Stochastic gauge theory for quantum many-body problems

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Motivation

- N-particle, M-mode Hilbertspace growth as M^N, making first principles calculations in many-body quantum mechanics extremely challenging.
- This limitation can sometimes be overcome by stochastic phase space methods [1].
- Stochastic methods work better if "gauge" freedom is exploited [2].
- We develop gauge techniques for systems with long-range interactions.

Gauge-P Method

- Expresses the density matrix in a modified P-representation.
- Quantum correlations are represented by stochastic correlations in an ensemble of trajectories, allowing a massive reduction in basis size.
- Gauge techniques allow a tuning of the resulting stochastic equations of motion to reduce the sampling error.
- Method can easily be adapted to treat open quantum systems.

Phase space representation

- We define many-mode coherent states $|\boldsymbol{\alpha}\rangle$ with the crucial property $\hat{a}_n|\boldsymbol{\alpha}\rangle = \alpha_n|\boldsymbol{\alpha}\rangle$. $\hat{a}_n$ destroys a boson in the single particle mode $|n\rangle$.
- The density operator is expanded in terms of the many-mode Gauge-P representation

$$\hat{\rho} = \int d^{4M}\boldsymbol{\alpha} \int d^{4M}\boldsymbol{\beta} \int d^2\Omega \left[\Omega \frac{|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\beta}^*|}{\langle\boldsymbol{\beta}^*|\boldsymbol{\alpha}\rangle}\right] G(\boldsymbol{\alpha},\boldsymbol{\beta},\Omega). \quad (1)$$

- We wish to solve the quantum dynamics of the following many-body Hamiltonian from first principles:

$$\hat{H} = \sum_{nm}\left[\hat{a}_n^\dagger \tilde{\omega}_{nm}\hat{a}_m + \frac{1}{2}\hat{a}_n^\dagger\hat{a}_m^\dagger \tilde{W}_{nm}\hat{a}_n\hat{a}_m\right]. \quad (2)$$

Stochastic equations of motion

- We begin from a master-equation such like:

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \sum_j \frac{\kappa_j}{2}\left(2\hat{O}_j\hat{\rho}\,\hat{O}_j^\dagger - \hat{O}_j^\dagger\hat{O}_j\hat{\rho} - \hat{\rho}\,\hat{O}_j^\dagger\hat{O}_j\right), \quad (3)$$

including coupling to some baths via the operators $\hat{O}_j$.

- Inserting Eq. (1) into Eq. (3) we obtain an equation of motion for $G(\boldsymbol{\alpha},\boldsymbol{\beta},\Omega)$ of the Fokker-Planck type:

$$\frac{\partial G}{\partial t} = -\sum_j \frac{\partial}{\partial\gamma_j}A_j G + \frac{1}{2}\sum_{nj}\frac{\partial}{\partial\gamma_n}\frac{\partial}{\partial\gamma_j}D_{nj}G, \quad (4)$$

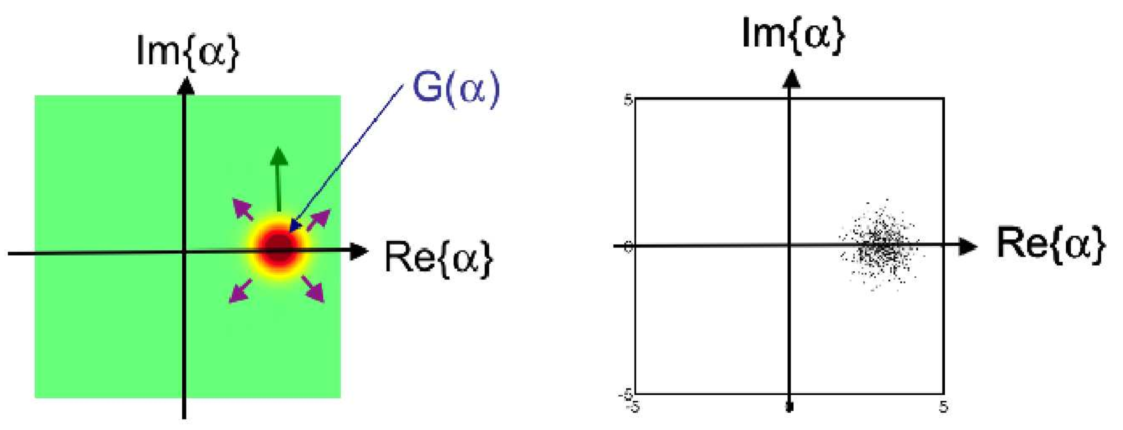
where we have introduced the notation $\boldsymbol{\gamma}^T = (\boldsymbol{\alpha}^T,\boldsymbol{\beta}^T,\Omega)$. The first term on the rhs. is called *drift* term, the second *diffusion* term.

- The solution of a Fokker-Planck equation (FPE) corresponds exactly to the solution of the stochastic differential equations (SDEs) [3]

$$d\gamma_n = A_n dt + \sum_j B_{nj}d\eta_j(t). \quad (5)$$

The matrix B is the "square-root" of the diffusion matrix $D = BB^T$.

- The γ_n is a stochastic wave function and the $d\eta_j(t)$ are *real* gaussian noises with correlations $\overline{d\eta_j(t)d\eta_k(t')} = \delta_{j,k}\delta(t-t')$.
- The distribution of the γ_n within an ensemble of trajectories reproduces the functional form of $G(\boldsymbol{\gamma},t)$:



(left) Exemplary $G(\boldsymbol{\gamma},t)$ for single mode, considering variable α only. (right) Corresponding distribution of α in the ensemble of trajectories.

Quantum field observables

- Using Eq. (1), we can write the stochastic correspondence of any normally ordered quantum expectation value:

$$\langle(a_n^\dagger)^p(a_m)^q\rangle = \overline{\Re\mathrm{e}[\,\Omega\beta^p\alpha^q]}/\overline{\Re\mathrm{e}[\Omega]}. \quad (6)$$

- $\overline{\cdots}$ denotes a stochastic average of trajectories. Due to the finite ensemble size the average has an error called the *sampling error*. It is usually well estimated by the standard deviation of the average.

Drift Gauges

- From Eq. (1) we have

$$f(\boldsymbol{\alpha},\boldsymbol{\beta},\Omega)\left[1 - \Omega\frac{\partial}{\partial\Omega}\right]\Lambda = 0, \quad \Lambda \equiv \Omega\frac{|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\beta}^*|}{\langle\boldsymbol{\beta}^*|\boldsymbol{\alpha}\rangle}. \quad (7)$$

- $f(\boldsymbol{\alpha},\boldsymbol{\beta},\Omega)$ is arbitrary function of $\boldsymbol{\gamma}$, which can thus be inserted into the FPE.
- It can be shown that this allows modifications of the drift terms of Eq. (5) without affecting the noise terms [2].
- Commonly for Bose-Einstein condensates:

$$i\frac{\partial\alpha}{\partial t} = \ldots g[\alpha\beta]\alpha \rightarrow i\frac{\partial\alpha}{\partial t} = \ldots g\Re\mathrm{e}[\alpha\beta]\alpha. \quad (8)$$

Diffusion gauges

- For B fulfilling $D = BB^T$, this is also true for $B' = BO$, where O is an arbitrary *complex orthogonal matrix* defined by $\mathbb{1} = OO^T$. O is called diffusion gauge.
- A useful simple *local* diffusion gauge is:

$$O = \begin{pmatrix} -\cosh a\mathbb{1} & -i\sinh a\mathbb{1} \\ -i\sinh a\mathbb{1} & \cosh a\mathbb{1}\end{pmatrix}. \quad (9)$$

- Diffusion gauges with $a > 0$ shift the noise from $\alpha\beta$ to α/β.
- The parameter a can be adjusted to minimize the sampling error at a time instant of interest.

Gauged equations of motion

- Using both types of gauges, the full stochastic equations of motion for the Hamiltonian Eq. (2) without any bath-coupling are:

$$d\gamma_n = i\left[\sum_l \omega_{nl}\gamma_l + \sum_l \gamma_n W_{nl}(n_l - m_l)\right] + \sqrt{i}\sum_{lp}\gamma_n S_{nl}O_{lp}d\eta_p, \quad 0 < n \le 2M \quad (10)$$

$$d\gamma_{2M+1} = d\Omega = \sqrt{i}\Omega\sum_{plk} d\eta_p O_{lp}S_{kl}m_k. \quad (11)$$

We used $\bar{\gamma} = (\boldsymbol{\beta}^T,\boldsymbol{\alpha}^T,\Omega)$, $n_k = \alpha_k\beta_k$ and have defined $2M\times 2M$ matrices

$$\omega = \begin{pmatrix}-\tilde{\omega} & 0\\ 0 & \tilde{\omega}\end{pmatrix},\quad W = \begin{pmatrix}-\tilde{W} & 0\\ 0 & \tilde{W}\end{pmatrix},\quad S = \begin{pmatrix}-i\sqrt{\tilde{W}} & 0\\ 0 & \sqrt{\tilde{W}}\end{pmatrix}. \quad (12)$$

- The function m_k parametrizes the drift gauge. We choose $m_k = \Im\mathrm{m}[n_k]$ to stabilize the equations.

Optimization of stochastic gauges

- We define a characteristic variance

$$\mathcal{V} = \frac{1}{2M}\sum_n^{2M}\mathrm{var}[\log|\Omega\gamma_n|], \quad (13)$$

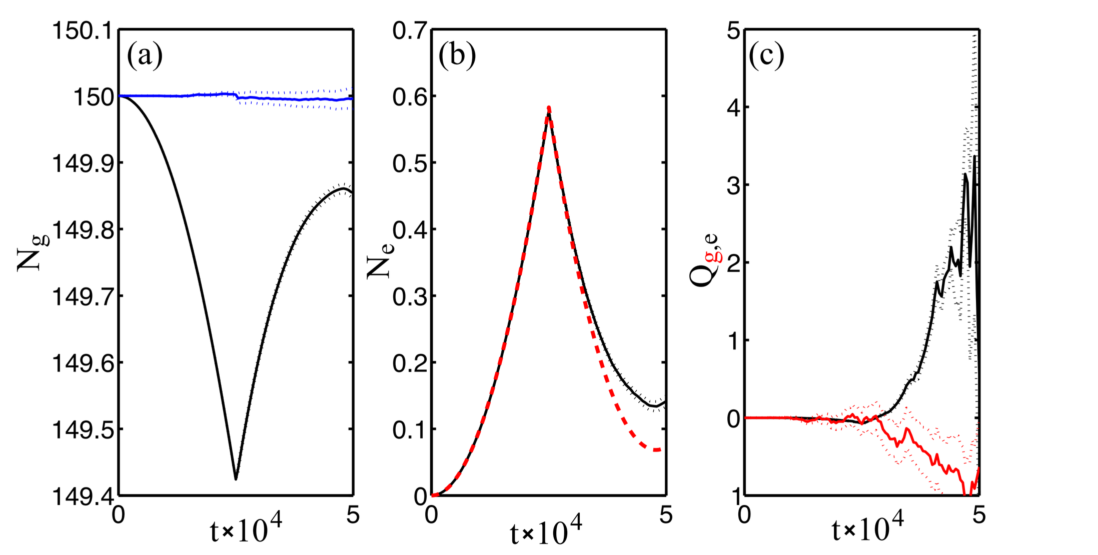
which must not get much larger than 10 to obtain a useful sampling error.

- Using stochastic calculus, we calculate the time evolution of $\mathcal{V}$ that follows from Eqs. (10) and (11). One obtains $\mathcal{V}(t, O, \tilde{W}, n(t=0))$.
- The expression allowed us to tune constant local diffusion gauges as in Eq. (9), by minimizing $\mathcal{V}$ with respect to a. This can yield an adaptive local diffusion gauge $a(t)$.
- It also could be used to devise fully nonlocal diffusion gauges with more complicated forms of O. So far these do not seem to be better than local gauges.

Applications (work in progress)

Echo sequences in strongly interacting Rydberg Gases

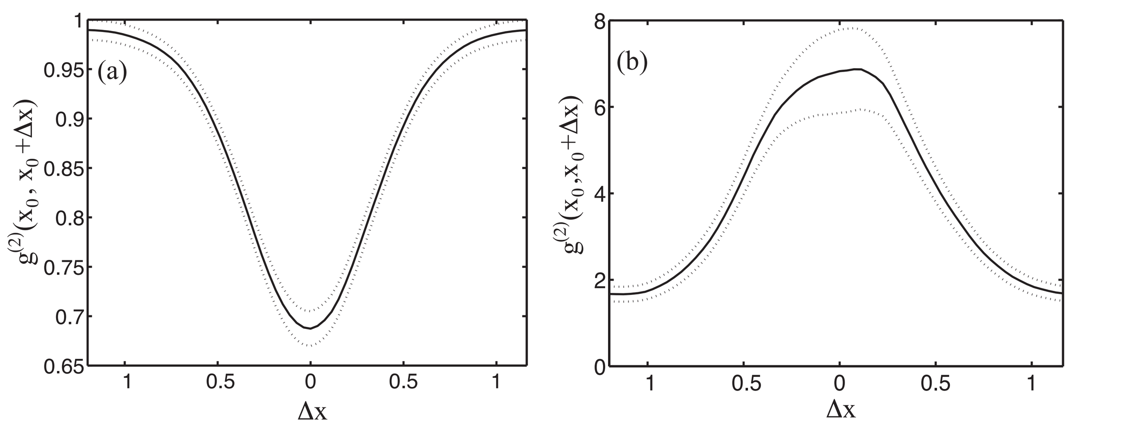
- We study Rydberg state ($|e\rangle$) excitation and de-excitation in a Bose-condensed gas of ground state atoms ($|g\rangle$).
- Conversion is modeled with a Rabi-coupling term $\hat{H} = \cdots + \omega\sum_n \hat{a}_{e,n}^\dagger\hat{a}_{g,n}$.
- We consider an echo sequence as in the experiment [4], where after an excitation time $\tau/2$, the sign of the Rabi coupling is flipped $\omega \rightarrow -\omega$.
- Without interactions, the system would return to its initial state. Due to dephasing by the long range interactions within the Rydberg component, a residual excited state population remains.



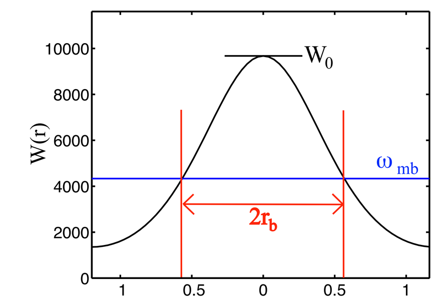
(a) (black) Atom number in the ground state N_g during echo sequence with $\tau = 5\times10^{-4}$. (blue) Total number. Dotted lines indicate sampling error. (b) (black) Excited state number N_e form stochastic quantum field theory. (red) Mean field simulation. (c) Mandel-Q parameter for ground and excited state. $Q = (\langle\hat{N}_{e,g}^2\rangle - \langle\hat{N}_{e,g}\rangle^2)/\langle\hat{N}_{e,g}\rangle - 1$.

- During the de-excitation part of the echo sequence, strong quantum correlation develop, indicating the formation of "clumps" of atoms.
- To show this we plot the Rydberg-Rydberg correlation function

$$g^{(2)}(x,y) = \langle:\hat{N}_e(x)\hat{N}_e(y):\rangle/(\langle\hat{N}_e(x)\rangle\langle\hat{N}_e(y)\rangle). \quad (14)$$



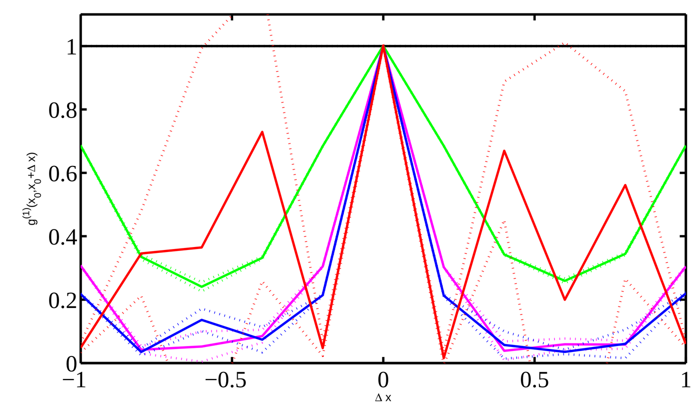
(a) Rydberg-Rydberg correlation function $g^{(2)}(x,y)$ as defined in the text at time $t = \tau/2$. (b) The same at $t = 3\tau/4$.



So far, only for the unrealistic potential on the left tractable sampling errors were achieved.

Interaction quench in the extended Bose-Hubbard model

- Instead of the continuous transfer of population from the $|g\rangle$ to the $|e\rangle$ component as before, let us ignore $|g\rangle$ and begin with a nonzero initial population in $|e\rangle$, which is in a coherent state (superfluid).
- We then consider the effect of long-range interactions, corresponding to a sudden quench.
- Our Hamiltonian corresponds to the extended Bose-Hubbard model. For the local Bose-Hubbard model the quench was studied eg. in [5].
- The interaction dephases correlations between different sites. Without hopping $\tilde{\omega}_{ij} = 0$ there will be an exact quantum revival.
- Inter-site hopping causes an eventual cessation of revival oscillations and can establish an equilibrium [5].
- We look at the one-body density matrix $g^{(1)}(x,y) = \langle\hat{a}_e(x)^\dagger\hat{a}_e(y)\rangle/\sqrt{\langle\hat{N}_e(x)\rangle\langle\hat{N}_e(y)\rangle}$ to look for similar effects in the presence of long-range interactions.



(a) Off-diagonal one-body density matrix (coherence) $g^{(1)}(x,y)$ as defined in the text. Plots are from $t = 0$, to $t = 12\times10^{-4}$ with increasing time: (black), (green), (magenta), (blue), (red).

- Currently, Gauge-P simulations of this scenario reach well after the decoherence time but fail (just?) before the first revival time.

Outlook

These preliminary results should be improved in the following ways:

- Make a definite statement as to whether nonlocal diffusion gauges can be advantageous over local ones.
- Simulate the Rydberg excitation echo sequence for more realistic Coulombic potentials. To this end we currently investigate using the Gauge-freedom to distribute the Coulomb potential among deterministic and noise terms.
- Investigate observables that show interesting behaviour well before the revival time for the quench scenario.

Conclusions

- We have extended the stochastic Gauge-P formalism to long-range interacting systems by deriving an expression for a characteristic variance and developing adaptive local diffusion gauges from that.
- We have applied the method to echo type Rydberg excitations and de-excitations in Bose-Einstein condensates.
- For a toy-model potential, we find the formation of a strongly anti-blockaded gas of Rydberg atoms during the de-excitation phase.
- We trialled simulating interaction-quenches in the extended Bose-Hubbard model. The Gauge-P formalism can model the initial destruction of long-range phase-coherence, but fails before the first quantum revival.

References

[1] P.D. Drummond *et al.*, *J. Mod. Opt.* **54**, 2499 (2007).

[2] P. Deuar *et al.*, *Phys. Rev. A* **66**, 033812 (2002); *J. Opt. B* **5**, S281 (2003); *PhD-thesis*, cond-mat/0507023 (2004).

[3] C.W. Gardiner, Handbook of Stochastic Methods, Springer (2003).

[4] U. Raitzsch *et al.*, *Phys. Rev. Lett.* **100**, 013002 (2008).

[5] C. Kollath *et al.*, *Phys. Rev. Lett.* **98**, 180601 (2007).