magnetically ordered phases. Using $\mathbb{Z}_2$ Berry phase as local order parameter, we have successfully characterized the dimer and plaquette singlet phases.
Quantum Phase Transition of 4He in Nanoporous Gelsil Glass

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In experiments on 4He on nanoporous Gelsil glass with average pore diameter of 2.5 nm a suppression of the $\lambda$- transition under pressurization has been observed. The novel feature of this suppression with respect to similar effects in other porous media observed in the past, Vycor glass for example, is that for a pressure of about 3.4 MPa the superfluid transition decreases to zero Kelvin. We argue that this system indeed exhibits quantum critical phenomena. The mapping of the effective model of the system, the 3D quantum rotor model, to a (3+1)D classical XY model yields a phase boundary between the superfluid and the normal fluid regime of the form $p_c(0) - p_c(T) \sim T^2$. This is in remarkable agreement with experiment as are also the expressions we obtain for the superfluid density as a function of pressure in the limit of zero temperature. It is known that disorder and particle-hole symmetry breaking are relevant perturbations and would alter the universality class. However, we show that in the accessible temperature range the perturbations do not yield sizable effects and thus establish the validity of the (3+1)D XY model picture. Furthermore we present an argument that explains why quantum phenomena have not been observed in 4He filled in porous media with pore sizes larger than Gelsil.
effective pair potentials using an \textit{ab initio} variational approach

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We used a variational approach adapted to a quantum molecular dynamics code to determine the best reference potential for warm dense aluminum. This \textit{ab initio} variational approach was based on the Gibbs-Bogolyubov inequality. We used many-body reference systems interacting through hard-sphere and inverse-power-law potentials, among which the Coulomb potential was a particular case defining the classical one-component plasma model. Comparisons with full quantum molecular dynamics simulations are shown. This work is intended to be a demonstration of feasibility of extracting analytical potentials from first-principles using quantum molecular dynamics simulations.
Reducing the cost of tensor networks algorithms using variational Monte Carlo

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Quantum many-body problems are notoriously difficult to solve, primarily because the information contained in a wave-function grows exponentially in the number of particles and/or spatial modes. Fortunately, it is possible to represent certain states, such as the ground states of typical Hamiltonians, efficiently and accurately using a network of tensors with a greatly reduced amount of information. Another approach is that of Monte Carlo, where the most important configurations are sampled directly; however, this approach becomes very inefficient when encountering the sign problem. Combining these two techniques can potentially reduce the cost of the tensor network contractions while still providing a sign-problem-free method.

For example, a tensor network ansatz called the MERA can efficiently represent critical systems. We present our progress on using variational Monte Carlo with the 1D MERA, which formally reduces the cost from $O(\chi^8)$ for an exact approach to $O(\chi^4)$ per Monte Carlo sample, where $\chi$ is a parameter that monotonically increases with the entanglement in the system. We discuss the advantages and disadvantages of this scheme, analyzing its performance and accuracy. Finally, we will provide a brief outlook on possible applications of Monte Carlo sampling to 2D tensor networks, where even greater reductions in the computational cost may be possible.
Growth of spin correlation owing to quantum charge fluctuation

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We study a mechanism in which a quantum charge fluctuation on the A-site mediates the spin correlation among the spins on the B-sites. We consider simple charge transfer models for it and study the temperature dependence of the spin correlation among the spins on the B-sites, and found peculiar non-monotonic dependences. We will discuss their physical mechanisms.
Melting temperature for the Mott insulator-like phase in the Bose-Hubbard model

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The Bose-Hubbard model describes ultracold atoms in periodic potentials such as optical or magnetic lattices. At zero temperature, the Mott insulator phase with an integer for the average number of particles is defined by zero compressibility of the system

$$\kappa = \frac{\partial \langle \hat{n} \rangle}{\partial \mu} = 0$$

For ultracold atoms a Mott insulator-like phase has been introduced for which the average number of particles is slightly different from an integer. Different values $T \approx 0.2 \; U, 0.1 \; U$ and $0.06 \; U$ (based on a truncated number-state basis) have been reported as the melting temperature for the Mott insulator-like phase, where $U$ is the onsite interaction. The melting temperature of $0.06 \; U$ for the Mott insulator-like phase in the experiment of M. Greiner et. al. (Nature 415 39, 2002) is about $4 \; nK$.

We study ultracold atoms in the grand canonical ensemble. We perform accurate numerical calculations based on the exact diagonalisation in a truncated number-state basis. Using derivatives of the compressibility, we find that the melting temperature is close to $0.06 \; U$. 
Nonadiabatic transition between Floquet states

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A frequency of the Rabi oscillation driven by a periodic external field varies with parameters, e.g., frequency and amplitude, of the external field, and it becomes zero at some points of the parameters, which is called "coherent destruction of tunneling". This phenomenon is understood as a degeneracy of the Floquet quasienergies as a function of the parameters. We analyze asymmetrically periodically driven systems from the symmetrical point of view, and derive necessary conditions for the degeneracy of the quasienergies. We demonstrate the gap opening in the quasienergy spectrum. Moreover, an adiabatic transition between the Floquet states is demonstrated and the transition probability is analyzed in the analogy to the Landau-Zener-Stückelberg problem.
A point defect in graphene

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Defects in graphene give rise to zero modes that are often related to the sharp peak in the local density of states near the defect site. Here we solved all zero modes induced by a single defect in the finite-size graphene and show that their contributions to the local density of states vanish in the thermodynamic limit. Instead, lots of resonant states emerge at low energies and eventually lead to a power-law singularity in the local density of states. Our findings show that the impurity problem in graphene should be treated as a collective phenomenon rather than a single impurity state.
Nonequilibrium transport properties in an open quantum dot: exact many-electron scattering states

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We construct the exact two-electron scattering state in an open quantum dot. It is striking that the scattering state contains two-body bound states induced by the Coulomb interaction. The bound state describes a scattering process in which the set of momenta is not conserved and hence, it is not in the form of a Bethe eigenstate. Using this, we discuss the following two topics. 1. Nonequilibrium current-voltage characteristics in the interacting resonant level model (Ref. A. Nishino, T. Imamura and N. Hatano, Phys. Rev. Lett. 102, 146803 (2009).) 2. Entanglement generation in the Anderson model (Ref. T. Imamura, A. Nishino and N. Hatano, Phys. Rev. B. 80, 245323 (2009).) This is a joint work with Akinori Nishino and Naomichi Hatano.
Control of quantum transport in a spin chain by periodic driving

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Simple many-body Hamiltonian, such as Heisenberg and Hubbard models, include a hopping term. If such a system is driven by a spatially-linear oscillating field, the hopping strength takes an effective renormalized value. In the high-frequency regime, the inter-site transport is completely suppressed under a certain condition, which is often called coherent destruction of tunnelling (CDT). There is another similar transport effect called Dynamical Localization (DL), which requires no restriction on frequency.

We demonstrate CDT and DL phenomena in a doubly-excited spin chain under an spatially-linear oscillating field. The phenomena act selectively on bound pairs of spins, relative to magnon-like scattering states. Thus, one can spatially separate a mixture of the two components into bound-pair and magnon wavepackets. We show how to control the relative direction and speed of transport of them in the DL regime.
Numerically exact calculation of low-energy spectrum in quantum systems

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We study low-energy spectrum of a hard-core boson model and the Hubbard model in one dimension. Via Grosso et al.’s method with a modified Lanczos algorithm, we obtain the low-energy spectrum of the models. To understand the nature of quantum phase transitions, the behavior of energy gap between the ground state and the excited state should be correctly interpreted. We find that the spontaneous symmetry breaking of the system is very important to understand the meaning of those many-particle energy gaps. Finite-size scaling of the gap at the Heisenberg point in the hard-core boson model gives the dynamic critical exponent, $z = 0.975 \pm 0.002$. We also compare the energy gap of the doped case with that of the half-filled case for the one-dimensional Hubbard model.
Real-space renormalization group for the transverse-field Ising model

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We have developed a framework of a real-space renormalization group for the transverse-field Ising model in one dimension. As the renormalized spin, we adopt the two lowest-lying eigenstates of the 4x4 matrix generated by the interacting pair of two neighboring spins of the original system. By an ingenious choice of the decomposition of the system into blocks of pairs of spins to preserve the symmetry, we succeeded in deriving the exact location of the critical point and the exact value of the critical exponent $\nu$. The method is further applied to the evaluation of additional critical exponents as well as the ground-state energy. Generalizations to other systems will also be discussed.
Controlling conductance statistics of quantum wires by driving ac fields

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We calculate the entire distribution of the conductance of a one-dimensional disordered quantum wire in the presence of a time-dependent field. Our calculations are based on Floquet theory and a scaling approach to localization. Effects of the applied ac field on the conductance statistics can be strong and in some cases dramatic, as in the high-frequency regime where the conductance distribution shows a sharp cut-off. In this frequency regime, the conductance is written as a product of a frequency-dependent term and a field-independent term, the latter containing the information on the disorder in the wire. We thus use the solution of the Mel’nikov equation for time-independent transport to calculate the conductance distribution at any degree of disorder. At lower frequencies, we find that the conductance distribution and the correlations of the transmission of Floquet modes are described by a solution of the Dorokhov-Mello-Pereyra-Kumar equation with an effective number of channels. Our theoretical results are verified numerically using a single-band Anderson Hamiltonian.
Nontrivial eigenvalues of the Liouvillian for an open quantum system

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In the present study, we will discuss whether the Liouville equation has more information than the Schrödinger equation in the case of infinite systems. It is known [1] that the Schrödinger equation can have discrete complex eigenvalues if the Hamiltonian $H$ represents an infinite system. We then naturally expect that the Liouvillian in the equation $i\hbar \frac{\partial \rho}{\partial t} = L \rho = z \rho$ also has complex eigenvalues \{z\}. We know that, if $H$ has eigenvalues \{E_n\}, $L$ has at least eigenvalues \{znm = E_n - E_m\}. If the system is infinite, $L$ can have unexpected complex eigenvalues besides \{E_n - E_m\}, which may describe approach to equilibrium.

We can obtain the Hamiltonian spectrum rigorously for an infinite system, using the Feshbach formalism [2]. We here also obtain the Liouvillian spectrum with the Feshbach formalism, and then compare the results to see the relation.

References
Since P.W. Anderson’s 1973 paper, the search for a resonating valence bond (RVB) states has been one of the recurrent themes in research on frustrated antiferromagnets. Quantum Dimer Model (QDM) proposed by Rokhsar and Kivelson exhibits crystalline order on the square lattice, except at RK point. On the point, a short ranged RVB state is realized. Recently Moessner and Sondhi have revealed that there is a truly short ranged RVB phase for a finite range of parameters on the triangular lattice. Furthermore, they have mapped the QDM to an Ising gauge theory.

Stimulated by these researches, we propose Extended QDM defined by the S=1 Hilbert spaces. We have succeeded in deriving a S=1 spin Hamiltonian which is completely dual with EQDM and described by local interactions. We regard locality with dual spin Hamiltonian as leading principle on expanding QDM. We have then revealed that EQDM contains the phase transitions (e.g. from columnar to herringbone) pointed out by Papanikolaou et al. as well as the usual QDM transitions. Furthermore, this model exhibits 3 degeneracy in a region. There exists a triple point. One exotic phase is governed by a hidden order and we recognize it as the mix state of quantum solid and liquid.
Ground-state properties of symmetric electron-hole quantum bilayers

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The ground-state properties of the symmetric electron-hole quantum bilayers with a neutralizing background and zero magnetic field are explored by including unequal density of layers. The quantum self-consistent mean-field approximation of Singwi, Tosi, Land and Sjölander (qSTLS) is used to study the intra layer (within a layer) and inter layer (between the layer) properties, such as pair-correlation functions, static structure factors, static local-field correction factors and static density susceptibility over a wide range of layer density parameter \( r_s \) and layer spacing \( d \). We find that the inclusion of unequal density brings a phase transition from charge density wave (CDW) to coupled Wigner crystal (WC) ground state at the close proximity of the layers. The results are compared with recent findings of the equal density effects in symmetric electron-hole quantum bilayers.
Phase transition on hyperbolic lattices analyzed by corner transfer matrix renormalization group

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Thermodynamic functions and the entanglement entropy of two-dimensional classical models on hyperbolic lattices are calculated by means of the corner transfer matrix renormalization group (CTMRG), a combination of the density matrix renormalization group (DMRG) and Baxter's corner transfer matrix formalism. Phase transitions observed for Ising, Potts, and clock models are mean-field like, and the correlation length is always finite, even at the transition temperature. In accordance with these facts, the entanglement entropy does not diverge. We discuss the origin of the mean-field behavior based on the matrix product structure of these hyperbolic lattice models. As a quantum analogue, we propose hyperbolic deformation for one-dimensional quantum spin chains.
High Temperature Thermodynamics of the Multiferroic \( \text{Ni}_3 \text{V}_2 \text{O}_8 \)

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The nickel vanadate \( \text{Ni}_3 \text{V}_2 \text{O}_8 \) is a much studied multiferroic material, which shows simultaneous ferroelectric and magnetic order at low temperatures.

The material itself is rather complex, with a 'Kagome staircase' structure of coupled layers, and with 6 magnetic \( \text{Ni}^{2+} \) \( \text{S}=1 \) ions per unit cell. Ab-initio LDA electronic structure calculations have estimated values of 10 different exchange constants, of which 5 appear to be dominant.

In the present work we use high-temperature expansions to compute the specific heat and susceptibility for a 5-parameter Heisenberg model of this material. The results are compared to experimental data to test the adequacy of the model, and to try to refine the values of the exchange parameters.
Role of scale free property in Wilson numerical renormalization group

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We discuss an essential mechanism of the energy scale controlling in Wilson numerical renormalization group (NRG) for the Kondo impurity problem. We show that the gapless free fermion part of Wilson's effective Hamiltonian with exponentially modulated hopping parameters has a scale free property; the bulk eigenstate is represented as a wave-packet, and its lattice translation generates the exponential dependence of energy scale. We also show that an edge state emerges in the lowest energy scale of the Wilson's Hamiltonian, which has not been emphasized so far. On the basis of the wave-packet representation, the low-energy spectrum of the Kondo model is revisited. A generalization for one-dimensional quantum systems is also discussed.
Classical phase transitions in topological quantum codes suffering loss

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Many proposals for quantum information processing are subject to detectable loss errors. We show that topological error correcting codes, which have very high thresholds against logical errors, are also extremely robust against losses.

Previous work (Wang, Preskill, Harrington, Raussendorf and others) has shown that the optimum thresholds for error correction in these codes are coincident with the Nishimori point of the Random Bond Ising model (RBIM) in 2D and its generalisations in 3D. Heuristic decoding algorithms based on Edmonds’ matching do remarkably well, attaining a substantial fraction of the critical value at the Nishimori point. We show that these heuristic decoders may be further improved by accounting for degeneracy in the form of an entropy-like term in the free-energy of the RBIM.

In the presence of losses, we present analytic results showing that the maximum loss rate is set by the percolation threshold in the corresponding lattice: for a 2D topological code (useful as a quantum memory), the maximum tolerable loss rate is the same as the bond percolation threshold on a square lattice of 50\%, whilst in 3D (useful for full quantum computation), the maximum tolerable loss rate is the bond percolation threshold on a simple cubic lattice, $\sim 24.9\%$.

Numerical simulations support these results, and show a remarkably graceful tradeoff between tolerable rates of loss and computational errors, allowing us to compute a phase diagram showing correctable regions of parameter space.
We numerically investigate electron transfers in graphene by Nelson's quantum stochastic mechanics. Attempts to apply graphene to nanodevices have recently drawn attention. In past theoretical studies of electron transfers, discussions are based on transfer integrals, Kubo formula, Green's functions, etc. In this paper, we present a new approach by using quantum stochastic mechanical simulations.

Quantum stochastic mechanics provide the quantum motion of electrons from their wave functions. The wave functions are obtained as the molecular orbitals from quantum chemical calculations using the linear combination of local atomic orbitals. The time evolution of the quantum stochastic process is given by Ito type stochastic differential equation. From the analysis of the electron motion, we calculate electron mobilities in graphene directly.

Finally, we point out some merits of quantum dynamics approaches. Stochastic mechanics with given wavefunctions enable us to simulate electron dynamics directly. For the drift velocity $v$ of the electron depends on the wave function $\psi$ according to

$$v \propto \Re (\nabla \psi / |\psi|) + \Im (\nabla \psi / |\psi|),$$

the nodes of the molecular orbital accelerate the electron motion. It is shown that not only the extensity of the electron distribution but also the shape of the molecular orbital plays the important role of the electron transfer.
Quantum fidelity and dynamical scar in chaotic billiard

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Recently the time-evolution of quantum states is seriously considered to clarify the dynamical behavior of electrons in two dimensional (2D) nanostructures. By computer simulation, we have numerically studied the time-evolution of the Gaussian wavepacket in the stadium billiard, which is the typical 2D chaotic nanostructure. In order to measure the robustness of the quantum states against the perturbation, we have also examined the quantum fidelity.

The quantum fidelity is evaluated as the square of the inner product between the time-evolving wavefunction in the original billiard system and the slightly distorted system with some impurities which is Gaussian potentials. Increasing the perturbation, it is also known that the fidelity has the transition from the perturbation theory regime to the Fermi-golden-rule regime, and to the Lyapunov regime in the 2D stadium billiard as the simpler quantum system. In simpler quantum systems, the decay rate of the fidelity in the Lyapunov regime become the classical maximum Lyapunov exponent of the system, however, it is suppressed in our result.

We have found the enhancement of the wavefunction around unstable periodic orbits during the time-evolution of the wavepacket in the stadium billiard. We shall call it the dynamical scar and it is similar to the scars in the stationary states of the chaotic billiard. It is also found that, when the dynamical scar is observed, the diffusion of the wavepacket in the billiard is suppressed and the decay rate of the fidelity in the Lyapunov regime is smaller than the classical maximum Lyapunov exponent.
An exactly solvable model for strongly correlated electron pairs

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We start from a Hamiltonian describing non-interacting fermions and add bosons to the model, with a Jaynes-Cummings-like interaction between the bosons and fermions. This model can be solved analytically. In the ground state, part of the electrons form bound pairs with opposite momentum and spin. As a consequence of the Pauli exclusion principle, the model also shows a gap in the kinetic energy of the fermions, but not in the spectrum of the full Hamiltonian.
Non-BCS superconductivity for underdoped cuprates by spin-vortex attraction

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Within a gauge approach to the \( t-J \) model, we propose a new, non-BCS mechanism of superconductivity for underdoped cuprates. The gluing force of the superconducting mechanism is an attraction between spin vortices on two different Néel sublattices, centered around the empty sites (holes), which can be described in terms of fermionic holons. The spin fluctuations are described by bosonic spinons with a gap originating also from the spin vortices. Due to the no-double occupation constraint, there is a gauge interaction between holon and spinon, through which the spin vortex attraction induces the formation of spin-singlet (RVB) spin pairs with a lowering of the spinon gap. Lowering the temperature there appear two crossover temperatures. At the higher crossover, a finite density of incoherent holon pairs are formed, and it is identified with the pseudogap temperature. At the lower crossover temperature, a finite density of incoherent spinon RVB pairs are formed, and it is identified with the appearance of the Nernst signal. The true superconducting transition occurs at a even lower temperature, via a 3D XY-type transition. The superconducting mechanism is not of BCS-type, and it involves a gain in kinetic energy (for spinons) coming from the spin interactions. The main features of this non-BCS description of superconductivity agree with the experimental results in underdoped cuprates, especially the contour plot of the Nernst signal.
Conductance of single DNA molecules: effects of decoherence

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The influence of decoherence and bonding on the linear conductance of single double-stranded DNA molecules is examined by fitting a phenomenological statistical model developed recently (Eur. Phys. J. B, 68, 237 (2009)) to experimental results. The DNA molecule itself is described by a tight-binding ladder model with parameters obtained from ab-initio calculations available in the literature. Sequence and length dependence of experimental conductance values provide a crucial test of the model.
Bose-liquid interpretation of a classical limit of the noncommutative quantum mechanics

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We briefly review the formalism of the 2D quantum mechanics on noncommutative spaces and outline some of its striking features as compared to the conventional QM. By virtue of functional methods we define the classical limit of a quantum particle on a noncommutative plane and derive the classical action (which turns out to be non-local) and equations of motion for this object. It is shown that there exists a map between these equations and the equations of motion of a fluid element of the inviscid Bose liquid. Some arguments of why it may not be a coincidence are given.