

4. Second quantization in stochastic field theory

4.1 Second quantization for Fokker-Planck equation

■ **Probability densities of Markov processes.** We are dealing with Markov processes, therefore the joint probability density function (PDF) is completely expressed in terms of the conditional PDF and the single-event PDF:

$$\begin{aligned} p(\varphi_1, t_1; \varphi_2, t_2; \dots; \varphi_n, t_n) \\ = p(\varphi_1, t_1 | \varphi_2, t_2) p(\varphi_2, t_2 | \varphi_3, t_3) \cdots p(\varphi_{n-1}, t_{n-1} | \varphi_n, t_n) p(\varphi_n, t_n) \end{aligned}$$

provided $t_1 \geq t_2 \geq t_3 \geq \dots \geq t_{n-1} \geq t_n$. Consider now evolution generated by the Fokker-Planck equation

$$\begin{aligned} \frac{\partial}{\partial t} p(\varphi, t | \varphi_0, t_0) = -\frac{\partial}{\partial \varphi} \{[-K\varphi + U(\varphi)] p(\varphi, t | \varphi_0, t_0)\} \\ + \frac{1}{2} \frac{\partial^2}{\partial \varphi^2} [b(\varphi)Db(\varphi)p(\varphi, t | \varphi_0, t_0)]. \quad (4.1) \end{aligned}$$

Recall that the conditional probability density is the fundamental solution of this equation, i.e.

$$p(\varphi, t_0 | \varphi_0, t_0) = \delta(\varphi - \varphi_0)$$

and is also properly normalized

$$\int d\varphi p(\varphi, t | \varphi_0, t_0) = 1.$$

The probability density function $p(\varphi, t)$ is the solution of the FPE (4.1) as well, but with the initial condition $p(\varphi, t_0) = p_0(\varphi)$.

■ **Liouville operator.** Introduce now – in analogy with quantum mechanics – the state vector $|p_t\rangle$ according to representation

$$p(\varphi, t) := \langle \varphi | p_t \rangle.$$

To construct the evolution operator for the state vector, introduce the (nearly) quantum-mechanical momentum and coordinate operators by

$$\hat{\pi}f(\varphi) = -\frac{\partial}{\partial \varphi}f(\varphi), \quad \hat{\varphi}f(\varphi) = \varphi f(\varphi).$$

The non-trivial commutation relation is

$$[\widehat{\varphi}, \widehat{\pi}] = 1.$$

In these terms, the FPE for the PDF gives rise to the evolution equation for the state vector in the form

$$\frac{\partial}{\partial t} |p_t\rangle = \widehat{L} |p_t\rangle,$$

where the Liouville operator, according to (4.1), assumes the form

$$\widehat{L} = \widehat{\pi} [-K\widehat{\varphi} + U(\widehat{\varphi})] + \frac{1}{2} \widehat{\pi}^2 b(\widehat{\varphi}) Db(\widehat{\varphi}). \quad (4.2)$$

In this notation, the conditional PDF may be expressed as the matrix element

$$p(\varphi, t | \varphi_0, t_0) = \left\langle \varphi \left| e^{\widehat{L}(t-t_0)} \right| \varphi_0 \right\rangle. \quad (4.3)$$

Introduce time-dependent operators $\widehat{\varphi}(t)$ in the Heisenberg picture of imaginary time quantum mechanics (i.e. Euclidean quantum mechanics):

$$\widehat{\varphi}(t) = e^{-\widehat{L}t} \widehat{\varphi} e^{\widehat{L}t}, \quad (4.4)$$

and define the time-ordered product (chronological product, T product) of time-dependent operators

$$T \left[\widehat{A}_1(t_1) \cdots \widehat{A}_n(t_n) \right] = \sum_{P(1, \dots, n)} P \left[\theta(t_1 \dots t_n) \widehat{A}_1(t_1) \cdots \widehat{A}_n(t_n) \right], \quad (4.5)$$

where

$$\theta(t_1 \dots t_n) \equiv \theta(t_1 - t_2) \theta(t_2 - t_3) \cdots \theta(t_{n-1} - t_n).$$

In definition (4.5) the sum is taken over all permutations of the labels of the time arguments $\{t_i\}_{i=1}^n$ and the operators in each term are put in the order of growing time arguments from the right to the left. Thus, under the T -product sign operators commute. It should be noted that the definition of the time-ordered product should be amended for coinciding time arguments. We shall return to this point later and exclude this case for the time being.

■ **Green functions.** Introduce then the n -point Green function of the Euclidean fields (4.4)

$$G_n(t_1, t_2, \dots, t_n) := \text{Tr} \{ \widehat{p}_0 T [\widehat{\varphi}(t_1) \widehat{\varphi}(t_2) \cdots \widehat{\varphi}(t_n)] \} \quad (4.6)$$

with the density operator

$$\widehat{p}_0 := \int d\varphi |p_0\rangle \langle \varphi|. \quad (4.7)$$

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Choosing, for definiteness, the time sequence $t_1 > t_2 > t_3 > \dots > t_{n-1} > t_n > t_0$ it is readily seen by direct substitution of relations (4.3), (4.4) and (4.7) in (4.6) with the aid of the normalization conditions of the PDF and insertions of the resolution of the identity $\int d\varphi |\varphi\rangle\langle\varphi| = 1$ that

$$\int d\varphi_1 \dots \int d\varphi_n \varphi_1 \dots \varphi_n p(\varphi_1, t_1; \varphi_2, t_2; \dots; \varphi_n, t_n) = G_n(t_1, t_2, \dots, t_n), \quad (4.8)$$

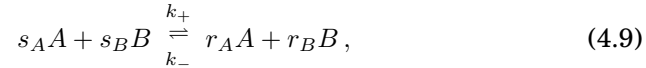
i.e. the Green function (4.6) is equal to the moment function (4.8). This relation connects the operator approach to evaluation of moments of the random process.

4.2 Second quantization for master equation

In the occupation-number basis and in the stationary field operators there is no explicit Planck constant. The ideas of the Fock-space representation and creation/annihilation operators may therefore as well be used in classical problems with a variable number of particles or some other entities.

■ **Rate equation.** Various processes in biology and chemistry are described in terms of variable numbers of some agents or representatives of species ("particle numbers" or "occupation numbers"). In many cases changes in the particle number are caused by interactions between colliding particles, i.e. *reactions*.

Description of a particular reaction may usually be given by the *reaction equation*. For instance, for a two species process with the *rate constants* k_+ and k_- the reaction equation is



where A and B denote the two species and s_A, s_B, r_A and r_B are coefficients (usually integers) describing in which proportions the agents react.

The simplest kinetic description of the dynamics of the average particle numbers is given by the *rate equation*. For the binary reaction (4.9), e.g.

$$\frac{d}{dt} c_A = k_+(r_A - s_A)c_A^{s_A} c_B^{s_B} + k_-(s_A - r_A)c_A^{r_A} c_B^{r_B},$$

where c_X is the concentration of the species X .

The rate equation is a deterministic differential equation for average particle numbers in a homogeneous system, therefore it does not take into account boundary conditions, spatial inhomogeneities and randomness in the individual reaction events.

■ **Master equation.** The inherent randomness of a reaction may be taken into account, when the evolution of the system is described as a *stochastic process*.

To keep things simple, consider a system with just one variable. A classic example is the *Verhulst (logistic) model* of population growth. The rate equation for the particle number n (the number of individuals in the population) may be written as

$$\frac{dn}{dt} = -\beta n + \lambda n - \gamma n^2, \quad (4.10)$$

where β is the death rate, λ the birth rate and γ the damping coefficient necessary to bring about a saturation for the population.

A complete (microscopic) description of a stochastic problem of random particle number is given by the evolution equations written for the probabilities $P(t, n)$ to find exactly n particles in the system at the time instant t . These *master equations* (forward Kolmogorov equations to mathematicians) are balance equations with the generic structure

$$\frac{dP_f}{dt} = \sum_i w(i \rightarrow f) P_i - \sum_i w(f \rightarrow i) P_f,$$

where $w(i \rightarrow f)$ is the *transition rate* from the state i to the state f , i.e. the probability per time unit that the system initially in the state i occurs in the state f . Transition rates of the master equation are related to coefficients of the rate equation, but the correspondence is not unambiguous: a given rate equations may generate different master equations, therefore a verbal description of the process is often necessary.

Master equations for the *stochastic Verhulst model* may be written as

$$\begin{aligned} \frac{dP(t, N)}{dt} &= \lambda(N-1)P(t, N-1) - (\beta N + \gamma N^2)P(t, N), \\ \frac{dP(t, n)}{dt} &= [\beta(n+1) + \gamma(n+1)^2]P(t, n+1) + \lambda(n-1)P(t, n-1) \\ &\quad - (\beta n + \lambda n + \gamma n^2)P(t, n), \quad 0 < n < N, \\ \frac{dP(t, 0)}{dt} &= (\beta + \gamma)P(t, 1). \end{aligned} \quad (4.11)$$

Here, boundary conditions for the particle number are made explicit in the equations for the probabilities of the boundary values of the particle number. Usually, the empty state ($n = 0$) is an *absorbing state* (once the system occurs in an absorbing state, it will stay there forever) and the state with the maximum sustainable population ($n = N$) a *reflecting state* (there no available states beyond a reflecting state, but the system does not get stuck to that state) as here.

Using master equations (4.11) a coupled set of evolution equations for the moments of the particle number $\langle n^m \rangle$ may be written. The evolution equation for the average particle number $\langle n \rangle$ coincides with the rate equation (4.10), when all correlations are neglected, i.e. moments replaced by corresponding powers of the average particle number $\langle n^m \rangle \rightarrow \langle n \rangle^m$. This, however, is not always the case, but only *if* the transition rates vanish with n .

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■ **Fock space.** Introduce the state vector

$$|\Phi\rangle = \sum_{n=0}^{\infty} P(t, n) |n\rangle. \quad (4.12)$$

Here, the basis vectors are defined as row and column vectors of the form

$$\langle n| = (0, 0, \dots, 0, \sqrt{n!}, 0, \dots), \quad |n\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \sqrt{n!} \\ 0 \\ \vdots \end{pmatrix}, \quad (4.13)$$

where the nonvanishing element appears in the column (row) number $n + 1$. The scalar product (denoted by $\langle m|n\rangle$) is defined in the usual way for real-number component vectors. With the standard scalar product, the basis vectors are orthogonal. Note, however, that – contrary to the quantum-mechanical convention – the basis vectors are not of unit length, but $\langle n|n\rangle = n!$. Therefore, the n -particle PDF (probability density function) may be extracted from the state vector through the following scalar product

$$P(t, n) = \frac{1}{n!} \langle n|\Phi\rangle. \quad (4.14)$$

All basis vectors (4.13) may be constructed from the "vacuum" vector

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix} \quad (4.15)$$

with the use of the creation operator \hat{a}^+ , which is a matrix of the form

$$\hat{a}^+ = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & \dots \\ 1 & 0 & 0 & \dots & 0 & \dots \\ 0 & \sqrt{2} & 0 & \dots & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 0 & 0 & \dots \\ 0 & 0 & 0 & \dots & \sqrt{n} & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}. \quad (4.16)$$

By direct matrix multiplication it may be readily seen that

$$\hat{a}^+|0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} = |1\rangle, \quad \hat{a}^+|n\rangle = |n+1\rangle. \quad (4.17)$$

Note that the coefficient is different from that in QM due to different normalization of the basis vectors.

The Hermitian conjugate to the creation operator (4.16) is the annihilation operator \hat{a} :

$$\hat{a} = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & \dots \\ 0 & 0 & \sqrt{2} & \dots & 0 & \dots \\ 0 & 0 & 0 & \dots & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 0 & \sqrt{n} & \dots \\ 0 & 0 & 0 & \dots & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}. \quad (4.18)$$

The action of the annihilation operator on basis vectors justifies its name (note the coefficient)

$$\hat{a}|0\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad \hat{a}|n\rangle = n|n-1\rangle. \quad (4.19)$$

An important operator is also the occupation number operator $\hat{a}^+\hat{a}$, since the basis vectors are its eigenvectors:

$$\langle n|\hat{a}^+\hat{a} = n\langle n|, \quad \hat{a}^+\hat{a}|n\rangle = n|n\rangle. \quad (4.20)$$

Liouville equation. The point of introducing all this machinery is that it allows to express the set of master equations for one-step processes ("birth-and-death processes") with an unoccupied absorbing state

$$\begin{aligned} \frac{dP(t, n)}{dt} &= r_{n+1}P(t, n+1) + g_{n-1}P(t, n-1) - (r_n + g_n)P(t, n), \\ \frac{dP(t, 0)}{dt} &= r_1P(t, 1), \end{aligned} \quad (4.21)$$

in the form of a single evolution equation for the state vector (4.12) without any explicit dependence on the occupation number:

$$\frac{d|\Phi\rangle}{dt} = \hat{L}(\hat{a}^+, \hat{a})|\Phi\rangle, \quad (4.22)$$

where the Liouville operator $\hat{L}(\hat{a}^+, \hat{a})$ may be constructed from operators \hat{a}^+ and \hat{a} by rules to be discussed a bit later.

The different terms on the right-hand-side of the master equation (4.21) allow for the following "transport process" interpretation: the terms $r_{n+1}P(t, n+1) + g_{n-1}P(t, n-1)$ describe the increase of the probability to observe the occupation number n due to transitions from states with occupation numbers $n+1$ and $n-1$, respectively, whereas the terms

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$-(r_n + g_n)P(t, n)$, describe the decrease of the probability of the occupation number n due to transitions to states with occupation numbers $n + 1$ and $n - 1$, respectively.

The formal solution of Eq. (4.22) is

$$|\Phi(t)\rangle = e^{t\hat{L}(\hat{a}^+, \hat{a})} |\Phi(0)\rangle, \quad (4.23)$$

where the initial state vector is determined by the initial condition for the probabilities: $|\Phi(0)\rangle = \sum_{n=0}^{\infty} P(0, n) |n\rangle$. In principle, the relation (4.23) may be used for a compact representation of the solution of the set of master equations (4.21), particularly if it is possible to calculate the matrix exponential in a closed form.

■ **Projection vector.** To represent expectation values of occupation-number dependent quantities in the operator formalism consider the projection vector $\langle P |$. It is defined as the coherent state vector

$$\langle P | = \sum_{n=0}^{\infty} \frac{1}{n!} \langle n | = \sum_{n=0}^{\infty} \frac{1}{n!} \langle 0 | \hat{a}^n = \langle 0 | e^{\hat{a}}. \quad (4.24)$$

The projection vector is a left eigenvector of the creation operator with the eigenvalue equal to unity

$$\langle P | \hat{a}^+ = \langle P |. \quad (4.25)$$

The explicit row-vector form of the projection vector is

$$\langle P | = \left(1, 1, \frac{1}{\sqrt{2}}, \dots, \frac{1}{\sqrt{n!}}, \dots \right). \quad (4.26)$$

From the property (4.25) or the representation (4.26) it can readily be seen that

$$\langle P | n \rangle = 1, \quad \forall n. \quad (4.27)$$

The basic relation for calculation of expectation values follows from the definition in terms of probabilities, which may be cast in the form of a matrix element between the projection vector $\langle P |$ and the state vector $|\Phi\rangle$:

$$\langle Q(n) \rangle = \sum_{n=0}^{\infty} Q(n) P(t, n) = \langle P | Q(\hat{a}^+ \hat{a}) | \Phi \rangle. \quad (4.28)$$

The last equality, again without explicit occupation-number dependence, comes from the the relation

$$\langle P | (\hat{a}^+ \hat{a})^m | n \rangle = n^m \langle P | n \rangle = n^m. \quad (4.29)$$

Thus, in the operator language the expectation value of an occupation-number dependent quantity $Q(n)$ may be written as

$$\langle Q(n) \rangle = \langle P | Q(\hat{a}^+ \hat{a}) e^{t\hat{L}(\hat{a}^+, \hat{a})} | \Phi(0) \rangle. \quad (4.30)$$

■ **Liouville operator.** Consider the Verhulst model (4.11) as an example of construction of the Liouville operator. The master equation for the state vector of the Verhulst model – for unlimited occupation number for simplicity – may be cast in the form

$$\begin{aligned} \frac{d|\Phi\rangle}{dt} = & (\beta + \gamma)P(t, 1)|0\rangle + \sum_{n=1}^{\infty} \left\{ [\beta(n+1) + \gamma(n+1)^2]P(t, n+1) \right. \\ & \left. + \lambda(n-1)P(t, n-1) - (\beta n + \gamma n^2 + \lambda n)P(t, n) \right\} |n\rangle \end{aligned}$$

Rewrite the right-hand side to obtain expressions like $P(t, n)|n\rangle$ (i.e. the occupation number in the state probability and the basis vector should be the same) multiplied by an independent of n operator (polynomial in \hat{a}^+ and \hat{a}). For instance

$$\begin{aligned} nP(t, n)|n\rangle &= \hat{a}^+ \hat{a} P(t, n)|n\rangle, \\ (n+1)P(t, n+1)|n\rangle &= \hat{a} P(t, n+1)|n+1\rangle, \\ (n-1)P(t, n-1)|n\rangle &= (\hat{a}^+)^2 \hat{a} P(t, n-1)|n-1\rangle. \end{aligned}$$

The right-hand side of the master equation for the state vector is thus transformed in the form in which an operator, the *Liouville operator* $\hat{L}(\hat{a}^+, \hat{a})$, constructed from the creation and annihilation operators is acting on the state vector. Thus, the master equation for the state vector then yields the *Liouville equation*

$$\frac{d|\Phi\rangle}{dt} = \hat{L}(\hat{a}^+, \hat{a})|\Phi\rangle,$$

where the Liouville operator for the Verhulst model is

$$\hat{L}(\hat{a}^+, \hat{a}) = \beta(I - \hat{a}^+) \hat{a} + \gamma(I - \hat{a}^+) \hat{a} \hat{a}^+ \hat{a} + \lambda(\hat{a}^+ - I) \hat{a}^+ \hat{a}.$$

In some situations it is convenient to transfer the operator exponential $e^{\hat{a}}$ of the projection vector (4.24) from the left to the right in Eq. (4.30) according to the rule

$$e^{\hat{a}} \hat{a}^+ = (\hat{a}^+ + I) e^{\hat{a}} \quad (4.31)$$

which is a direct consequence of the commutation relations. After this the expectation value of $Q(n)$ may be written as

$$\langle Q(n) \rangle = \langle 0 | Q[(\hat{a}^+ + I) \hat{a}] e^{t \hat{L}'(\hat{a}^+, \hat{a})} | \Phi'(0) \rangle, \quad (4.32)$$

where \hat{L}' and $|\Phi'(0)\rangle$ are the "shifted" Liouville operator and initial state vector, respectively:

$$\hat{L}'(\hat{a}^+, \hat{a}) = \hat{L}(\hat{a}^+ + I, \hat{a}), \quad (4.33)$$

$$|\Phi'(0)\rangle = \sum_{n=0}^{\infty} P(0, n) (\hat{a}^+ + I)^n |0\rangle. \quad (4.34)$$

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■ **Green functions.** Consider the Green function of occupation-number operators $\hat{n}_H(t) = \hat{a}_H^\dagger(t)\hat{a}_H(t)$:

$$G_m(t_1, t_2, \dots, t_m) = \text{Tr} \left\{ \hat{P}_0 T [\hat{n}_H(t_1)\hat{n}_H(t_2) \cdots \hat{n}_H(t_m)] \right\}, \quad (4.35)$$

with the density operator

$$\hat{P}_0 = |\Phi(0)\rangle\langle P|. \quad (4.36)$$

The definition (4.35) may be, of course, written in terms of the shifted operators as well, but then the "density operator" $|\Phi(0)\rangle\langle P|$ will not be a genuine density operator.

From definitions it follows that the conditional probability density function for the master equation may be written as (the factorial in front of the matrix element is due to the unusual normalization of the basis states)

$$P(n, t | n_0, t_0) = \frac{1}{n!} \left\langle n \left| e^{\hat{L}(t-t_0)} \right| n_0 \right\rangle. \quad (4.37)$$

Choosing, for definiteness, the time sequence $t_1 > t_2 > t_3 > \dots > t_{n-1} > t_n > t_0$ it is readily seen by direct substitution of relations (4.37) and (4.36) in (4.35) with the aid of the normalization conditions of the PDF and insertions of the resolution of the identity $\sum_n \frac{1}{n!} |n\rangle\langle n| = 1$ that

$$\sum_{n_1} \dots \sum_{n_m} n_1 \cdots n_m P(n_1, t_1; n_2, t_2; \dots; n_m, t_m) = G_m(t_1, t_2, \dots, t_m), \quad (4.38)$$

i.e. the Green function (4.35) is equal to the moment function (4.38). This relation connects the operator approach to evaluation of moments of the random process described by a master equation.

4.3 Problems

Problem 4.1. Consider the Liouville operator of a "free" Fokker-Planck system

$$\hat{L} = -K\hat{\pi}\hat{\varphi} + \frac{D}{2}\hat{\pi}^2.$$

Construct explicitly the time-dependent operators

$$\hat{\varphi}(t) = e^{-\hat{L}t}\hat{\varphi}e^{\hat{L}t}, \quad \hat{\pi}(t) = e^{-\hat{L}t}\hat{\pi}e^{\hat{L}t}.$$

Problem 4.2. With the use of definitions

$$\hat{\varphi}(t) = e^{-\hat{L}t}\hat{\varphi}e^{\hat{L}t},$$

$$T[\hat{A}_1(t_1) \cdots \hat{A}_n(t_n)] = \sum_{P(1, \dots, n)} P[\theta(t_1 \dots t_n) \hat{A}_1(t_1) \cdots \hat{A}_n(t_n)],$$

$$\hat{p}_0 := \int d\varphi |p_0\rangle \langle \varphi|,$$

and the relation

$$p(\varphi, t | \varphi_0, t_0) = \langle \varphi | e^{\hat{L}(t-t_0)} | \varphi_0 \rangle.$$

show that

$$\begin{aligned} & \text{Tr} \{ \hat{p}_0 T [\hat{\varphi}(t_1) \hat{\varphi}(t_2) \cdots \hat{\varphi}(t_n)] \} \\ &= \int d\varphi_1 \cdots \int d\varphi_n \varphi_1 \cdots \varphi_n p(\varphi_1, t_1; \varphi_2, t_2; \dots; \varphi_n, t_n), \end{aligned}$$

when $t_1 > t_2 > t_3 > \dots > t_{n-1} > t_n > t_0$.

Problem 4.3. Write down the set of master equations for the modification of the Verhulst model, in which the quadratic in the particle number term of the transition rate is interpreted as a consequence of an annihilation reaction $A + A \rightarrow \emptyset$ with the rate constant γ . Construct then the Liouville operator for this model.

Problem 4.4. Prove the transfer rule

$$e^{\hat{a}} \hat{a}^+ = (\hat{a}^+ + I) e^{\hat{a}}.$$