Stochastic Mean-field methods

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Part 1: Exact evolution of quantum systems

-Introduction to stochastic Schroedinger Equation

-illustration : system-environment

-application to self-interacting system

Part 2: Approximate evolution of quantum systems

-Dissipation and fluctuations beyond mean-field

-Quantum jump approach to the many-body problem



One Body space

What is a Stochastic Schroedinger equation?

Standard Schroedinger equation:

$$d\left|\Psi\right\rangle = \frac{dt}{i\hbar}H\left|\Psi\right\rangle$$



Deterministic evolution

Stochastic Schroedinger equation (SSE):

$$d |\Psi\rangle = \left\{ \frac{dt}{i\hbar} H + \frac{dB_{sto}}{I} \right\} |\Psi\rangle$$

$$\blacksquare$$
Stochastic operator :
$$dB_{sto} = \sum_{\alpha} x_{\alpha}(t)O_{\alpha}$$





Exact dynamics of a systems coupled to an environment with SSE



 \blacksquare Average density $D = \overline{|\Psi_1 \rangle \langle \Psi_2|}$



Introduction of mean-field:

Stochastic equation are not unique. One can take advantage of this flexibility (mean-field)



Lacroix, Phys. Rev. A72, 013805 (2005).

0

0.5

1.5

1.0

time

A two-level system interacting with a bath of spin systems

Simulation of self-interacting system with 'simple state': the nuclei case







³D TDHF-Sly4d (P. Bonche)

Critical aspects • Static: some important long range correlations are neglected. • Dynamics: correlations (fluctuations) are underestimated.

Exact Many-Body with SSE on "simple" state: the Functional integral method

General strategy

S. Levit, PRC21 (1980) 1594.

$$\left|\Phi\left(t+\Delta t\right)\right\rangle=\exp\left(\frac{\Delta t}{i\hbar}H\right)\left|\Phi\left(t\right)\right\rangle$$

$$H\left|\Phi\right\rangle = \left(H_{1}-O^{2}\right)\left|\Phi\right\rangle$$

$$\exp\left(-\frac{\Delta t}{i\hbar}O^{2}\right)|\Phi\left(t\right)\rangle = \int d\sigma G\left(\sigma\right)\exp(a\sigma O)\left|\Phi\left(t\right)\right\rangle$$
$$|\Phi\left(t+\Delta t\right)\rangle = \int d\sigma G\left(\sigma\right)\left|\Phi_{\sigma}\left(t+\Delta t\right)\right\rangle$$

The many-body problem

$$H = \sum_{ij} T_{ij} a_i^+ a_j + \frac{1}{4} \sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_l a_k$$
$$O_{ij} O_{il} O_{jk}$$

Example of application in nuclear physics: -Shell Model Monte-Carlo ...



Adapted from: S.E.Koonin, D.J.Dean, K.Langanke, Ann.Rev.Nucl.Part.Sci. 47, 463 (1997).

Recent progress for dynamics: stochastic mean-field



Carusotto, Y. Castin and J. Dalibard, PRA63 (2001)

O. Juillet and Ph. Chomaz, PRL 88 (2002)

- The link with observable evolution is not simple (D. Lacroix , PRC71, 064322 (2005))
- A systematic method is desirable
- The numerical effort is huge

Mean-field from variational principle

More insight in mean-field dynamics:

Exact state Trial states $|\Psi(t)\rangle \longrightarrow \begin{cases} |Q(t)\rangle \\ |Q + \delta Q\rangle = e^{\sum_{\alpha} \delta q_{\alpha} A_{\alpha}} |Q\rangle \end{cases}$

The approximate evolution is obtained by minimizing the action:

$$S = \int_{t_0}^{t_1} \mathrm{d}s \langle Q | \mathrm{i}\hbar\partial_t - H | Q \rangle$$



The idea is now to treat the missing information as the *Environment* for the Relevant part (*System*)

Good part: average evolution

$$i\hbar \frac{d\langle A_{\alpha} \rangle}{dt} = \langle [A_{\alpha}, H] \rangle \xrightarrow{\text{exact Ehrenfest}}_{\text{evolution}} H = \mathcal{P}_1 H + (1 - \mathcal{P}_1) H$$

Missing part: correlations

$$|dQ\rangle = \sum_{\alpha} dq_{\alpha} A_{\alpha} |dQ\rangle = \frac{dt}{i\hbar} \mathcal{P}_{1}(t) H |Q\rangle$$
$$\Longrightarrow i\hbar \frac{d\langle A_{\alpha} A_{\beta} \rangle}{dt} \neq \langle [A_{\alpha} A_{\beta}, H] \rangle$$

Hamiltonian splitting

$$H = \mathcal{P}_1 H + \frac{(1 - \mathcal{P}_1)H}{(1 - \mathcal{P}_1)H}$$

System Environment



Existence theorem : Optimal stochastic path from observable evolution

D. Lacroix, Annals of Physics (2006), in press.



Simple illustration: simulation of the free wave spreading with "quasi-classical states"



Reduction of the information:I want to simulate the expansion with Gaussian wave-
function having fixed widths. $\langle x^2 \rangle = cte$, $\langle p^2 \rangle = cte$ Mean-field evolution:t > 0Image: Constraint of the expansion of the expansion of freedom
 $\langle x \rangle$, $\langle p \rangle$ Missing information
 $\langle x^2 \rangle$, $\langle p^2 \rangle$, $\langle xp \rangle$ Trial statesRelevant degrees
of freedom
 $\langle x^2 \rangle$, $\langle p^2 \rangle$, $\langle xp \rangle$ Coherent states

 $\rangle, \langle a^2 \rangle, \langle a^+ a \rangle$

 $|\alpha + d\alpha|$



Guess of the SSE from the existence theorem

Densities

Stochastic c-number evolution from Ehrenfest theorem



Nature of the stochastic mechanics

$$\begin{cases} X = \frac{1}{\sqrt{2\eta}} (\alpha + \beta^*), \\ P = i\hbar\sqrt{\frac{\eta}{2}} (\beta^* - \alpha) \end{cases} \begin{cases} dX = \frac{P}{m} dt + d\chi_1 \\ dP = d\chi_2, \end{cases}$$

with
$$\overline{\mathrm{d}\chi_1\,\mathrm{d}\chi_2} = \frac{\hbar^2\eta}{2m}\,\mathrm{d}t$$

the quantum wave spreading can be simulated by a classical brownian motion in the complex plane



SSE for Many-Body Fermions and bosons

D. Lacroix, Annals of Physics (2006), in press.

Starting point:

$$H = \sum_{ii} \langle i|T|j\rangle a_i^+ a_j + \frac{1}{2} \sum_{ijkl} \langle ij|v_{12}|lk\rangle a_i^+ a_j^+ a_l a_k$$
$$D_{ab} = |\Phi_a\rangle \langle \Phi_b| \quad \text{with} \quad \langle \Phi_b \mid \Phi_a\rangle = 1$$
$$\rho_1 = \sum |\alpha_i\rangle \langle \beta_i|$$

Ehrenfest theorem BBGKY hierarchy $i\hbar \frac{d}{dt}\rho_1 = [h_{MF}, \rho_1], \qquad v_{12} = \sum_{\lambda} O_{\lambda}(1)O_{\lambda}(2)$ $i\hbar \frac{d}{dt}\rho_{12} = [h_{MF}(1) + h_{MF}(2), \rho_{12}] + (1 - \rho_1)(1 - \rho_2)v_{12}\rho_1\rho_2 - \rho_1\rho_2v_{12}(1 - \rho_1)(1 - \rho_2)$ Observables $\langle j|\rho_1|i\rangle = \langle a_i^+a_j\rangle$ Fluctuations $\langle ij|\rho_{12}|kl\rangle = \langle a_k^+a_l^+a_ja_i\rangle$

Stochastic one-body evolution

$$d\rho_1 = [h_{MF}, \rho_1] \\ + \sum_{\lambda} d\xi_{\lambda}^{[2]} (1 - \rho_1) O_{\lambda} \rho_1 + \sum_{\lambda} d\eta_{\lambda}^{[2]} (1 - \rho_1) O_{\lambda} \rho_1$$

with
$$\overline{d\xi_{\lambda}^{[2]}d\xi_{\lambda'}^{[2]}} = -\overline{d\eta_{\lambda}^{[2]}d\eta_{\lambda'}^{[2]}} = \delta_{\lambda\lambda'}\frac{dt}{i\hbar}$$



 The method is general. the SSE are deduced easily
 extension to Stochastic TDHFB D. Lacroix, arXiv nucl-th 0605033
 The mean-field appears naturally and the interpretation is easier
 the numerical effort can be reduced by reducing the number of observables

Part II Dissipation in Many-Body Systems with SSE

Quantum jump method -Dissipation

$$H = H_S + H_E + \sum_{\alpha} B_{\alpha}(S) \otimes C_{\alpha}(E)$$

Exact dynamics

with SSE on simple state $|\Psi
angle=|\Phi
angle\otimes|\chi
angle$



Then, the average dyn. identifies with the exact one

1 For total wave $\overline{d |\Psi\rangle} = \left\{ \frac{dt}{i\hbar} H + \mathcal{O}(dt) \right\} |\Psi\rangle$ 2 For total density $D = \overline{|\Psi_1\rangle \langle \Psi_2|}$

Application to self-interacting system Interpretation as a "system+environment"

Environmen System Approximate Dissipative dynamics At t=0 $D(t=0) = \rho_S \otimes \rho_E$ • Weak coupling approx. Projection technique • Markovian approx. Lindblad master equation: $i\hbar \frac{d}{dt}\rho_S = [H_S, \rho_S]$

$$+ \sum_{k} \gamma_k \left(A_k A_k \rho_S + \rho_S A_k A_k - 2A_k \rho_S A_k \right)$$

Can be simulated by stochastic eq. on $|\Phi\rangle$, The Master equation being recovered using :

$$\rho_{S} = \overline{\left|\Phi\right\rangle \left\langle\Phi\right|}$$

Gardiner and Zoller, *Quantum noise* (2000) Breuer and Petruccione, *The Theory of Open Quant. Syst.*

Dissipation in self-interacting systems

Y. Abe et al, Phys. Rep. 275 (1996) D. Lacroix et al, Progress in Part. and Nucl. Phys. 52 (2004)

Short time evolution

$$\begin{split} \mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}\rho_1 &= [h_{\mathrm{MF}},\rho_1],\\ \mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}\rho_{12} &= [h_{\mathrm{MF}}(1) + h_{\mathrm{MF}}(2),\rho_{12}]\\ &+ (1-\rho_1)(1-\rho_2)v_{12}\rho_1\rho_2 - \rho_1\rho_2v_{12}(1-\rho_1)(1-\rho_2)v_{12}\rho_1\rho_2 - \rho_1\rho_2v_{12}(1-\rho_1)(1-\rho_2)v_{12}(1-\rho_1)(1-\rho_1)(1-\rho_2)v_{12}(1-\rho_1)(1-\rho_1)(1-\rho_1)(1-\rho_1)(1-\rho_2)v_{12}(1-\rho_1)(1-\rho_1)(1-\rho_1)(1-\rho_1)(1$$

Correlation $C_{12} = \rho_{12} - (\rho_1 \rho_2)_A$



Approximate long time evolution+Projection

$$i\hbar \frac{d}{dt}\rho_{1} = [h_{MF}, \rho_{1}] + Tr_{2} [v_{12}, C_{12}]$$
with
$$C_{12}(t) = -\frac{i}{\hbar} \int_{t_{0}}^{t} U_{12}(t, s) F_{12}(s) U_{12}^{\dagger}(t, s) ds + \delta \mathcal{O}(t)$$
projected two-body
propagated initial
correlation

Dissipation $i\hbar \frac{d}{dt}\rho = [h_{MF}, \rho] + K(\rho)$

Semiclassical version for approaches in Heavy-Ion collisions



Application in quantum systems





D. Lacroix et al, Progress in Part. and Nucl. Phys. (2004)

Alternative formulation with Stochastic Schroedinger equations

GOAL: Restarting from an uncorrelated state $D = |\Phi_0\rangle \langle \Phi_0|$ we should:

1-have an estimate of $D = |\Psi(t)\rangle \langle \Psi(t)|$

2-interpret it as an average over jumps between "simple" states

Weak coupling approximation : perturbative treatment R.-G. Reinhard and E. Suraud, Ann. of Phys. 216, 98 (1992) $|\Psi(t')\rangle = |\Phi(t')\rangle - \frac{i}{\hbar} \int \delta v_{12}(s) |\Phi(s)\rangle \, ds - \frac{1}{2\hbar^2} T \left(\int \int \delta v_{12}(s) \delta v_{12}(s') ds ds' \right) |\Phi(s)\rangle$ Residual interaction in the mean-field interaction picture

Statistical assumption in the Markovian limit :



We assume that the residual interaction can be treated as an ensemble of two-body interaction:

$$\begin{cases} \overline{\delta v_{12}(s)} = 0\\ \overline{\delta v_{12}(s)\delta v_{12}(s')} \propto \overline{\delta v_{12}^2(s)} e^{-(s-s')^2/2\tau^2} \end{cases}$$

Time-scale and Markovian dynamics



Hypothesis : $\tau \ll \Delta t \ll \tau_{2coll}$

Two strategies can be considered:

- Considering waves directly (philosophy of exact treatment)
- Considering densities directly (philosophy of dissipative treatment) $\overline{\Delta D} = \frac{\Delta t}{i\hbar} [H_{MF}, D] - \frac{\tau \Delta t}{2\hbar^2} \overline{[\delta v_{12}, [\delta v_{12}, D]]}$

 $\overline{\Delta |\Psi\rangle} = \frac{\Delta t}{i\hbar} H_{MF} |\Phi(t)\rangle - \frac{\tau \Delta t}{2\hbar^2} \overline{\delta v_{12}^2} |\Phi(t)\rangle$

Quantum jump with dissipation: link between Extended TDHF and Lindblad eq.

One-body density Master equation step by step

Initial simple state

 $D = |\Phi\rangle \langle \Phi|$ $\rho = \sum_{\alpha} |\alpha\rangle \langle \alpha|$



Separability of the interaction $v_{12} = \sum_{\lambda} O_{\lambda}(1)O_{\lambda}(2)$

$$\begin{split} \overline{\Delta D} &= \frac{\Delta t}{i\hbar} [H_{MF}, D] - \frac{\tau \Delta t}{2\hbar^2} \overline{[\delta v_{12}, [\delta v_{12}, D]]} \\ i\hbar \frac{d}{dt} \rho &= [h_{MF}, \rho] - \frac{\tau}{2\hbar^2} \mathcal{D}(\rho) \\ \text{with } \langle j | \mathcal{D} | i \rangle &= \overline{\langle \left[\left[a_i^+ a_j, \delta v_{12} \right], \delta v_{12} \right] \rangle} \\ \mathcal{D}(\rho) &= Tr_2 \left[v_{12}, C_{12} \right] \\ \text{with } C_{12} &= (1 - \rho_1)(1 - \rho_2)v_{12}\rho_1\rho_2 \\ -\rho_1\rho_2 v_{12}(1 - \rho_1)(1 - \rho_2) \end{split}$$
$$\end{split}$$

• Dissipation contained in Extended TDHF is included

• The master equation is a Lindblad equation

• Associated SSE D. Lacroix, PRC73 (2006)



Application to Bose condensate

1D bose condensate with gaussian two-body interaction N-body density: $D = |N : \alpha\rangle \langle N : \alpha|$

SSE on single-particle state :

Summary Quantum Jump (QJ) methods (or SSE) to extend mean-field

Approximate evolution

Mean-field $D=\left \Phi ight angle\left\langle \Phi ight $	Simplified QJ $D = \overline{\ket{\Phi_1}ra{\Phi_2}}$	Generalized QJ $D = \overline{ \Phi\rangle \langle \Phi }$	${\sf Exact} \ {\sf QJ} \ D = \overline{\ket{\Phi_1}ra{\Phi_2}}$	variational QJ $D = \overline{ Q_1\rangle \langle Q_2 }$ $ Q_1\rangle = q_1, \cdots, q_N\rangle$
- Eluctuation- - Dissipation-	Fluctuation 🗸 Dissipation	Fluctuation 🗸 Dissipation 🗸	Everything 🗸	Partially everything 🗸
Numerical iss	ues			
	Flexible	Fixed	Fixed	Flexible
$t=0 \text{ fm/c} \qquad t=48 \text{ fm/c} \qquad t=90 \text{ fm/c}$ $\begin{bmatrix} t & t & t & t \\ t & t & t \\ t & t & t \\ t & t &$		U.K.	s ka, o ka, o	



Simplified scenario for introducing fluctuations beyond Mean-field

Interpretation of the equation on waves as an average over jumps:

SSE in one-body space

Assuming $D_{ab} = |\Phi_a\rangle \langle \Phi_b|$ with $\langle \Phi_b | \Phi_a \rangle = 1$ and $\langle a_i^+ a_j \delta v_{12}^2 \rangle \simeq \langle a_i^+ a_j \rangle \langle \delta v_{12}^2 \rangle + 2 \langle a_i^+ a_j \delta v_{12} \rangle \langle \delta v_{12} \rangle - 2 \langle a_i^+ a_j \rangle \langle \delta v_{12} \rangle^2$ $d\rho = \frac{dt}{i\hbar} [h_{MF}, \rho] + dB_a(1 - \rho)U_\delta(\rho)\rho + dB_b^* \rho U_\delta(\rho)(1 - \rho)$ D. Lacroix, PRC73 (2006)Application Monopole vibration in ⁴⁰Ca External t < 0 $\delta v_{12} = \sigma_0 \delta(\mathbf{r}_1 - \mathbf{r}_2)$ $\delta v_{12} = \sigma_0 \delta(\mathbf{r}_1 - \mathbf{r}_2)$ $\delta v_{12} = \sigma_0 \delta(\mathbf{r}_1 - \mathbf{r}_2)$ $\delta v_{12} = \sigma_0 \delta(\mathbf{r}_1 - \mathbf{r}_2)$

3.15

0

150

⁵⁰ *time (fm/c)*



Summary and Critical discussion on the simplified scenario

- The stochastic method is directly applicable to nuclei
- It provide an easy way to introduce fluctuations beyond mean-field
- It does not account for dissipation.
- In nuclear physics the two particle-two-hole components dominates the residual interaction, but $U_{\delta_{2p2h}}(\rho) = 0$!!!

Coming back to the system+environment picture

