



The Dynamics of the Hubbard Model Through Stochastic Calculus and Girsanov Transformation

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Abstract

As a typical quantum many body problem, we consider the time evolution of density matrix elements in the Bose-Hubbard model. For an arbitrary initial state, these quantities can be obtained from an SDE or stochastic differential equation system. To this SDE system, a Girsanov transformation can be applied. This has the effect that all the information from the initial state moves into the drift part, into the mean field part, of the transformed system. In the large N limit with $g = UN$ fixed, the diffusive part of the transformed system vanishes and as a result, the exact quantum dynamics is given by an ODE system which turns out to be the time dependent discrete Gross Pitaevskii equation. For the two site Bose-Hubbard model, the GP equation reduces to the mathematical pendulum and the difference of expected number of particles at the two lattice sites is equal to the velocity of that pendulum which is either oscillatory or it can have rollovers which then corresponds to the self trapping or insulating phase. As a by-product, we also find an equivalence of the mathematical pendulum with a quartic double well potential. Collapse and revivals are a more subtle phenomenon, in order to see these the diffusive part of the SDE system or quantum corrections have to be taken into account. This can be done with an approximation and collapse and revivals can be reproduced, numerically and also through an analytic calculation. Since expectation values of Fresnel or Wiener diffusion processes, we write the density matrix elements exactly in this way, can be obtained from parabolic second order PDEs, we also obtain various exact PDE representations. The paper has been written with the goal to come up with an efficient calculation scheme for quantum many body systems and as such the formalism is generic and applies to arbitrary dimension, arbitrary hopping matrices and, with suitable adjustments, to fermionic models.

Keywords Quantum many-body problem · Bose-Hubbard model · Correlation functions · Stochastic differential equations · Gross-Pitaevskii equation · Collapse and revivals

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1 General Setup and SDE Representation

We consider the d -dimensional Bose-Hubbard model with Hamiltonian

$$H = -J \sum_{\langle i, j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_j a_j^\dagger a_j^\dagger a_j a_j + \sum_j \epsilon_j a_j^\dagger a_j \quad (1.1)$$

with bosonic annihilation and creation operators $a_j, a_j^\dagger$ satisfying the commutation relations

$$[a_i, a_j^\dagger] = \delta_{i, j} \quad (1.2)$$

As usual, $\langle i, j \rangle$ denotes the sum over nearest neighbors and to be specific, we choose a cubic lattice Γ given by

$$j = (j_1, \dots, j_d) \in \{1, 2, \dots, L\}^d =: \Gamma \quad (1.3)$$

We find it convenient to work in the Bargmann-Segal representation [1] where the $a_j, a_j^\dagger$ are realized through the operators

$$a_j = \frac{\partial}{\partial z_j}, \quad a_j^\dagger = z_j \quad (1.4)$$

which act on the Hilbert space of analytic functions of $|\Gamma| = L^d$ complex variables

$$\mathcal{F} := \left\{ f = f(\{z_j\}) : \mathbb{C}^{|\Gamma|} \rightarrow \mathbb{C} \text{ analytic} \mid \|f\|_{\mathcal{F}}^2 = (f, f)_{\mathcal{F}} < \infty \right\} \quad (1.5)$$

with scalar product

$$(f, g)_{\mathcal{F}} := \int_{\mathbb{C}^{|\Gamma|} = \mathbb{R}^{2|\Gamma|}} f(z) \overline{g(z)} d\mu(z) \quad (1.6)$$

$$d\mu(z) := \prod_j e^{-|z_j|^2} \frac{d\operatorname{Re} z_j d\operatorname{Im} z_j}{\pi} \quad (1.7)$$

In the following, sums $\sum_j$ or $\sum_{i, j}$ or products $\prod_j$ are always meant to be sums and products over all lattice sites if not specified otherwise. That is, we use the notation

$$\sum_j \dots := \sum_{j \in \Gamma} \dots \quad (1.8)$$

$$\prod_j \dots := \prod_{j \in \Gamma} \dots \quad (1.9)$$

and $\sum_{i, j} := \sum_{i, j \in \Gamma}$. Actually we can allow for a general hopping matrix which should be real and symmetric,

$$\varepsilon := (\varepsilon_{ij}) \in \mathbb{R}^{|\Gamma| \times |\Gamma|} \quad (1.10)$$

with $\varepsilon_{ij} = \varepsilon_{ji}$. With that, the final Hamiltonian, we use a small h instead of a capital H , reads

$$h = h_0 + h_{\text{int}} \quad (1.11)$$

with a quadratic part

$$h_0 = \sum_{i, j} \varepsilon_{ij} z_i \frac{\partial}{\partial z_j} \quad (1.12)$$

and a quartic part

$$h_{\text{int}} = u \sum_j z_j^2 \frac{\partial^2}{\partial z_j^2} \quad (1.13)$$

where we substituted the capital U by a small u according to (the capital U 's we use later for a unitary evolution matrix)

$$u := \frac{U}{2} \quad (1.14)$$

For a nearest neighbor hopping J and trapping potentials ϵ_j as in (1.1) we have

$$\epsilon_{ij} = \begin{cases} -J & \text{if } |i - j| = 1 \\ +\epsilon_j & \text{if } i = j \\ 0 & \text{otherwise} . \end{cases} \quad (1.15)$$

1.1 Time Evolution of States as Fresnel Expectation Values

The time evolution $e^{-ith} = e^{-it(h_0+h_{\text{int}})}$ we calculate through the Trotter formula. That is, we discretize time

$$t = t_k = k dt \quad (1.16)$$

and write

$$e^{-ith} = e^{-ikdt(h_0+h_{\text{int}})} \approx (e^{-idt h_{\text{int}}} e^{-idt h_0})^k \quad (1.17)$$

where the approximate equality becomes exact in the limit $dt \rightarrow 0$ which we implicitly assume from now on. The action of $e^{-idt h_0}$ is given by

$$(e^{-idt h_0} f)(z) = f(e^{-idt \epsilon} z) \quad (1.18)$$

The action of $e^{-idt h_{\text{int}}}$ we write as follows: First, on monomials $\prod_j z_j^{n_j}$ we have

$$e^{-idt h_{\text{int}}} \prod_j z_j^{n_j} = e^{iudt \sum_j n_j} e^{-iudt \sum_j n_j^2} \prod_j z_j^{n_j} \quad (1.19)$$

Recall the Fresnel integral

$$\int_{\mathbb{R}} e^{-i\lambda\phi} e^{i\frac{\phi^2}{2}} \frac{d\phi}{\sqrt{2\pi i}} = e^{-i\frac{\lambda^2}{2}} \quad (1.20)$$

with $\sqrt{i} = e^{i\frac{\pi}{4}}$. We can write

$$e^{-idt h_{\text{int}}} \prod_j z_j^{n_j} = \int_{\mathbb{R}^{|\Gamma|}} \prod_j (e^{iudt - i\sqrt{2udt}\phi_j} z_j)^{n_j} \prod_j e^{i\frac{\phi_j^2}{2}} \frac{d\phi_j}{\sqrt{2\pi i}} \quad (1.21)$$

Thus, for any analytic f (by slight abuse of notation, we temporarily label the lattice sites with natural numbers from 1 to $|\Gamma|$ in the middle of the next line)

$$f(z) = f(\{z_j\}) = \sum_{n_1, \dots, n_{|\Gamma|} \geq 0} c_{n_1, \dots, n_{|\Gamma|}} z_1^{n_1} \cdots z_{|\Gamma|}^{n_{|\Gamma|}} \equiv \sum_{\{n_j\}} c_{\{n_j\}} \prod_j z_j^{n_j} \quad (1.22)$$

we have

$$\begin{aligned}
 (e^{-i dt h_{\text{int}}} f)(z) &= \sum_{\{n_j\}} c_{\{n_j\}} e^{-i dt h_{\text{int}}} \prod_j z_j^{n_j} \\
 &= \sum_{\{n_j\}} c_{\{n_j\}} \int_{\mathbb{R}^{|\Gamma|}} \prod_j (e^{i u dt - i \sqrt{2 u dt} \phi_j z_j})^{n_j} \prod_j e^{i \frac{\phi_j^2}{2}} \frac{d\phi_j}{\sqrt{2\pi i}} \\
 &= \int_{\mathbb{R}^{|\Gamma|}} f(\{e^{i u dt - i \sqrt{2 u dt} \phi_j z_j}\}_{j \in \Gamma}) \prod_j e^{i \frac{\phi_j^2}{2}} \frac{d\phi_j}{\sqrt{2\pi i}} \\
 &=: \int_{\mathbb{R}^{|\Gamma|}} f(e^{-i d D_\phi} z) \prod_j e^{i \frac{\phi_j^2}{2}} \frac{d\phi_j}{\sqrt{2\pi i}} \quad (1.23)
 \end{aligned}$$

with the $|\Gamma| \times |\Gamma|$ diagonal matrix

$$dD_\phi := \text{diag}(\{\sqrt{2 u dt} \phi_j - u dt\}_{j \in \Gamma}) \in \mathbb{C}^{|\Gamma| \times |\Gamma|} \quad (1.24)$$

Thus, a single Trotter step is given by

$$\begin{aligned}
 (e^{-i dt h} f)(z) &= [e^{-i dt h_{\text{int}}} (e^{-i dt h_0} f)](z) \\
 &= \int_{\mathbb{R}^{|\Gamma|}} (e^{-i dt h_0} f)(e^{-i d D_\phi} z) \prod_j e^{i \frac{\phi_j^2}{2}} \frac{d\phi_j}{\sqrt{2\pi i}} \\
 &= \int_{\mathbb{R}^{|\Gamma|}} f(e^{-i dt \varepsilon} e^{-i d D_\phi} z) e^{i \sum_j \frac{\phi_j^2}{2}} \prod_j \frac{d\phi_j}{\sqrt{2\pi i}} \\
 &=: \int_{\mathbb{R}^{|\Gamma|}} f(e^{-i dt \varepsilon} e^{-i d D_\phi} z) e^{i \frac{\phi^2}{2}} \frac{d^{|\Gamma|} \phi}{(2\pi i)^{|\Gamma|/2}} \quad (1.25)
 \end{aligned}$$

Iterating,

$$(e^{-i k dt h} f)(z) = \int_{\mathbb{R}^{k|\Gamma|}} f(e^{-i dt \varepsilon} e^{-i d D_{\phi_1}} \dots e^{-i dt \varepsilon} e^{-i d D_{\phi_k}} z) \prod_{\ell=1}^k e^{i \frac{\phi_\ell^2}{2}} \frac{d^{|\Gamma|} \phi_\ell}{(2\pi i)^{|\Gamma|/2}} \quad (1.26)$$

with the notations

$$\begin{aligned}
 \phi_\ell &:= (\{\phi_{j,\ell}\}_{j \in \Gamma}) \in \mathbb{R}^{|\Gamma|} \\
 \phi_\ell^2 &:= \sum_j \phi_{j,\ell}^2 \in \mathbb{R} \\
 d^{|\Gamma|} \phi_\ell &:= \prod_j d\phi_{j,\ell}
 \end{aligned} \quad (1.27)$$

That is, on the (real, scalar) integration variable $\phi_{j,\ell} \in \mathbb{R}$, the first index $j = (j_1, \dots, j_d)$ is a lattice site index and the second index $\ell \in \mathbb{N}$ is a time index. Furthermore

$$dD_{\phi_\ell} = \text{diag}(\{\sqrt{2 u dt} \phi_{j,\ell} - u dt\}_{j \in \Gamma}) \in \mathbb{R}^{|\Gamma| \times |\Gamma|} \quad (1.28)$$

Let us summarize the above formula in part (a) of the following

Theorem 1 Let $h = h_0 + h_{\text{int}} : \mathcal{F} \rightarrow \mathcal{F}$ be the Bose-Hubbard Hamiltonian given by (1.12) and (1.13) and let $\psi \in \mathcal{F}$ be any initial state. Then:

a) In the limit $dt \rightarrow 0$ with $t = t_k = kdt$ fixed, there is the formula

$$(e^{-ikdt} h \psi)(z) = \mathbb{E}[\psi(U_{kdt} z)] \quad (1.29)$$

with unitary evolution matrix

$$U_{kdt} := e^{-idt \varepsilon} e^{-i d D_{\phi_1}} \dots e^{-idt \varepsilon} e^{-i d D_{\phi_k}} \in \mathbb{C}^{|\Gamma| \times |\Gamma|} \quad (1.30)$$

and Fresnel expectation value

$$\mathbb{E}[\cdot] := \int_{\mathbb{R}^{k|\Gamma|}} \cdot \prod_{\ell=1}^k e^{i \frac{\phi_\ell^2}{2}} \frac{d^{|\Gamma|} \phi_\ell}{(2\pi i)^{|\Gamma|/2}} \quad (1.31)$$

b) The evolution matrix $U_{t_k} = U_{kdt}$ is a solution of the following stochastic differential equation (SDE)

$$dU_{t_k} := U_{t_k} - U_{t_{k-1}} = -i U_{t_{k-1}} (\varepsilon dt + \sqrt{2u} dx_{t_k}) \quad (1.32)$$

where dx_{t_k} is the diagonal matrix of Fresnel Brownian motions given by (1.44) below.

Let's consider part (b) of the theorem. Suppose we would have Gaussian densities, let's say 1-dimensional, $e^{-\phi_\ell^2/2} d\phi_\ell/\sqrt{2\pi}$ instead of Fresnel kernels $e^{i \phi_\ell^2/2} d\phi_\ell/\sqrt{2\pi i}$. Then the combination of integration variables

$$x_{t_k} := \sqrt{dt} \sum_{\ell=1}^k \phi_\ell \quad (1.33)$$

would be a standard Brownian motion, the product (with $x_{t_0} := 0$)

$$dW := \prod_{\ell=1}^k e^{-\frac{\phi_\ell^2}{2}} \frac{d\phi_\ell}{\sqrt{2\pi}} = \prod_{\ell=1}^k e^{-\frac{(x_{t_\ell} - x_{t_{\ell-1}})^2}{2dt}} \frac{dx_{t_\ell}}{\sqrt{2\pi} dt} =: \prod_{\ell=1}^k p_{dt}(x_{t_\ell}, x_{t_{\ell-1}}) dx_{t_\ell} \quad (1.34)$$

would be standard Wiener measure and in the limit $dt \rightarrow 0$ there would be the standard Brownian motion calculation rule (Appendix A.1 has a quick reminder)

$$(dx_t)^2 = dt \quad (1.35)$$

and $dx_t dt = dt dt = 0$. In the presence of Fresnel kernels, we can make the same definitions. That is, the combination of integration variables

$$x_{t_k} := \sqrt{dt} \sum_{\ell=1}^k \phi_\ell \quad (1.36)$$

we call a one-dimensional Fresnel Brownian motion if the ϕ_ℓ 's are to be integrated against the product of one-dimensional Fresnel kernels (again with $x_{t_0} := 0$)

$$dF := \prod_{\ell=1}^k e^{i \frac{\phi_\ell^2}{2}} \frac{d\phi_\ell}{\sqrt{2\pi i}} = \prod_{\ell=1}^k e^{i \frac{(x_{t_\ell} - x_{t_{\ell-1}})^2}{2dt}} \frac{dx_{t_\ell}}{\sqrt{2\pi i} dt} =: \prod_{\ell=1}^k q_{dt}(x_{t_\ell}, x_{t_{\ell-1}}) dx_{t_\ell} \quad (1.37)$$

which we then refer to as Fresnel measure. Observe that for both Fresnel and Gaussian kernels we have the equations

$$\int_{\mathbb{R}} k_t(x, y) k_s(y, z) dy = k_{t+s}(x, z) \quad (1.38)$$

$$\int_{\mathbb{R}} k_t(x, y) dy = 1 \quad (1.39)$$

with $k_t \in \{p_t, q_t\}$. Now, what we can use is the fact that in the limit $dt \rightarrow 0$ there are analog calculation rules for Fresnel Brownian motions. That is, there are the following formulae (see Appendices A.1 and A.4 for more background)

$$(dx_t)^2 = i dt \quad (1.40)$$

and $dx_t dt = dt dt = 0$.

Now let's return to the time evolution formula (1.29) of Theorem 1. Instead of 1-dimensional Fresnel kernels we have $|\Gamma|$ -dimensional Fresnel kernels and accordingly $|\Gamma|$ -dimensional Fresnel Brownian motions

$$x_{j,t_k} = x_{j,kdt} := \sqrt{dt} \sum_{\ell=1}^k \phi_{j,\ell} \quad (1.41)$$

where $j \in \Gamma$ again denotes some lattice site. With

$$dx_{j,kdt} := x_{j,kdt} - x_{j,(k-1)dt} = \sqrt{dt} \phi_{j,k} \quad (1.42)$$

we can write

$$\begin{aligned} dD_{\phi_k} &= \text{diag}(\{\sqrt{2u} dx_{j,kdt} - u dt\}_{j \in \Gamma}) \\ &=: \sqrt{2u} dx_{kdt} - u dt Id \end{aligned} \quad (1.43)$$

where we introduced the diagonal matrix of Fresnel Brownian motions

$$dx_{kdt} := \text{diag}(\{dx_{j,kdt}\}_{j \in \Gamma}) \in \mathbb{C}^{|\Gamma| \times |\Gamma|} \quad (1.44)$$

and Id is the $|\Gamma| \times |\Gamma|$ identity matrix. From the calculation rule (1.40) we get the matrix equation

$$(dx_{kdt})^2 = \text{diag}(\{(dx_{j,kdt})^2\}_{j \in \Gamma}) = i dt Id \quad (1.45)$$

Thus, up to terms $O(dt^{3/2})$,

$$\begin{aligned} e^{-i dD_{\phi_k}} &= 1 - i dD_{\phi_k} - \frac{1}{2} (dD_{\phi_k})^2 \\ &= 1 - i\sqrt{2u} dx_{kdt} + i u dt Id - \frac{1}{2} (\sqrt{2u} dx_{kdt} - u dt Id)^2 \\ &= 1 - i\sqrt{2u} dx_{kdt} + i u dt Id - \frac{1}{2} (\sqrt{2u} dx_{kdt})^2 \\ &= 1 - i\sqrt{2u} dx_{kdt} \end{aligned} \quad (1.46)$$

and we arrive at the following SDE for the evolution matrix U_t :

$$\begin{aligned} U_{kdt} &= e^{-idt\varepsilon} e^{-i dD_{\phi_1}} \times \dots \times e^{-idt\varepsilon} e^{-i dD_{\phi_{k-1}}} \times e^{-idt\varepsilon} e^{-i dD_{\phi_k}} \\ &= U_{(k-1)dt} \times e^{-idt\varepsilon} e^{-i dD_{\phi_k}} \\ &\stackrel{(1.46)}{=} U_{(k-1)dt} (1 - i dt \varepsilon) (1 - i\sqrt{2u} dx_{kdt}) \\ &= U_{(k-1)dt} (1 - i dt \varepsilon - i\sqrt{2u} dx_{kdt}) \end{aligned} \quad (1.47)$$

or, with $t_k = kdt$,

$$dU_{t_k} := U_{t_k} - U_{t_{k-1}} = -i U_{t_{k-1}} (dt \varepsilon + \sqrt{2u} dx_{t_k}) \quad (1.48)$$

which completes the derivation of part (b) of Theorem 1. More compactly, this could be written as

$$dU_t = -i U_t (\varepsilon dt + \sqrt{2u} dx_t) \quad (1.49)$$

but we want to remind at this place that when discretizing stochastic differential equations or stochastic integrals it is usually crucial whether a particular time index is a t_k or a t_{k-1} . Throughout this paper, we use the Ito definition which is as follows: If some quantity Q_t satisfies the stochastic differential equation

$$dQ_t = A_t dt + B_t dx_t \quad (1.50)$$

then this is equivalent to the following discrete time update rule

$$Q_{t_k}(\phi_1, \dots, \phi_k) = Q_{t_{k-1}}(\phi_1, \dots, \phi_{k-1}) + A_{t_{k-1}}(\phi_1, \dots, \phi_{k-1}) dt + B_{t_{k-1}}(\phi_1, \dots, \phi_{k-1}) \sqrt{dt} \phi_k \quad (1.51)$$

That is, the new random number or integration variable ϕ_k which enters when going from time t_{k-1} to t_k enters in an explicitly given way, namely through the explicit ϕ_k on the very right of (1.51). There are no ϕ_k 's in the A , B or $Q_{t_{k-1}}$ on the right hand side of (1.51). This then for example has the immediate consequence that

$$E[Q_{t_k}] = E[Q_{t_{k-1}}] + E[A_{t_{k-1}}] dt \quad (1.52)$$

since the diffusive part does not contribute to the expectation value because of $E[\phi_k] = 0$. Thus, quantities Q_t which have a vanishing drift part $A = 0$ are of special importance since their expectation value does not change over time and they are called martingales. Appendix A.2 has a quick reminder on Ito and Stratonovich integrals and why there are different definitions at all.

1.2 Density Matrix Elements from Stochastic Differential Equations

We consider the following normalized initial state with $\lambda = \{\lambda_j\} \in \mathbb{C}^{|\Gamma|}$

$$\psi_0(z) = \psi_0(\{z_j\}) := \prod_j e^{\lambda_j z_j} e^{-\frac{|\lambda_j|^2}{2}} =: e^{\lambda z} e^{-\frac{|\lambda|^2}{2}} \quad (1.53)$$

This is a product of coherent states. The expected number of particles at site j is

$$(\psi_0, a_j^\dagger a_j \psi_0)_{\mathcal{F}} = |\lambda_j|^2 \quad (1.54)$$

which means that $|\lambda_j| = \sqrt{N_j}$ would be a natural choice if we want to have N_j particles at site j . The total number of particles N is given by

$$N = \sum_j N_j = \sum_j |\lambda_j|^2 = |\lambda|^2 \quad (1.55)$$

Let's consider the time evolution of this ψ_0 . According to Theorem 1, we have

$$\psi_t(z) = (e^{-ith} \psi_0)(z) = E[\psi_0(U_t z)] \quad (1.56)$$

where the evolution matrix U_t is given by the SDE

$$dU_t = -i U_t (dt \varepsilon + \sqrt{2u} dx_t) \quad (1.57)$$

with initial condition $U_0 = Id$ and x_t being a Fresnel Brownian motion. We want to calculate the time evolution of the density matrix elements

$$\begin{aligned} (\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} &= (\psi_t, [a_j a_i^+ - \delta_{i,j}] \psi_t)_{\mathcal{F}} \\ &= (a_j^+ \psi_t, a_i^+ \psi_t)_{\mathcal{F}} - \delta_{i,j} (\psi_t, \psi_t)_{\mathcal{F}} \\ &= \int_{\mathbb{C}^{|\Gamma|}} z_j \bar{z}_i |\psi_t(z)|^2 d\mu(z) - \delta_{i,j} \end{aligned} \quad (1.58)$$

From Theorem 1 we have the representations (with $t = t_k = kdt$)

$$\begin{aligned} \psi_t(z) &= \mathbb{E}[\psi_0(U_t z)] = \int \psi_0(U_{x,t} z) dF(\{x_t\}) \\ \overline{\psi_t(z)} &= \overline{\mathbb{E}[\psi_0(U_t z)]} = \int \overline{\psi_0(U_{y,t} z)} d\bar{F}(\{y_t\}) \end{aligned} \quad (1.59)$$

with

$$\begin{aligned} dF &= \prod_{\ell=1}^k e^{+i \frac{\phi_{\ell}^2}{2}} \frac{d^{|\Gamma|} \phi_{\ell}}{(2\pi i)^{|\Gamma|/2}} = \prod_{\ell=1}^k e^{+i \frac{(x_{t_{\ell}} - x_{t_{\ell-1}})^2}{2dt}} \frac{d^{|\Gamma|} x_{t_{\ell}}}{(2\pi i dt)^{|\Gamma|/2}} \\ d\bar{F} &= \prod_{\ell=1}^k e^{-i \frac{\theta_{\ell}^2}{2}} \frac{d^{|\Gamma|} \theta_{\ell}}{[2\pi(-i)]^{|\Gamma|/2}} = \prod_{\ell=1}^k e^{-i \frac{(y_{t_{\ell}} - y_{t_{\ell-1}})^2}{2dt}} \frac{d^{|\Gamma|} y_{t_{\ell}}}{[2\pi(-i)dt]^{|\Gamma|/2}} \end{aligned} \quad (1.60)$$

where $\sqrt{-i} := \bar{\sqrt{i}} = e^{-i \frac{\pi}{4}}$ and $x_{t_{\ell}}$ and $y_{t_{\ell}}$ are $|\Gamma|$ -dimensional Fresnel Brownian motions given by

$$\begin{aligned} x_{t_{\ell}} &= \sqrt{dt} \sum_{m=1}^{\ell} \phi_m \\ y_{t_{\ell}} &= \sqrt{dt} \sum_{m=1}^{\ell} \theta_m \end{aligned} \quad (1.61)$$

With that, we can write

$$\begin{aligned} &\int_{\mathbb{C}^{|\Gamma|}} z_j \bar{z}_i |\psi_t(z)|^2 d\mu(z) \\ &= \int_{\mathbb{C}^{|\Gamma|}} z_j \bar{z}_i \int \psi_0(U_{x,t} z) dF(\{x_t\}) \int \overline{\psi_0(U_{y,t} z)} d\bar{F}(\{y_t\}) d\mu(z) \\ &= \int \int \left\{ \int_{\mathbb{C}^{|\Gamma|}} z_j \bar{z}_i \psi_0(U_{x,t} z) \overline{\psi_0(U_{y,t} z)} d\mu(z) \right\} dF(\{x_t\}) d\bar{F}(\{y_t\}) \end{aligned} \quad (1.62)$$

and in the same way

$$\begin{aligned} \|\psi_t\|_{\mathcal{F}}^2 &= \int_{\mathbb{C}^{|\Gamma|}} |\psi_t(z)|^2 d\mu(z) \\ &= \int \int \left\{ \int_{\mathbb{C}^{|\Gamma|}} \psi_0(U_{x,t} z) \overline{\psi_0(U_{y,t} z)} d\mu(z) \right\} dF(\{x_t\}) d\bar{F}(\{y_t\}) \end{aligned} \quad (1.63)$$

The wavy brackets above are the expectations over the bosonic Fock space, written in the Bargmann-Segal representation, and can be calculated. Since

$$\psi_0(U_{x,t} z) \overline{\psi_0(U_{y,t} z)} = \exp\{U_{x,t}^T \lambda \cdot z\} \exp\{\bar{U}_{y,t}^T \bar{\lambda} \cdot \bar{z}\} e^{-|\lambda|^2} \quad (1.64)$$

with U^T denoting the transpose of U , and because of the formulae

$$\int_{\mathbb{C}^{|\Gamma|}} e^{\lambda z + \bar{\lambda} \bar{z}} d\mu(z) = e^{\lambda \bar{\lambda}}$$

$$\int_{\mathbb{C}^{|\Gamma|}} z_j \bar{z}_i e^{\lambda z + \bar{\lambda} \bar{z}} d\mu(z) = \frac{\partial}{\partial \lambda_j} \frac{\partial}{\partial \bar{\lambda}_i} e^{\lambda \bar{\lambda}} = (\lambda_i \bar{\lambda}_j + \delta_{i,j}) e^{\lambda \bar{\lambda}} \quad (1.65)$$

we obtain the following representations: The norm of ψ_t is given by

$$\|\psi_t\|_{\mathcal{F}}^2 = \mathbb{E}_x \bar{\mathbb{E}}_y \left[\exp \{ U_{x,t}^T \lambda \cdot \bar{U}_{y,t}^T \bar{\lambda} \} \right] e^{-|\lambda|^2} \quad (1.66)$$

and density matrix elements can be written as

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = \mathbb{E}_x \bar{\mathbb{E}}_y \left[[U_{x,t}^T \lambda]_i [\bar{U}_{y,t}^T \bar{\lambda}]_j \exp \{ U_{x,t}^T \lambda \cdot \bar{U}_{y,t}^T \bar{\lambda} \} \right] e^{-|\lambda|^2} \quad (1.67)$$

where we used the notation

$$\mathbb{E}_x \bar{\mathbb{E}}_y [\dots] = \int \int \dots dF(\{x_t\}) d\bar{F}(\{y_t\}) \quad (1.68)$$

for the Fresnel expectations.

Now recall that

$$dU_{x,t} = -i U_{x,t} (dt \varepsilon + \sqrt{2u} dx_t) \quad (1.69)$$

or, since $\varepsilon_{ij} = \varepsilon_{ji}$ or $\varepsilon^T = \varepsilon$,

$$dU_{x,t}^T = -i (dt \varepsilon + \sqrt{2u} dx_t) U_{x,t}^T \quad (1.70)$$

Thus,

$$d(U_{x,t}^T \lambda) = -i (dt \varepsilon + \sqrt{2u} dx_t) U_{x,t}^T \lambda \quad (1.71)$$

and in the same way

$$d(\bar{U}_{y,t}^T \bar{\lambda}) = +i (dt \varepsilon + \sqrt{2u} dy_t) \bar{U}_{y,t}^T \bar{\lambda} \quad (1.72)$$

Thus, if we abbreviate the quantities (where the $\bar{v}$ at this stage is not the complex conjugate of v since it has different integration variables)

$$v = v_{x,t} := U_{x,t}^T \lambda \in \mathbb{C}^{|\Gamma|} \quad (1.73)$$

$$\bar{v} = \bar{v}_{y,t} := \bar{U}_{y,t}^T \bar{\lambda} \in \mathbb{C}^{|\Gamma|}$$

we obtain the SDE system

$$dv = -i (dt \varepsilon + \sqrt{2u} dx_t) v \quad (1.74)$$

$$d\bar{v} = +i (dt \varepsilon + \sqrt{2u} dy_t) \bar{v}$$

with initial conditions

$$v_0 = \lambda \quad (1.75)$$

$$\bar{v}_0 = \bar{\lambda}$$

In coordinates, this reads

$$\begin{aligned} dv_j &= -i dt (\varepsilon v)_j - i \sqrt{2u} v_j dx_j \\ d\bar{v}_j &= +i dt (\varepsilon \bar{v})_j + i \sqrt{2u} \bar{v}_j dy_j \end{aligned} \quad (1.76)$$

or even more explicitly, making also the times and the Fresnel integration variables x and y explicit at the $v, \bar{v}$,

$$\begin{aligned} dv_{j,x,t} &= -i dt \sum_i \varepsilon_{ji} v_{i,x,t} - i \sqrt{2u} v_{j,x,t} dx_{j,t} \\ d\bar{v}_{j,y,t} &= +i dt \sum_i \varepsilon_{ji} \bar{v}_{i,y,t} + i \sqrt{2u} \bar{v}_{j,y,t} dy_{j,t} \end{aligned} \quad (1.77)$$

Then, from (1.67) we obtain the density matrix elements as

$$(\psi_t, a_i^\dagger a_j \psi_t)_{\mathcal{F}} = \mathbb{E}_x \bar{\mathbb{E}}_y [v_i \bar{v}_j e^{v\bar{v}}] e^{-|\lambda|^2} \quad (1.78)$$

if we use the notation

$$v\bar{v} := \sum_j v_j \bar{v}_j = v^T \bar{v} \quad (1.79)$$

Finally, the norm of ψ_t has the representation

$$\|\psi_t\|_{\mathcal{F}}^2 = \mathbb{E}_x \bar{\mathbb{E}}_y [e^{v\bar{v}}] e^{-|\lambda|^2} \quad (1.80)$$

We summarize the results in the following

Theorem 2 *Let ψ_0 be the initial state*

$$\psi_0(z) = \psi_0(\{z_j\}) = \prod_j e^{\lambda_j z_j} e^{-\frac{|\lambda_j|^2}{2}} =: e^{\lambda z} e^{-\frac{|\lambda|^2}{2}} \quad (1.81)$$

and let $\psi_t = e^{-it\hbar} \psi_0$ be the time evolved state with Bose-Hubbard Hamiltonian $h = h_0 + h_{\text{int}}$ given by (1.12) and (1.13). Then there are the following representations:

$$(\psi_t, a_i^\dagger a_j \psi_t)_{\mathcal{F}} = \mathbb{E}_x \bar{\mathbb{E}}_y [v_{i,x,t} \bar{v}_{j,y,t} e^{v_{x,t} \bar{v}_{y,t}}] e^{-|\lambda|^2} \quad (1.82)$$

$$\|\psi_t\|_{\mathcal{F}}^2 = \mathbb{E}_x \bar{\mathbb{E}}_y [e^{v_{x,t} \bar{v}_{y,t}}] e^{-|\lambda|^2} \quad (1.83)$$

with Fresnel expectations $\mathbb{E}_x \bar{\mathbb{E}}_y [\cdot]$ given by (1.68) and (1.60) above, and the $v, \bar{v} \in \mathbb{C}^{|\Gamma|}$ are given by the SDE system

$$\begin{aligned} dv_j &= -i dt (\varepsilon v)_j - i \sqrt{2u} v_j dx_j \\ d\bar{v}_j &= +i dt (\varepsilon \bar{v})_j + i \sqrt{2u} \bar{v}_j dy_j \end{aligned} \quad (1.84)$$

with initial conditions $v_{x,0} = \lambda, \bar{v}_{y,0} = \bar{\lambda}$.

Now, in the next chapter we will see that the combination $v_{x,t} \bar{v}_{y,t}$ is a martingale and as a consequence, the exponential $e^{v_{x,t} \bar{v}_{y,t}}$ can be absorbed into the Fresnel integration measure. This has the effect that the density matrix elements are then simply given by

$$(\psi_t, a_i^\dagger a_j \psi_t)_{\mathcal{F}} = \mathbb{E}_{\tilde{x}} \bar{\mathbb{E}}_{\tilde{y}} [v_{i,\tilde{x},t} \bar{v}_{j,\tilde{y},t}]$$

where the $v_{\tilde{x},t}, \bar{v}_{\tilde{y},t}$ are given by the transformed SDE system

$$\begin{aligned} dv_j &= -i dt (\varepsilon v)_j - i 2u dt v_j \bar{v}_j v_j - i \sqrt{2u} v_j d\tilde{x}_j \\ d\bar{v}_j &= +i dt (\varepsilon \bar{v})_j + i 2u dt v_j \bar{v}_j \bar{v}_j + i \sqrt{2u} \bar{v}_j d\tilde{y}_j \end{aligned}$$

with transformed Fresnel Brownian motions

$$\begin{aligned} d\tilde{x}_{j,t_\ell} &:= dx_{j,t_\ell} - \sqrt{2u} dt (v_j \bar{v}_j)_{t_{\ell-1}} \\ d\tilde{y}_{j,t_\ell} &:= dy_{j,t_\ell} - \sqrt{2u} dt (v_j \bar{v}_j)_{t_{\ell-1}} \end{aligned}$$

So, let's look at the details.

2 Martingale Property and Girsanov Transformation

2.1 Unitary Time Evolution as a Martingale

Recall from Theorem 1 that the time evolution $\psi_t = e^{-it(h_0 + h_{\text{int}})} \psi_0$ of some initial state $\psi_0 = \psi_0(z)$ can be written as a Fresnel expectation value

$$\psi_t(z) = \mathbb{E}[\psi_0(U_t z)] = \mathbb{E}_x[\psi_0(U_{x,t} z)] = \int \psi_0(U_{x,t} z) dF(\{x_s\}_{0 \leq s \leq t}) \quad (2.1)$$

where the unitary evolution matrix is given by the SDE

$$dU_{x,t} = -i U_{x,t} (dt \varepsilon + \sqrt{2u} dx_t) \quad (2.2)$$

with initial value $U_{x,0} = Id$. The norm of ψ_t is given by

$$\|\psi_t\|_{\mathcal{F}}^2 = (\psi_t, \psi_t)_{\mathcal{F}} = \int_{\mathbb{C}^{|\Gamma|}} \psi_t(z) \overline{\psi_t(z)} d\mu(z) \quad (2.3)$$

with $d\mu(z)$ given by (1.7). For the complex conjugated ψ_t we use integration variables or Fresnel Brownian motions $\{y_s\}_{0 \leq s \leq t}$ and write

$$\overline{\psi_t(z)} = \bar{\mathbb{E}}_y[\overline{\psi_0(U_{y,t} z)}] = \int \overline{\psi_0(U_{y,t} z)} d\bar{F}(\{y_s\}_{0 \leq s \leq t}) \quad (2.4)$$

such that, as in (1.63) of the last chapter,

$$\begin{aligned} \|\psi_t\|_{\mathcal{F}}^2 &= \int_{\mathbb{C}^{|\Gamma|}} \psi_t(z) \overline{\psi_t(z)} d\mu(z) \\ &= \int_{\mathbb{C}^{|\Gamma|}} \mathbb{E}_x[\psi_0(U_{x,t} z)] \bar{\mathbb{E}}_y[\overline{\psi_0(U_{y,t} z)}] d\mu(z) \\ &= \mathbb{E}_x \bar{\mathbb{E}}_y \left[\int_{\mathbb{C}^{|\Gamma|}} \psi_0(U_{x,t} z) \overline{\psi_0(U_{y,t} z)} d\mu(z) \right] \end{aligned} \quad (2.5)$$

Now we have

$$d\mu(Uz) = d\mu(z) \quad (2.6)$$

for any unitary U . Thus, with the substitution $z = U_{y,t}^+ w$ with $U^+ = \bar{U}^T$ being the adjoint matrix, and renaming the w back to z , we obtain

$$\|\psi_t\|_{\mathcal{F}}^2 = \mathbb{E}_x \bar{\mathbb{E}}_y \left[\int_{\mathbb{C}^{|\Gamma|}} \psi_0(U_{x,t} U_{y,t}^+ z) \overline{\psi_0(z)} d\mu(z) \right] \quad (2.7)$$

This quantity has to be independent of t , we have to have

$$\begin{aligned}\|\psi_t\|_{\mathcal{F}}^2 &= \mathbb{E}_x \bar{\mathbb{E}}_y \left[\int_{\mathbb{C}^{|\Gamma|}} \psi_0(U_{x,t} U_{y,t}^+) \overline{\psi_0(z)} d\mu(z) \right] \\ &\stackrel{!}{=} \int_{\mathbb{C}^{|\Gamma|}} \psi_0(z) \overline{\psi_0(z)} d\mu(z) = \|\psi_0\|_{\mathcal{F}}^2\end{aligned}\quad (2.8)$$

How can this be understood from a stochastic calculus point of view? We have

$$\begin{aligned}dU_{x,t} &= -i U_{x,t} (dt \varepsilon + \sqrt{2u} dx_t) \\ dU_{y,t}^+ &= +i (dt \varepsilon + \sqrt{2u} dy_t) U_{y,t}^+\end{aligned}\quad (2.9)$$

Since $dx_t dy_t = 0$, we also have $dU_{x,t} dU_{y,t}^+ = 0$ such that

$$\begin{aligned}d(U_{x,t} U_{y,t}^+) &= dU_{x,t} U_{y,t}^+ + U_{x,t} dU_{y,t}^+ + dU_{x,t} dU_{y,t}^+ \\ &= -i U_{x,t} (dt \varepsilon + \sqrt{2u} dx_t) U_{y,t}^+ + i U_{x,t} (dt \varepsilon + \sqrt{2u} dy_t) U_{y,t}^+ + 0 \\ &= -i \sqrt{2u} U_{x,t} (dx_t - dy_t) U_{y,t}^+ \\ &= -i \sqrt{4u} U_{x,t} d\xi_t U_{y,t}^+\end{aligned}\quad (2.10)$$

if we put (the eta's will be used later, not now)

$$d\xi_t := \frac{dx_t - dy_t}{\sqrt{2}}, \quad d\eta_t := \frac{dx_t + dy_t}{\sqrt{2}}\quad (2.11)$$

Equation (2.10) means that the matrix $U_{x,t} U_{y,t}^+$ is a martingale, its $d(U_{x,t} U_{y,t}^+)$ has no drift part, no dt part, but only a diffusive part, a $d\xi_t$ or dy_t part. And since

$$\mathbb{E}[dx_t] = \bar{\mathbb{E}}[dy_t] = 0\quad (2.12)$$

one then has

$$\mathbb{E}\bar{\mathbb{E}}[d(U_{x,t} U_{y,t}^+)] = 0\quad (2.13)$$

which results in

$$\mathbb{E}\bar{\mathbb{E}}[U_{x,t} U_{y,t}^+] = U_{x,0} U_{y,0}^+ = Id\quad (2.14)$$

However, in (2.8) we have not directly an expectation of the matrix $U_{x,t} U_{y,t}^+$ itself, but we have an arbitrary function of it, so we have to consider an expectation of the form

$$\mathbb{E}_x \bar{\mathbb{E}}_y \left[f(U_{x,t} U_{y,t}^+) \right]\quad (2.15)$$

where $f : \mathbb{C}^{|\Gamma| \times |\Gamma|} \rightarrow \mathbb{C}$ is an arbitrary function. These quantities should also be time independent, how can we understand that? Let's abbreviate for the moment

$$M_t := U_{x,t} U_{y,t}^+ = (M_{ij})_{i,j \in \Gamma}\quad (2.16)$$

Then, with the Ito formula (Appendix A.2 has a quick reminder),

$$df(M_t) = \sum_{i,j \in \Gamma} \frac{\partial f}{\partial M_{ij}} dM_{ij} + \frac{1}{2} \sum_{i,j \in \Gamma} \sum_{k,\ell \in \Gamma} \frac{\partial^2 f}{\partial M_{ij} \partial M_{k\ell}} dM_{ij} dM_{k\ell}\quad (2.17)$$

In the equation above, also the k, ℓ are temporarily used as lattice site indices, they are no time indices here. The first sum is purely diffusive since

$$dM_{ij} = -i \sqrt{4u} [U_{x,t} d\xi_t U_{y,t}^+]_{i,j}\quad (2.18)$$

has no dt part. And the second sum actually vanishes since

$$\begin{aligned} dM_{ij} dM_{k\ell} &= -4u [U_{x,t} d\xi_t U_{y,t}^+]_{i,j} [U_{x,t} d\xi_t U_{y,t}^+]_{k,\ell} \\ &= -4u \sum_{m,n \in \Gamma} [U_{x,t}]_{i,m} d\xi_{m,t} [U_{y,t}^+]_{m,j} [U_{x,t}]_{k,n} d\xi_{n,t} [U_{y,t}^+]_{n,\ell} \\ d\xi_{m,t} d\xi_{n,t} &\stackrel{=}{=} 0 \end{aligned} \quad (2.19)$$

Namely,

$$\begin{aligned} d\xi_{m,t} d\xi_{n,t} &= \frac{1}{2} (dx_{m,t} - dy_{m,t}) (dx_{n,t} - dy_{n,t}) \\ &= \frac{1}{2} (dx_{m,t} dx_{n,t} + dy_{m,t} dy_{n,t} - dx_{m,t} dy_{n,t} - dy_{m,t} dx_{n,t}) \\ &= \frac{1}{2} (dx_{m,t} dx_{n,t} + dy_{m,t} dy_{n,t} - 0 - 0) \end{aligned} \quad (2.20)$$

For $m = n$, this becomes

$$\begin{aligned} d\xi_{m,t} d\xi_{m,t} &= \frac{1}{2} ((dx_{m,t})^2 + (dy_{m,t})^2) \\ &= \frac{1}{2} (i dt - i dt) = 0 \end{aligned} \quad (2.21)$$

And for $m \neq n$, this is simply

$$d\xi_{m,t} d\xi_{n,t} = \frac{1}{2} (0 + 0) = 0 \quad (2.22)$$

Thus we end up with

$$df(M_t) = -i\sqrt{4u} \sum_{i,j} \frac{\partial f}{\partial M_{ij}} [U_{x,t} d\xi_t U_{y,t}^+]_{i,j} \quad (2.23)$$

which is purely diffusive and this results in

$$\mathbb{E}_x \bar{\mathbb{E}}_y [df(M_t)] = 0 \quad (2.24)$$

and accordingly

$$\mathbb{E}_x \bar{\mathbb{E}}_y [f(M_t)] = f(M_0) + \int_0^t \mathbb{E}_x \bar{\mathbb{E}}_y [df(M_s)] = f(M_0) \quad (2.25)$$

for arbitrary f . Let's summarize these observations in the following

Theorem 3 Let $U_{x,t}$ be the unitary evolution matrix of Theorem 1 such that the time evolution of an arbitrary state $\psi \in \mathcal{F}$ can be written as

$$(e^{-ikdt} \psi)(z) = \mathbb{E}_x [\psi(U_{x,kdt} z)] \quad (2.26)$$

with Fresnel expectation $\mathbb{E}_x[\cdot]$ given by (1.60) and (1.68). Then, for arbitrary $f: \mathbb{C}^{|\Gamma| \times |\Gamma|} \rightarrow \mathbb{C}$, the quantity $f(U_{x,t} U_{y,t}^+)$ is a martingale, its $df(U_{x,t} U_{y,t}^+)$ has no dt -part, and we have the following identity:

$$\mathbb{E}_x \bar{\mathbb{E}}_y [f(U_{x,t} U_{y,t}^+)] = f(U_0 U_0^+) = f(\text{Id}) \quad (2.27)$$

In particular, for any time evolved state $\psi_t = e^{-it h} \psi_0$,

$$\begin{aligned} \|\psi_t\|_{\mathcal{F}}^2 &= \int_{\mathbb{C}^{|\Gamma|}} \mathbb{E}_x \bar{\mathbb{E}}_y [\psi_0(U_{x,t} U_{y,t}^+ \overline{\psi_0(z)})] d\mu(z) \\ &= \int_{\mathbb{C}^{|\Gamma|}} \psi_0(z) \overline{\psi_0(z)} d\mu(z) = \|\psi_0\|_{\mathcal{F}}^2. \end{aligned} \quad (2.28)$$

2.2 Girsanov Transformed SDE System for the Density Matrix Elements

Recall the representations of Theorem 2, for the initial state $\psi_0(z) = e^{\lambda z} e^{-\frac{|\lambda|^2}{2}}$, the density matrix elements can be written as

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = \mathbb{E}_x \bar{\mathbb{E}}_y [v_{i,x,t} \bar{v}_{j,y,t} e^{v_{x,t} \bar{v}_{y,t}}] e^{-|\lambda|^2} \quad (2.29)$$

with vector valued functions $v = v_{x,t} \in \mathbb{C}^{|\Gamma|}$ and $\bar{v} = \bar{v}_{y,t} \in \mathbb{C}^{|\Gamma|}$ which are given by the SDE system

$$\begin{aligned} dv &= -i(dt \varepsilon + \sqrt{2u} dx_t) v \\ d\bar{v} &= +i(dt \varepsilon + \sqrt{2u} dy_t) \bar{v} \end{aligned} \quad (2.30)$$

with initial conditions $v_{x,0} = \lambda$, $\bar{v}_{y,0} = \bar{\lambda}$. Since $dx_{j,t} dy_{j,t} = 0$, we obtain

$$\begin{aligned} d(v^T \bar{v}) &= dv^T \bar{v} + v^T d\bar{v} + dv^T d\bar{v} \\ &= -i v^T (dt \varepsilon + \sqrt{2u} dx_t) \bar{v} + i v^T (dt \varepsilon + \sqrt{2u} dy_t) \bar{v} + 0 \\ &= -i \sqrt{2u} v^T (dx_t - dy_t) \bar{v} \\ &= -i \sqrt{2u} \sum_j v_j \bar{v}_j (dx_{j,t} - dy_{j,t}) \end{aligned} \quad (2.31)$$

That is, the quantity $v^T \bar{v} = \sum_j v_j \bar{v}_j \equiv v \bar{v}$, we omit the transpose sign in the following, is a martingale. Now we write

$$\begin{aligned} (v \bar{v})_{kdt} &= (v \bar{v})_0 + \sum_{\ell=1}^k [(v \bar{v})_{\ell dt} - (v \bar{v})_{(\ell-1)dt}] \\ &= (v \bar{v})_0 + \sum_{\ell=1}^k d(v \bar{v})_{\ell dt} \\ &= (v \bar{v})_0 - i \sqrt{2u} \sum_{\ell=1}^k \sum_j (v_j \bar{v}_j)_{(\ell-1)dt} (dx_{j,\ell dt} - dy_{j,\ell dt}) \\ &= |\lambda|^2 - i \sqrt{2u} \sum_{\ell=1}^k \sum_j (v_j \bar{v}_j)_{(\ell-1)dt} (\phi_{j,\ell} - \theta_{j,\ell}) \end{aligned} \quad (2.32)$$

such that

$$e^{(v \bar{v})_{kdt}} e^{-|\lambda|^2} = e^{(v \bar{v})_{kdt} - (v \bar{v})_0} = \exp \left\{ -i \sqrt{2u} \sum_{\ell=1}^k \sum_j (v_j \bar{v}_j)_{(\ell-1)dt} (\phi_{j,\ell} - \theta_{j,\ell}) \right\} \quad (2.33)$$

with integration variables

$$\begin{aligned} dx_{j,\ell dt} &= \sqrt{dt} \phi_{j,\ell} \\ dy_{j,\ell dt} &= \sqrt{dt} \theta_{j,\ell} \end{aligned} \quad (2.34)$$

In terms of the $\phi_{j,\ell}, \theta_{j,\ell}$ variables, the Fresnel measure reads

$$\mathbb{E}_x \bar{\mathbb{E}}_y [\dots] = \int_{\mathbb{R}^{k|\Gamma|}} \int_{\mathbb{R}^{k|\Gamma|}} \dots \prod_{\ell=1}^k e^{\frac{i}{2} \sum_j (\phi_{j,\ell}^2 - \theta_{j,\ell}^2)} \frac{d^{|\Gamma|} \phi_\ell d^{|\Gamma|} \theta_\ell}{(2\pi)^{|\Gamma|}} \quad (2.35)$$

Consider the ℓ 'th term on the right hand side of (2.33),

$$\sum_j (v_j \bar{v}_j)_{(\ell-1)dt} (\phi_{j,\ell} - \theta_{j,\ell}) \quad (2.36)$$

The ϕ_ℓ and θ_ℓ show up in an explicit linear form, since the quantities

$$(v_j \bar{v}_j)_{(\ell-1)dt} = (v_j \bar{v}_j)_{(\ell-1)dt} \left(\{\phi_m, \theta_m\}_{m=1}^{\ell-1} \right) \quad (2.37)$$

depend only on ϕ 's and θ 's at earlier times $t_1, \dots, t_{\ell-1}$. Thus, we can absorb them into the integration measure simply by completing the square. In the mathematics literature, the corresponding change of variables then is called a Girsanov transformation. Thus, this is a very elementary calculation, but, since this is a key step, let us be very explicit and proceed line by line. The result is summarized in Theorem 4 below.

We have at time $t = t_k = kdt$

$$\begin{aligned} (\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} &= \mathbb{E} \bar{\mathbb{E}} [v_i \bar{v}_j e^{v \bar{v}}] e^{-|\lambda|^2} \\ &= \int_{\mathbb{R}^{2k|\Gamma|}} v_{i,kdt} \bar{v}_{j,kdt} \prod_{\ell=1}^k \exp \left\{ -i\sqrt{2udt} \sum_j (v_j \bar{v}_j)_{(\ell-1)dt} (\phi_{j,\ell} - \theta_{j,\ell}) \right\} \times \\ &\quad \prod_{\ell=1}^k \exp \left\{ \frac{i}{2} \sum_j (\phi_{j,\ell}^2 - \theta_{j,\ell}^2) \right\} \frac{d^{|\Gamma|} \phi_\ell d^{|\Gamma|} \theta_\ell}{(2\pi)^{|\Gamma|}} \end{aligned} \quad (2.38)$$

Consider the ℓ -th factor. The exponentials with the ϕ_ℓ variables combine to

$$\begin{aligned} &\exp \left\{ -i\sqrt{2udt} \sum_j (v_j \bar{v}_j)_{(\ell-1)dt} \phi_{j,\ell} \right\} \times \exp \left\{ \frac{i}{2} \sum_j \phi_{j,\ell}^2 \right\} \\ &= \exp \left\{ \frac{i}{2} \sum_j \left[\phi_{j,\ell}^2 - 2\sqrt{2udt} (v_j \bar{v}_j)_{(\ell-1)dt} \phi_{j,\ell} \right] \right\} \\ &= \exp \left\{ \frac{i}{2} \sum_j \left[\phi_{j,\ell} - \sqrt{2udt} (v_j \bar{v}_j)_{(\ell-1)dt} \right]^2 \right\} \times \exp \left\{ -\frac{i}{2} \sum_j 2udt (v_j \bar{v}_j)_{(\ell-1)dt}^2 \right\} \end{aligned} \quad (2.39)$$

The exponentials with the θ_ℓ variables combine to

$$\begin{aligned} & \exp \left\{ +i\sqrt{2udt} \sum_j (v_j \bar{v}_j)_{(\ell-1)dt} \theta_{j,\ell} \right\} \times \exp \left\{ -\frac{i}{2} \sum_j \theta_{j,\ell}^2 \right\} \\ &= \exp \left\{ -\frac{i}{2} \sum_j \left[\theta_{j,\ell}^2 - 2\sqrt{2udt} (v_j \bar{v}_j)_{(\ell-1)dt} \theta_{j,\ell} \right] \right\} \\ &= \exp \left\{ -\frac{i}{2} \sum_j \left[\theta_{j,\ell} - \sqrt{2udt} (v_j \bar{v}_j)_{(\ell-1)dt} \right]^2 \right\} \times \exp \left\{ +\frac{i}{2} \sum_j 2udt (v_j \bar{v}_j)_{(\ell-1)dt}^2 \right\} \end{aligned} \quad (2.40)$$

Observe that the last exponentials in (2.39) and (2.40)

$$\exp \left\{ -\frac{i}{2} \sum_j 2udt (v_j \bar{v}_j)_{(\ell-1)dt}^2 \right\} \times \exp \left\{ +\frac{i}{2} \sum_j 2udt (v_j \bar{v}_j)_{(\ell-1)dt}^2 \right\} = 1 \quad (2.41)$$

cancel each other.

Now we make the substitution of variables

$$\begin{aligned} \tilde{\phi}_{j,\ell} &:= \phi_{j,\ell} - \sqrt{2udt} (v_j \bar{v}_j)_{(\ell-1)dt} \\ \tilde{\theta}_{j,\ell} &:= \theta_{j,\ell} - \sqrt{2udt} (v_j \bar{v}_j)_{(\ell-1)dt} \end{aligned} \quad (2.42)$$

or equivalently

$$\begin{aligned} d\tilde{x}_{j,t_\ell} &:= dx_{j,t_\ell} - \sqrt{2u} dt (v_j \bar{v}_j)_{(\ell-1)dt} \\ d\tilde{y}_{j,t_\ell} &:= dy_{j,t_\ell} - \sqrt{2u} dt (v_j \bar{v}_j)_{(\ell-1)dt} \end{aligned} \quad (2.43)$$

Then we can write

$$\begin{aligned} (\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} &= E_x \bar{E}_y [v_i \bar{v}_j e^{v\bar{v}}] e^{-|\lambda|^2} \\ &= E_{\tilde{x}} \bar{E}_{\tilde{y}} [v_i \bar{v}_j] \end{aligned} \quad (2.44)$$

where in terms of the transformed variables $\tilde{x}$, $\tilde{y}$ the v_j and $\bar{v}_j$ are given by the transformed SDE system

$$\begin{aligned} dv_j &= -i dt (\varepsilon v)_j - i\sqrt{2u} v_j dx_j \\ &= -i dt (\varepsilon v)_j - i\sqrt{2u} v_j [d\tilde{x}_j + \sqrt{2u} dt v_j \bar{v}_j] \\ &= -i dt (\varepsilon v)_j - i2u dt v_j \bar{v}_j v_j - i\sqrt{2u} v_j d\tilde{x}_j \end{aligned} \quad (2.45)$$

and

$$\begin{aligned} d\bar{v}_j &= +i dt (\varepsilon \bar{v})_j + i\sqrt{2u} \bar{v}_j dy_j \\ &= +i dt (\varepsilon \bar{v})_j + i\sqrt{2u} \bar{v}_j [d\tilde{y}_j + \sqrt{2u} dt v_j \bar{v}_j] \\ &= +i dt (\varepsilon \bar{v})_j + i2u dt v_j \bar{v}_j \bar{v}_j + i\sqrt{2u} \bar{v}_j d\tilde{y}_j \end{aligned} \quad (2.46)$$

with initial conditions

$$\begin{aligned} v_{j,0} &= \lambda_j \\ \bar{v}_{j,0} &= \bar{\lambda}_j \end{aligned} \quad (2.47)$$

Recall that

$$|\lambda|^2 = N \quad (2.48)$$

has the meaning of total number of particles. Thus, if we divide (2.45) and (2.46) through $|\lambda| = \sqrt{N}$ and put

$$\begin{aligned} w_j &:= v_j / |\lambda| \\ \bar{w}_j &:= \bar{v}_j / |\lambda| \end{aligned} \quad (2.49)$$

we obtain

$$\begin{aligned} dw_j &= -i dt (\varepsilon w)_j - i 2uN dt w_j \bar{w}_j w_j - i \sqrt{2u} w_j d\tilde{x}_j \\ d\bar{w}_j &= +i dt (\varepsilon \bar{w})_j + i 2uN dt w_j \bar{w}_j \bar{w}_j + i \sqrt{2u} \bar{w}_j d\tilde{y}_j \end{aligned} \quad (2.50)$$

or, with

$$g := uN \quad (2.51)$$

$$\begin{aligned} dw_j &= -i dt (\varepsilon w)_j - i 2g dt w_j \bar{w}_j w_j - i \sqrt{2g/N} w_j d\tilde{x}_j \\ d\bar{w}_j &= +i dt (\varepsilon \bar{w})_j + i 2g dt w_j \bar{w}_j \bar{w}_j + i \sqrt{2g/N} \bar{w}_j d\tilde{y}_j \end{aligned} \quad (2.52)$$

Thus, in the limit $N \rightarrow \infty$ with $g = uN$ fixed, the diffusive part vanishes, the SDE reduces to a deterministic ODE system and the exact density matrix elements are given by

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = \mathbb{E}_{\tilde{x}} \bar{\mathbb{E}}_{\tilde{y}} [v_i \bar{v}_j] = N \times w_i(t) \bar{w}_j(t) \quad (2.53)$$

with the $w, \bar{w}$ given by the ODE system

$$\begin{aligned} \dot{w}_j &= -i (\varepsilon w)_j - i 2g w_j \bar{w}_j w_j \\ \dot{\bar{w}}_j &= +i (\varepsilon \bar{w})_j + i 2g w_j \bar{w}_j \bar{w}_j \end{aligned} \quad (2.54)$$

with initial conditions

$$\begin{aligned} w_j(0) &= \lambda_j / |\lambda| \\ \bar{w}_j(0) &= \bar{\lambda}_j / |\lambda| \end{aligned} \quad (2.55)$$

Observe that now the $\bar{w}_j$ are the true complex conjugates of the w_j . Before we proceed to the analog calculation for number states in the next section, let's summarize the results in the following

Theorem 4 Recall the SDE representation of Theorem 2 above,

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = \mathbb{E}_{\tilde{x}} \bar{\mathbb{E}}_{\tilde{y}} [v_{i,x,t} \bar{v}_{j,y,t} e^{v_{x,t} \bar{v}_{y,t}}] e^{-|\lambda|^2} \quad (2.56)$$

with

$$\begin{aligned} dv_j &= -i dt (\varepsilon v)_j - i \sqrt{2u} v_j dx_j \\ d\bar{v}_j &= +i dt (\varepsilon \bar{v})_j + i \sqrt{2u} \bar{v}_j dy_j \end{aligned} \quad (2.57)$$

Then, with the Girsanov transformation

$$\begin{aligned} d\tilde{x}_{j,t_\ell} &:= dx_{j,t_\ell} - \sqrt{2u} dt (v_j \bar{v}_j)_{(\ell-1)dt} \\ d\tilde{y}_{j,t_\ell} &:= dy_{j,t_\ell} - \sqrt{2u} dt (v_j \bar{v}_j)_{(\ell-1)dt} \end{aligned} \quad (2.58)$$

the exponential $e^{(v\bar{v})_t - |\lambda|^2} = e^{(v\bar{v})_t - (v\bar{v})_0}$ can be absorbed into the Fresnel integration measure, there is the identity

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = E_{\tilde{x}} \bar{E}_{\tilde{y}} [v_{i, \tilde{x}, t} \bar{v}_{j, \tilde{y}, t}] \quad (2.59)$$

with

$$\begin{aligned} dv_j &= -i dt (\varepsilon v)_j - i 2u dt v_j \bar{v}_j v_j - i \sqrt{2u} v_j d\tilde{x}_j \\ d\bar{v}_j &= +i dt (\varepsilon \bar{v})_j + i 2u dt v_j \bar{v}_j \bar{v}_j + i \sqrt{2u} \bar{v}_j d\tilde{y}_j \end{aligned} \quad (2.60)$$

In the limit $N \rightarrow \infty$ with $g = uN$ fixed, we have the exact representation

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = N \times w_i(t) \bar{w}_j(t) \quad (2.61)$$

with $\bar{w}_j$ now being the true complex conjugate of w_j and the w_j are given by the ODE system

$$\dot{w}_j = -i (\varepsilon w)_j - i 2g w_j \bar{w}_j w_j \quad (2.62)$$

with initial conditions $w_j(0) = \lambda_j / |\lambda|$. Equation (2.62) is the time dependent discrete Gross Pitaevskii equation, here with a general hopping matrix $\varepsilon = (\varepsilon_{ij})_{i,j \in \Gamma}$ which may also include some on-diagonal trapping potentials $\epsilon_j = \varepsilon_{jj}$ from the Hamiltonian (1.1).

2.3 Number States

Let's consider the dynamics of number states which are used to describe the dynamics of Bose-Einstein condensates. They are given by the following initial state

$$\psi_0(z) = \psi_0(\{z_j\}) = \frac{1}{\sqrt{N!} |\lambda|^N} \left(\sum_j \lambda_j z_j \right)^N = \frac{(\lambda z)^N}{\sqrt{N!} |\lambda|^N} \quad (2.63)$$

with

$$|\lambda|^2 = \sum_j |\lambda_j|^2 = N \quad (2.64)$$

There are the following formulae which are standard expectations over the bosonic Fock space, here written again in the Bargmann-Segal representation:

$$\frac{1}{N!} \int_{\mathbb{C}^{|\Gamma|}} (\lambda z)^N (\bar{\lambda} \bar{z})^N d\mu(z) = (|\lambda|^2)^N \quad (2.65)$$

$$\frac{1}{N!} \int_{\mathbb{C}^{|\Gamma|}} z_i \bar{z}_j (\lambda z)^N (\bar{\lambda} \bar{z})^N d\mu(z) = \delta_{i,j} (|\lambda|^2)^N + N \bar{\lambda}_i \lambda_j (|\lambda|^2)^{N-1} \quad (2.66)$$

Thus, with the condition (2.64), we have the following time zero expectations:

$$(\psi_0, \psi_0)_{\mathcal{F}} = \int_{\mathbb{C}^{|\Gamma|}} |\psi_0(z)|^2 d\mu(z) = \frac{|\lambda|^{2N}}{N^N} = 1 \quad (2.67)$$

$$(\psi_0, a_i^+ a_j \psi_0)_{\mathcal{F}} = \int_{\mathbb{C}^{|\Gamma|}} z_j \bar{z}_i |\psi_0(z)|^2 d\mu(z) = \delta_{i,j} = N \frac{\lambda_i \bar{\lambda}_j}{|\lambda|^2} = \lambda_i \bar{\lambda}_j \quad (2.68)$$

Now, let's consider the time t formulae. From (1.58) and (1.62) we have for an arbitrary initial state ψ_0

$$\begin{aligned} (\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} &= \int_{\mathbb{C}^{|\Gamma|}} z_j \bar{z}_i |\psi_t(z)|^2 d\mu(z) = \delta_{i,j} \\ &= \int \int \left\{ \int_{\mathbb{C}^{|\Gamma|}} z_j \bar{z}_i \psi_0(U_{x,t} z) \overline{\psi_0(U_{y,t} z)} d\mu(z) \right\} dF(\{x_t\}) d\bar{F}(\{y_t\}) = \delta_{i,j} \end{aligned} \quad (2.69)$$

The wavy bracket we can evaluate with the formulae from above. We obtain

$$\begin{aligned} & \int_{\mathbb{C}^{|\Gamma|}} z_j \bar{z}_i \psi_0(U_{x,t} z) \overline{\psi_0(U_{y,t} \bar{z})} d\mu(z) \\ &= \frac{1}{N!N^N} \int_{\mathbb{C}^{|\Gamma|}} z_j \bar{z}_i (U_{x,t}^T \lambda \cdot z)^N (\bar{U}_{y,t}^T \bar{\lambda} \cdot \bar{z})^N d\mu(z) \\ &= \frac{1}{N^N} \left\{ \delta_{i,j} (\lambda \cdot U_{x,t} U_{y,t}^+ \bar{\lambda})^N + N [U_{x,t}^T \lambda]_i [\bar{U}_{y,t}^T \bar{\lambda}]_j (\lambda \cdot U_{x,t} U_{y,t}^+ \bar{\lambda})^{N-1} \right\} \end{aligned} \quad (2.70)$$

Thus,

$$\begin{aligned} (\psi_0, a_i^+ a_j \psi_0)_{\mathcal{F}} &= \\ & \frac{1}{N^N} \mathbb{E}_x \bar{\mathbb{E}}_y \left[\delta_{i,j} (\lambda \cdot U_{x,t} U_{y,t}^+ \bar{\lambda})^N + N [U_{x,t}^T \lambda]_i [\bar{U}_{y,t}^T \bar{\lambda}]_j (\lambda \cdot U_{x,t} U_{y,t}^+ \bar{\lambda})^{N-1} \right] - \delta_{i,j} \\ &= \mathbb{E}_x \bar{\mathbb{E}}_y \left[[U_{x,t}^T \lambda]_i [\bar{U}_{y,t}^T \bar{\lambda}]_j (U_{x,t}^T \lambda \cdot U_{y,t}^+ \bar{\lambda})^{N-1} \right] / (\lambda \cdot \bar{\lambda})^{N-1} \end{aligned} \quad (2.71)$$

since

$$\frac{1}{N^N} \mathbb{E}_x \bar{\mathbb{E}}_y \left[\delta_{i,j} (\lambda \cdot U_{x,t} U_{y,t}^+ \bar{\lambda})^N \right] = \delta_{i,j} \quad (2.72)$$

because of Theorem 3 of Section 2.1. Now we can proceed as in the preceeding Section 2.2. We introduce the variables

$$\begin{aligned} v_j &= v_{x,t,j} := [U_{x,t}^T \lambda]_j \\ \bar{v}_j &= \bar{v}_{y,t,j} := [\bar{U}_{y,t}^T \bar{\lambda}]_j \end{aligned} \quad (2.73)$$

and from the matrix equations

$$\begin{aligned} dU_{x,t}^T &= -i (dt \varepsilon + \sqrt{2u} dx_t) U_{x,t}^T \\ d\bar{U}_{y,t}^T &= +i (dt \varepsilon + \sqrt{2u} dy_t) \bar{U}_{y,t}^T \end{aligned} \quad (2.74)$$

we obtain

$$\begin{aligned} dv_j &= -i dt (\varepsilon v)_j + \sqrt{2u} dx_{j,t} v_j \\ d\bar{v}_j &= +i dt (\varepsilon \bar{v})_j + \sqrt{2u} dy_{j,t} \bar{v}_j \end{aligned} \quad (2.75)$$

Furthermore,

$$(U_{x,t}^T \lambda \cdot U_{y,t}^+ \bar{\lambda})^{N-1} = \left(\sum_j v_j \bar{v}_j \right)^{N-1} =: (v \bar{v})^{N-1} \quad (2.76)$$

Thus, for the density matrix elements we obtain the following representation:

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = \mathbb{E} \bar{\mathbb{E}} [v_i \bar{v}_j (v \bar{v})^{N-1}] / (\lambda \bar{\lambda})^{N-1} \quad (2.77)$$

As in the last section, we can make a Girsanov transformation and absorb the quantity $(v \bar{v})^{N-1}$ into the Fresnel measure. Since the $v, \bar{v}$ obey exactly the same SDEs as in the last section with the same initial conditions

$$\begin{aligned} v_0 &= \lambda \\ \bar{v}_0 &= \bar{\lambda} \end{aligned} \quad (2.78)$$

Equation (2.31) remains unchanged:

$$d(v\bar{v}) = -i\sqrt{2u} \sum_j v_j \bar{v}_j (dx_{j,t} - dy_{j,t}) \quad (2.79)$$

Now we abbreviate

$$P(v\bar{v}) := (v\bar{v})^{N-1} \quad (2.80)$$

$$p(v\bar{v}) := P'(v\bar{v})/P(v\bar{v}) = [\log P]'(v\bar{v}) = (N-1)/(v\bar{v}) \quad (2.81)$$

Then, since $(v\bar{v})_0 = \lambda\bar{\lambda}$ and, more importantly, $[d(v\bar{v})]^2 = 0$, we can write

$$\frac{(v_t \bar{v}_t)^{N-1}}{(\lambda\bar{\lambda})^{N-1}} = e^{\log P(v_t \bar{v}_t) - \log P(v_0 \bar{v}_0)} = e^{\int_0^t p(v_s \bar{v}_s) d(v\bar{v})_s} \quad (2.82)$$

With the discrete time variables of Section 2.2, the exponent reads as follows:

$$\begin{aligned} \int_0^{t_k} p(v_s \bar{v}_s) d(v\bar{v})_s &= \sum_{\ell=1}^k p[(v\bar{v})_{(\ell-1)dt}] d(v\bar{v})_{\ell dt} \\ &= -i\sqrt{2u} \sum_{\ell=1}^k p[(v\bar{v})_{(\ell-1)dt}] \sum_j (v_j \bar{v}_j)_{(\ell-1)dt} (dx_{j,\ell dt} - dy_{j,\ell dt}) \\ &= -i\sqrt{2udt}(N-1) \sum_{\ell=1}^k \sum_j \left(\frac{v_j \bar{v}_j}{v\bar{v}}\right)_{(\ell-1)dt} (\phi_{j,\ell} - \theta_{j,\ell}) \end{aligned} \quad (2.83)$$

Thus, now we have to make the following substitution of variables:

$$\begin{aligned} \tilde{\phi}_{j,\ell} &:= \phi_{j,\ell} - \sqrt{2udt}(N-1) (v_j \bar{v}_j / v\bar{v})_{(\ell-1)dt} \\ \tilde{\theta}_{j,\ell} &:= \theta_{j,\ell} - \sqrt{2udt}(N-1) (v_j \bar{v}_j / v\bar{v})_{(\ell-1)dt} \end{aligned} \quad (2.84)$$

or equivalently

$$\begin{aligned} d\tilde{x}_{j,t_\ell} &:= dx_{j,t_\ell} - \sqrt{2u}(N-1) dt (v_j \bar{v}_j / v\bar{v})_{(\ell-1)dt} \\ d\tilde{y}_{j,t_\ell} &:= dy_{j,t_\ell} - \sqrt{2u}(N-1) dt (v_j \bar{v}_j / v\bar{v})_{(\ell-1)dt} \end{aligned} \quad (2.85)$$

Then we can write

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = E_x \bar{E}_y [v_i \bar{v}_j (v\bar{v})^{N-1}] / (\lambda\bar{\lambda})^{N-1} = E_x \bar{E}_y [v_i \bar{v}_j] \quad (2.86)$$

where in terms of the transformed variables $\tilde{x}, \tilde{y}$ the v_j and $\bar{v}_j$ are given by the transformed SDE system

$$\begin{aligned} dv_j &= -i dt (\varepsilon v)_j - i\sqrt{2u} v_j dx_j \\ &= -i dt (\varepsilon v)_j - i2u(N-1) dt \frac{v_j \bar{v}_j}{v\bar{v}} v_j - i\sqrt{2u} v_j d\tilde{x}_j \end{aligned} \quad (2.87)$$

and

$$\begin{aligned} d\bar{v}_j &= +i dt (\varepsilon \bar{v})_j + i\sqrt{2u} \bar{v}_j dy_j \\ &= +i dt (\varepsilon \bar{v})_j + i2u(N-1) dt \frac{v_j \bar{v}_j}{v\bar{v}} \bar{v}_j + i\sqrt{2u} \bar{v}_j d\tilde{y}_j \end{aligned} \quad (2.88)$$

with initial conditions $(v, \bar{v})_0 = (\lambda, \bar{\lambda})$. Dividing the system through $|\lambda| = \sqrt{N}$ and introducing again the normalized quantities

$$\begin{aligned} w &:= v / |\lambda| \\ \bar{w} &:= \bar{v} / |\lambda| \end{aligned} \quad (2.89)$$

we obtain the following ODE system in the limit $N \rightarrow \infty$ with $g = UN$ fixed:

$$\begin{aligned}\dot{w}_j &= -i(\varepsilon w)_j - i2g \frac{w_j \bar{w}_j}{w \bar{w}} w_j \\ \dot{\bar{w}}_j &= +i(\varepsilon \bar{w})_j + i2g \frac{w_j \bar{w}_j}{w \bar{w}} \bar{w}_j\end{aligned}\quad (2.90)$$

In particular, for a symmetric hopping matrix $\varepsilon = \varepsilon^T$

$$\begin{aligned}\frac{d}{dt}(w \bar{w}) &= \sum_j \{ \dot{w}_j \bar{w}_j + w_j \dot{\bar{w}}_j \} \\ &= -i \sum_j \{ (\varepsilon w)_j \bar{w}_j - w_j (\varepsilon \bar{w})_j \} - i2g \sum_j \left\{ \frac{w_j \bar{w}_j}{w \bar{w}} w_j \bar{w}_j - w_j \frac{w_j \bar{w}_j}{w \bar{w}} \bar{w}_j \right\} \\ &= 0\end{aligned}\quad (2.91)$$

Thus we have $(w \bar{w})_t = 1$ for all t and the ODE system (2.90) reduces again to the time dependent discrete Gross-Pitaevskii equation. We summarize in the following

Theorem 5 Consider the following normalized initial number state,

$$\psi_0(z) = \psi_0(\{z_j\}) = \frac{1}{\sqrt{N!} |\lambda|^N} \left(\sum_j \lambda_j z_j \right)^N = \frac{(\lambda z)^N}{\sqrt{N!} |\lambda|^N} \quad (2.92)$$

with $|\lambda|^2 = N$. Then the time t density matrix elements can be written as

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = \mathbb{E} \bar{\mathbb{E}}[v_i \bar{v}_j] \quad (2.93)$$

where the $v_j, \bar{v}_j$ are given by the SDE system

$$\begin{aligned}dv_j &= -i(\varepsilon v)_j dt - i2u(N-1) \frac{v_j \bar{v}_j}{v \bar{v}} v_j dt - i\sqrt{2u} v_j dx_j \\ d\bar{v}_j &= +i(\varepsilon \bar{v})_j dt + i2u(N-1) \frac{v_j \bar{v}_j}{v \bar{v}} \bar{v}_j dt + i\sqrt{2u} \bar{v}_j dy_j\end{aligned}\quad (2.94)$$

with initial conditions $(v, \bar{v})_0 = (\lambda, \bar{\lambda})$. In the large N limit with $g = uN$ fixed, this reduces again, as in Theorem 4 where the initial state was a coherent state, to the time dependent discrete Gross-Pitaevskii equation

$$\begin{aligned}\dot{w}_j &= -i(\varepsilon w)_j - i2g w_j \bar{w}_j w_j \\ \dot{\bar{w}}_j &= +i(\varepsilon \bar{w})_j + i2g w_j \bar{w}_j \bar{w}_j\end{aligned}\quad (2.95)$$

with normalized quantities $(w, \bar{w}) := (v, \bar{v})/|\lambda|$, initial conditions $(w, \bar{w})_0 = (\lambda, \bar{\lambda})/|\lambda|$ and density matrix elements given by $(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = N w_{i,t} \bar{w}_{j,t}$.

The results of Theorems 4 and 5 are in line with rigorous results in the continuous case in the large N limit. In [2], Benedikter, Porta and Schlein give an overview on rigorous derivations of effective evolution equations and results concerning the continuous time dependent Gross-Pitaevskii equation are summarized in chapter 5. The article [3] focusses solely on the GP equation. Pickl [4, 5] and more recently Jeblick, Leopold and Pickl [6] also gave rigorous derivations of the continuous time dependent GP equation. The issue has a longer history with more people involved, more background can be found in [2]. The fact that the coherent states and the number states of Theorem 4 and 5 show similar dynamics in the large N limit has also been observed by Schachenmayer, Daley and Zoller in [7].

3 PDE Representations

3.1 Untransformed Case, before Girsanov Transformation

In the untransformed case, the SDE representation for the density matrix elements is given by Theorem 2 of Section 1.2. We have

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = \mathbb{E} \mathbb{E}[v_i \bar{v}_j e^{v\bar{v}}] e^{-|\lambda|^2} \quad (3.1)$$

with

$$\begin{aligned} dv_j &= -i dt (\varepsilon v)_j - i \sqrt{2u} v_j dx_j \\ d\bar{v}_j &= +i dt (\varepsilon \bar{v})_j + i \sqrt{2u} \bar{v}_j dy_j \end{aligned} \quad (3.2)$$

According to the Fresnel version of Kolmogorov's backward equation, a one dimensional version is given in formula (A.81) with Fresnel expectation (A.74) in Appendix A.4, the quantity (3.1) has a PDE representation. In order to write it down, we need the operator A which is associated with the SDE system (3.2). To this end, we consider some arbitrary complex-valued function f of $2|\Gamma|$ arguments,

$$f = f(\{v_j\}, \{\bar{v}_j\}) : \mathbb{C}^{2|\Gamma|} \rightarrow \mathbb{C} \quad (3.3)$$

Because of

$$\begin{aligned} (dv_j)^2 &= \{-i dt (\varepsilon v)_j - i \sqrt{2u} v_j dx_j\}^2 \\ &= \{-i \sqrt{2u} v_j dx_j\}^2 \\ &= -2u v_j^2 (dx_j)^2 \\ &= -i 2u dt v_j^2 \end{aligned} \quad (3.4)$$

and

$$\begin{aligned} (d\bar{v}_j)^2 &= \{+i dt (\varepsilon \bar{v})_j + i \sqrt{2u} \bar{v}_j dy_j\}^2 \\ &= \{+i \sqrt{2u} \bar{v}_j dy_j\}^2 \\ &= -2u \bar{v}_j^2 (dy_j)^2 \\ &= +i 2u dt \bar{v}_j^2 \end{aligned} \quad (3.5)$$

and, for $i \neq j$,

$$dv_i d\bar{v}_i = dv_i d\bar{v}_j = dv_i dv_j = d\bar{v}_i d\bar{v}_j = 0 \quad (3.6)$$

we obtain with the Fresnel version of the Ito lemma

$$\begin{aligned} df &= \sum_j \left\{ \frac{\partial f}{\partial v_j} dv_j + \frac{\partial f}{\partial \bar{v}_j} d\bar{v}_j \right\} + \frac{1}{2} \sum_j \left\{ \frac{\partial^2 f}{\partial v_j^2} (dv_j)^2 + \frac{\partial^2 f}{\partial \bar{v}_j^2} (d\bar{v}_j)^2 \right\} \\ &= -i dt \sum_j \left\{ (\varepsilon v)_j \frac{\partial f}{\partial v_j} - (\varepsilon \bar{v})_j \frac{\partial f}{\partial \bar{v}_j} \right\} \\ &\quad - iu dt \sum_j \left\{ v_j^2 \frac{\partial^2 f}{\partial v_j^2} - \bar{v}_j^2 \frac{\partial^2 f}{\partial \bar{v}_j^2} \right\} + \text{diffusive} \\ &=: Af + \text{diffusive} \end{aligned} \quad (3.7)$$

Thus, the expectation

$$F_t := \mathbb{E}\mathbb{E}\left[f(\{v_{j,x,t}\}, \{\bar{v}_{j,y,t}\})\right] \quad (3.8)$$

considered as a function of its initial values $(v_0, \bar{v}_0) = (\{v_{j,0}\}, \{\bar{v}_{j,0}\}) = (\lambda, \bar{\lambda})$,

$$F_t = F_t(\{v_{j,0}\}, \{\bar{v}_{j,0}\}) \quad (3.9)$$

can be obtained as the solution of the parabolic second order PDE (the zero subscripts on the v 's are then usually omitted in the notation, $v_{j,0} \rightarrow v_j$ in the following PDE)

$$\frac{\partial F}{\partial t} = AF = -i \sum_j \left\{ (\varepsilon v)_j \frac{\partial F}{\partial v_j} - (\varepsilon \bar{v})_j \frac{\partial F}{\partial \bar{v}_j} \right\} - iu \sum_j \left\{ v_j^2 \frac{\partial^2 F}{\partial v_j^2} - \bar{v}_j^2 \frac{\partial^2 F}{\partial \bar{v}_j^2} \right\} \quad (3.10)$$

with initial condition

$$F_0 = f(\{v_j\}, \{\bar{v}_j\}) \quad (3.11)$$

If we introduce the differential operators

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\text{int}} \quad (3.12)$$

with

$$\mathcal{L}_0 := \sum_j \left\{ (\varepsilon v)_j \frac{\partial}{\partial v_j} - (\varepsilon \bar{v})_j \frac{\partial}{\partial \bar{v}_j} \right\} \quad (3.13)$$

$$\mathcal{L}_{\text{int}} := u \sum_j \left\{ v_j^2 \frac{\partial^2}{\partial v_j^2} - \bar{v}_j^2 \frac{\partial^2}{\partial \bar{v}_j^2} \right\} \quad (3.14)$$

the solution may be written as

$$F_t = e^{-it\mathcal{L}} F_0 \quad (3.15)$$

which one could try to evaluate through small or approximate large Trotter steps according to

$$F_t = e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}})} F_0 \approx \left(e^{-i\frac{t}{k}\mathcal{L}_0} e^{-i\frac{t}{k}\mathcal{L}_{\text{int}}} \right)^k F_0 \quad (3.16)$$

For the density matrix elements, we have to calculate the expectation (3.1) and hence the initial condition $F_0 = f$ is given by

$$F_0(\{v_j\}, \{\bar{v}_j\}) = v_i \bar{v}_j e^{v\bar{v} - |\lambda|^2} \quad (3.17)$$

The time evolution is then obtained through

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}})} \left\{ v_i \bar{v}_j e^{v\bar{v} - |\lambda|^2} \right\} \Big|_{v=\lambda, \bar{v}=\bar{\lambda}} \quad (3.18)$$

In particular, the solution of the PDE (3.10) is not needed in the whole $(v, \bar{v})$ -space, but only at one specific point

$$(\{v_j\}, \{\bar{v}_j\}) = (\{\lambda_j\}, \{\bar{\lambda}_j\}) . \quad (3.19)$$

3.2 Transformed Case, after Girsanov Transformation

After Girsanov transformation, we have the SDE representation which is given by Theorem 4 of Section 2.2,

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = \mathbb{E} \bar{\mathbb{E}}[v_i \bar{v}_j] \quad (3.20)$$

with

$$\begin{aligned} dv_j &= -i dt (\varepsilon v)_j - i 2u dt v_j \bar{v}_j v_j - i \sqrt{2u} v_j dx_j \\ d\bar{v}_j &= +i dt (\varepsilon \bar{v})_j + i 2u dt v_j \bar{v}_j \bar{v}_j + i \sqrt{2u} \bar{v}_j dy_j \end{aligned} \quad (3.21)$$

We still have

$$\begin{aligned} (dv_j)^2 &= -i 2u dt v_j^2 \\ (d\bar{v}_j)^2 &= +i 2u dt \bar{v}_j^2 \end{aligned} \quad (3.22)$$

and, for $i \neq j$,

$$dv_i d\bar{v}_i = dv_i d\bar{v}_j = dv_i dv_j = d\bar{v}_i d\bar{v}_j = 0 \quad (3.23)$$

Thus, again with the Ito lemma, for some arbitrary $f = f(\{v_j\}, \{\bar{v}_j\})$,

$$\begin{aligned} df &= \sum_j \left\{ \frac{\partial f}{\partial v_j} dv_j + \frac{\partial f}{\partial \bar{v}_j} d\bar{v}_j \right\} + \frac{1}{2} \sum_j \left\{ \frac{\partial^2 f}{\partial v_j^2} (dv_j)^2 + \frac{\partial^2 f}{\partial \bar{v}_j^2} (d\bar{v}_j)^2 \right\} \\ &= -i dt \sum_j \left\{ (\varepsilon v)_j \frac{\partial f}{\partial v_j} - (\varepsilon \bar{v})_j \frac{\partial f}{\partial \bar{v}_j} \right\} - i 2u dt \sum_j \left\{ v_j \bar{v}_j v_j \frac{\partial f}{\partial v_j} - v_j \bar{v}_j \bar{v}_j \frac{\partial f}{\partial \bar{v}_j} \right\} \\ &\quad - i u dt \sum_j \left\{ v_j^2 \frac{\partial^2 f}{\partial v_j^2} - \bar{v}_j^2 \frac{\partial^2 f}{\partial \bar{v}_j^2} \right\} + \text{diffusive} \end{aligned} \quad (3.24)$$

such that the expectation

$$F_t := \mathbb{E} \bar{\mathbb{E}} \left[f(\{v_{j,x,t}\}, \{\bar{v}_{j,y,t}\}) \right] \quad (3.25)$$

considered again as a function of its initial values $(v_0, \bar{v}_0) = (\{v_{j,0}\}, \{\bar{v}_{j,0}\}) = (\lambda, \bar{\lambda})$,

$$F_t = F_t(\{v_{j,0}\}, \{\bar{v}_{j,0}\}) \quad (3.26)$$

and omitting the subscripts 0 on the $v, \bar{v}$ in the following, can be obtained as the solution of the second order PDE

$$\begin{aligned} \frac{\partial F}{\partial t} &= -i \sum_j \left\{ (\varepsilon v)_j \frac{\partial F}{\partial v_j} - (\varepsilon \bar{v})_j \frac{\partial F}{\partial \bar{v}_j} \right\} - i 2u \sum_j v_j \bar{v}_j \left\{ v_j \frac{\partial F}{\partial v_j} - \bar{v}_j \frac{\partial F}{\partial \bar{v}_j} \right\} \\ &\quad - i u \sum_j \left\{ v_j^2 \frac{\partial^2 F}{\partial v_j^2} - \bar{v}_j^2 \frac{\partial^2 F}{\partial \bar{v}_j^2} \right\} \end{aligned} \quad (3.27)$$

with initial condition

$$F_0 = f(\{v_j\}, \{\bar{v}_j\}) \quad (3.28)$$

We write $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\text{int}}$ as in the untransformed case and abbreviate the additional term, which is due to the exponential $e^{v\bar{v}}$ which in turn comes from the initial state ψ_0 which was chosen to be a product of coherent states, as

$$\mathcal{L}_{\psi_0} := 2u \sum_j v_j \bar{v}_j \left\{ v_j \frac{\partial}{\partial v_j} - \bar{v}_j \frac{\partial}{\partial \bar{v}_j} \right\} \quad (3.29)$$

Then the solution of the PDE (3.27) can be written as

$$F_t = e^{-it(\mathcal{L} + \mathcal{L}_{\psi_0})} F_0 \quad (3.30)$$

For the density matrix elements, we now have to calculate the expectation (3.20) instead of (3.1) and hence the initial condition F_0 is simply given by

$$F_0(\{v_j\}, \{\bar{v}_j\}) = v_i \bar{v}_j \quad (3.31)$$

instead of the $v_i \bar{v}_j e^{v\bar{v} - |\lambda|^2}$ which we had in the untransformed case. Thus, the time evolved density matrix elements are obtained through

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_{\psi_0})} \{v_i \bar{v}_j\} \Big|_{v=\lambda, \bar{v}=\bar{\lambda}} \quad (3.32)$$

Again, the solution of the PDE (3.27) is not needed in the whole $(v, \bar{v})$ -space, but only at one specific point $(v, \bar{v}) = (\lambda, \bar{\lambda})$.

3.3 The PDE Version of the Girsanov Transformation Formula

By comparison of (3.18) and (3.32), apparently there has to be the identity

$$e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}})} \{f(v, \bar{v}) e^{v\bar{v} - |\lambda|^2}\} \Big|_{v=\lambda, \bar{v}=\bar{\lambda}} = e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_{\psi_0})} \{f(v, \bar{v})\} \Big|_{v=\lambda, \bar{v}=\bar{\lambda}} \quad (3.33)$$

for arbitrary functions $f(v, \bar{v})$. This identity has the following generalization which can be obtained by redoing the calculations of chapter 1 and 2 for an arbitrary initial state, not necessarily for a coherent state: Let $P = P(v\bar{v})$ be some (usually positive when restricted to real values, since it come from a $\|\psi_t\|^2$) arbitrary function of one real or complex variable. Then

$$e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}})} \{f(v, \bar{v}) \frac{P(v\bar{v})}{P(\lambda\bar{\lambda})}\} \Big|_{v=\lambda, \bar{v}=\bar{\lambda}} = e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P)} \{f(v, \bar{v})\} \Big|_{v=\lambda, \bar{v}=\bar{\lambda}} \quad (3.34)$$

or equivalently

$$e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}})} \{P(v\bar{v}) f(v, \bar{v})\} = P(v\bar{v}) \times e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P)} \{f(v, \bar{v})\} \quad (3.35)$$

with

$$\mathcal{L}_P := 2u \frac{P'(v\bar{v})}{P(v\bar{v})} \sum_j v_j \bar{v}_j \left\{ v_j \frac{\partial}{\partial v_j} - \bar{v}_j \frac{\partial}{\partial \bar{v}_j} \right\} \quad (3.36)$$

and $P'(x) = dP/dx$.

Since (3.35) is completely independent of any stochastics, just some algebraic statement concerning derivatives, let us also give an independent proof, thereby confirming the validity of the stochastic formalism¹ which has been used so far: First, one calculates that for any $P = P(v\bar{v}) = P(\sum_j v_j \bar{v}_j)$, one has, using $\varepsilon_{ij} = \varepsilon_{ji}$ for the $\mathcal{L}_0$ equation,

$$\mathcal{L}_0 P = 0 \quad (3.37)$$

$$\mathcal{L}_{\text{int}} P = 0 \quad (3.38)$$

Since $\mathcal{L}_0$ is a first order operator, one has for arbitrary $f = f(\{v_j\}, \{\bar{v}_j\})$

$$\mathcal{L}_0(Pf) = \mathcal{L}_0(P) \times f + P \times \mathcal{L}_0(f) = P \times \mathcal{L}_0(f) \quad (3.39)$$

¹ recall that we are using the stochastic calculus formalism with respect to Fresnel measure, not with Wiener measure, which is not part of standard rigorous textbook mathematics

Furthermore,

$$\begin{aligned}
 \mathcal{L}_{\text{int}}(Pf) &= u \sum_j \left\{ v_j^2 \frac{\partial^2}{\partial v_j^2} - \bar{v}_j^2 \frac{\partial^2}{\partial \bar{v}_j^2} \right\} (Pf) \\
 &= \mathcal{L}_{\text{int}}(P) \times f + P \times \mathcal{L}_{\text{int}}(f) + 2u \sum_j \left\{ v_j^2 \frac{\partial P}{\partial v_j} \frac{\partial f}{\partial v_j} - \bar{v}_j^2 \frac{\partial P}{\partial \bar{v}_j} \frac{\partial f}{\partial \bar{v}_j} \right\} \\
 &= P \times \mathcal{L}_{\text{int}}(f) + 2u \sum_j \left\{ v_j^2 P' \bar{v}_j \frac{\partial f}{\partial v_j} - \bar{v}_j^2 P' v_j \frac{\partial f}{\partial \bar{v}_j} \right\} \\
 &= P \times \mathcal{L}_{\text{int}}(f) + 2u P' \sum_j v_j \bar{v}_j \left\{ v_j \frac{\partial f}{\partial v_j} - \bar{v}_j \frac{\partial f}{\partial \bar{v}_j} \right\} \\
 &= P \times [\mathcal{L}_{\text{int}}(f) + \mathcal{L}_P(f)] \tag{3.40}
 \end{aligned}$$

Thus,

$$(\mathcal{L}_0 + \mathcal{L}_{\text{int}})(Pf) = P \times (\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P)(f) \tag{3.41}$$

and by induction

$$\begin{aligned}
 (\mathcal{L}_0 + \mathcal{L}_{\text{int}})^{n+1}(Pf) &= (\mathcal{L}_0 + \mathcal{L}_{\text{int}}) \{ (\mathcal{L}_0 + \mathcal{L}_{\text{int}})^n(Pf) \} \\
 &= (\mathcal{L}_0 + \mathcal{L}_{\text{int}}) \{ P \times (\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P)^n(f) \} \\
 &\stackrel{(3.41)}{=} P \times (\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P) \{ (\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P)^n(f) \} \\
 &= P \times (\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P)^{n+1}(f) \tag{3.42}
 \end{aligned}$$

This proves (3.35). Let us summarize the results of this chapter in the following

Theorem 6 For an arbitrary real symmetric hopping matrix $\varepsilon = (\varepsilon_{ij}) = (\varepsilon_{ji})$, define the differential operators

$$\mathcal{L}_0 := \sum_j \left\{ (\varepsilon v)_j \frac{\partial}{\partial v_j} - (\varepsilon \bar{v})_j \frac{\partial}{\partial \bar{v}_j} \right\} = \sum_{i,j} \varepsilon_{ij} \left\{ v_i \frac{\partial}{\partial v_j} - \bar{v}_i \frac{\partial}{\partial \bar{v}_j} \right\} \tag{3.43}$$

$$\mathcal{L}_{\text{int}} := u \sum_j \left\{ v_j^2 \frac{\partial^2}{\partial v_j^2} - \bar{v}_j^2 \frac{\partial^2}{\partial \bar{v}_j^2} \right\} \tag{3.44}$$

Furthermore, for some arbitrary function of one variable $P = P(v\bar{v}) = P(\sum_j v_j \bar{v}_j)$, put

$$\mathcal{L}_P := 2u \frac{P'(v\bar{v})}{P(v\bar{v})} \sum_j v_j \bar{v}_j \left\{ v_j \frac{\partial}{\partial v_j} - \bar{v}_j \frac{\partial}{\partial \bar{v}_j} \right\} \tag{3.45}$$

Then:

a) The density matrix elements of Theorem 2 can be calculated through the following formula, this is the untransformed case before Girsanov transformation:

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}})} \left\{ v_i \bar{v}_j e^{v\bar{v} - |\lambda|^2} \right\} \Big|_{v=\lambda, \bar{v}=\bar{\lambda}} \tag{3.46}$$

b) The density matrix elements of Theorem 2 can be calculated through the following equivalent formula, obtained from the SDE representation (2.59), (2.60) after Girsanov transformation:

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P)} \left\{ v_i \bar{v}_j \right\} \Big|_{v=\lambda, \bar{v}=\bar{\lambda}} \tag{3.47}$$

with $P(x) = e^x$.

c) For an arbitrary function $P = P(x)$ of one variable, there is the following general identity:

$$e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}})} \{ P(v\bar{v}) f(v, \bar{v}) \} = P(v\bar{v}) \times e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P)} \{ f(v, \bar{v}) \} \quad (3.48)$$

with $f = f(v, \bar{v}) = f(\{v_j\}, \{\bar{v}_j\})$ being an arbitrary function of $2|\Gamma|$ variables.

4 An Explicit Solvable Test Case: The 0D Bose-Hubbard Model

Since stochastic calculus with Fresnel Brownian motions instead of standard Brownian motions is not part of rigorous textbook mathematics, let's make an additional check of the formalism by applying it to an explicit solvable test case, the 0D Bose-Hubbard model. The term 0D Bose-Hubbard model we borrowed from the paper [8] of Ray, Ostmann, Simon, Grossmann and Strunz, where the model also had to serve as a test example. Besides of just being a test case, the purpose of this chapter is also to give some intuition for the approximation which will be used in Section 5.3 to take the diffusive part of the SDE system into account.

In the Bargmann-Segal representation (1.4), the Hamiltonian of the 0D Bose-Hubbard model is simply

$$h = h_0 + h_{\text{int}} := \varepsilon z \frac{d}{dz} + u z^2 \frac{d^2}{dz^2} \quad (4.1)$$

We choose the initial state

$$\psi_0(z) := e^{\lambda z} e^{-|z|^2/2} \quad (4.2)$$

with $\lambda \in \mathbb{C}$ and consider the time evolution

$$\psi_t := e^{-ith} \psi_0 \quad (4.3)$$

We want to calculate the quantity, with $a = d/dz$, $a^+ = z$,

$$\begin{aligned} (\psi_t, a \psi_t)_{\mathcal{F}} &= (a^+ \psi_t, \psi_t)_{\mathcal{F}} = \int_{\mathbb{C}} d\mu(z) z |\psi_t(z)|^2 \\ &= \int_{\mathbb{R}^2} \frac{d\text{Re}z d\text{Im}z}{\pi} e^{-|z|^2} z |\psi_t(z)|^2 \end{aligned} \quad (4.4)$$

Since

$$h z^n = \{\varepsilon n + u n(n-1)\} z^n =: h_n z^n \quad (4.5)$$

we have

$$\psi_t(z) = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} e^{-ith_n} z^n e^{-|z|^2/2} \quad (4.6)$$

such that

$$\begin{aligned}
 (\psi_t, a \psi_t)_{\mathcal{F}} &= \sum_{n,m=0}^{\infty} e^{-it(h_n-h_m)} \frac{\lambda^n \bar{\lambda}^m}{n! m!} \int_{\mathbb{R}^2} \frac{d^2 z}{\pi} e^{-|z|^2} z^{n+1} \bar{z}^m e^{-|\lambda|^2} \\
 &= \sum_{n=0}^{\infty} e^{-it(h_n-h_{n+1})} \frac{\lambda^n \bar{\lambda}^{n+1}}{n! (n+1)!} \int_{\mathbb{R}^2} \frac{d^2 z}{\pi} e^{-|z|^2} |z|^{2(n+1)} e^{-|\lambda|^2} \\
 &= \sum_{n=0}^{\infty} e^{+it(h_{n+1}-h_n)} \frac{\lambda^n \bar{\lambda}^{n+1}}{n!} e^{-|\lambda|^2}
 \end{aligned} \quad (4.7)$$

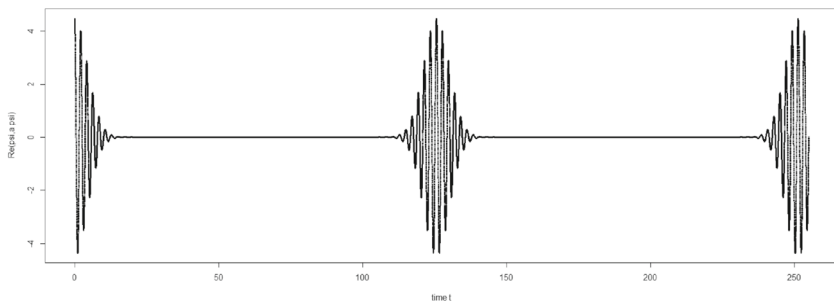
Since

$$h_{n+1} - h_n = \varepsilon - u + u(2n+1) = \varepsilon + 2un \quad (4.8)$$

we end up with

$$\begin{aligned}
 (\psi_t, a \psi_t)_{\mathcal{F}} &= \bar{\lambda} \sum_{n=0}^{\infty} e^{+it(\varepsilon+2un)} \frac{(\lambda \bar{\lambda})^n}{n!} e^{-|\lambda|^2} \\
 &= \bar{\lambda} e^{i\varepsilon t} \exp\{-(1 - e^{2iut}) |\lambda|^2\}
 \end{aligned} \quad (4.9)$$

This quantity has already collapse and revivals, if we plot $\text{Re}(\psi_t, a \psi_t)_{\mathcal{F}}$ for $\varepsilon = 2$, $u = g/N$ with $g = 0.5$ and $N = |\lambda|^2 = 20$, we get



Let's apply Theorem 2. We get the following representation:

$$(\psi_t, a \psi_t)_{\mathcal{F}} = \mathbb{E}_x \bar{\mathbb{E}}_y \left[\bar{v}_{y,t} e^{v_{x,t} \bar{v}_{y,t}} \right] e^{-|\lambda|^2} \quad (4.10)$$

where the $v_t, \bar{v}_t \in \mathbb{C}$ are given by the SDEs

$$\begin{aligned}
 dv_t &= -i dt \varepsilon v_t - i \sqrt{2u} v_t dx_t \\
 d\bar{v}_t &= +i dt \varepsilon \bar{v}_t + i \sqrt{2u} \bar{v}_t dy_t
 \end{aligned} \quad (4.11)$$

with initial conditions $v_0 = \lambda$, $\bar{v}_0 = \bar{\lambda}$. If we would have Wiener measure instead of Fresnel measure, this would be a geometric Brownian motion. Here we have Fresnel measure with calculation rules

$$\begin{aligned}
 (dx_t)^2 &= +i dt \\
 (dy_t)^2 &= -i dt
 \end{aligned} \quad (4.12)$$

and obtain the solutions

$$\begin{aligned} v_t &= v_0 e^{-i(\varepsilon-u)t - i\sqrt{2u}x_t} \\ \bar{v}_t &= \bar{v}_0 e^{+i(\varepsilon-u)t + i\sqrt{2u}y_t} \end{aligned} \quad (4.13)$$

Namely, the Ito formula applied to $v_t = v_0 e^{-i(\varepsilon-u)t - i\sqrt{2u}x_t} = v(x_t, t)$ gives

$$\begin{aligned} dv_t &= \frac{\partial v}{\partial x} dx_t + \frac{1}{2} \frac{\partial^2 v}{\partial x^2} (dx_t)^2 + \frac{\partial v}{\partial t} dt \\ &= -i\sqrt{2u} v_t dx_t + \frac{1}{2} (-i\sqrt{2u})^2 v_t (dx_t)^2 - i(\varepsilon - u) v_t dt \\ &\stackrel{(4.12)}{=} -i\sqrt{2u} v_t dx_t + \frac{1}{2} (-i\sqrt{2u})^2 v_t (+i) dt - i(\varepsilon - u) v_t dt \\ &= -i\sqrt{2u} v_t dx_t - i\varepsilon dt v_t \end{aligned} \quad (4.14)$$

For some integrand which depends on x_t only and not on earlier $\{x_{t'}\}_{t' < t}$, Fresnel or Wiener expectations reduce to 1-dimensional integrals (Appendix A.4 has a general formula in (A.84)). We have

$$\begin{aligned} \mathbb{E}_x \bar{\mathbb{E}}_y [f(x_t, y_t)] &= \int_{\mathbb{R}^2} f(x_t, y_t) e^{i\frac{x_t^2 - y_t^2}{2t}} \frac{dx_t dy_t}{2\pi t} \\ &= \int_{\mathbb{R}^2} f(\sqrt{t}x, \sqrt{t}y) e^{i\frac{x^2 - y^2}{2}} \frac{dx dy}{2\pi} \end{aligned} \quad (4.15)$$

Now we substitute

$$\xi = \frac{x - y}{\sqrt{2}}, \quad \eta = \frac{x + y}{\sqrt{2}} \quad (4.16)$$

which gives

$$e^{i\frac{x^2 - y^2}{2}} \frac{dx dy}{2\pi} = e^{i\xi\eta} \frac{d\xi d\eta}{2\pi} \quad (4.17)$$

The quantities in the integrand in (4.15) are given by (4.10),

$$e^{v_{x,t} \bar{v}_{y,t}} = \exp\{|\lambda|^2 e^{-i\sqrt{2u}(x_t - y_t)}\} = \exp\{|\lambda|^2 e^{-i\sqrt{4ut}\xi}\} \quad (4.18)$$

and

$$\begin{aligned} \bar{v}_{y,t} e^{v_{x,t} \bar{v}_{y,t}} &= \bar{\lambda} e^{+i(\varepsilon-u)t + i\sqrt{2u}y_t} \times \exp\{|\lambda|^2 e^{-i\sqrt{4ut}\xi}\} \\ &= \bar{\lambda} e^{+i(\varepsilon-u)t} e^{+i\sqrt{ut}(\eta - \xi)} \times \exp\{|\lambda|^2 e^{-i\sqrt{4ut}\xi}\} \end{aligned} \quad (4.19)$$

Thus we have to evaluate

$$\begin{aligned}
 (\psi_t, a \psi_t)_{\mathcal{F}} &= E_x \bar{E}_y [\bar{v}_{y,t} e^{v_{x,t} \bar{v}_{y,t}}] e^{-|\lambda|^2} \\
 &= \int_{\mathbb{R}^2} \bar{\lambda} e^{+i(\varepsilon-u)t} e^{+i\sqrt{u}(\eta-\xi)} \times \exp\{|\lambda|^2 (e^{-i\sqrt{4u}t}\xi - 1)\} e^{i\xi\eta} \frac{d\xi d\eta}{2\pi} \\
 &= \bar{\lambda} e^{+i(\varepsilon-u)t} \int_{\mathbb{R}} d\xi e^{-i\sqrt{u}t\xi} \int_{\mathbb{R}} e^{+i(\xi+\sqrt{u}t)\eta} \frac{d\eta}{2\pi} \times \exp\{|\lambda|^2 (e^{-i\sqrt{4u}t}\xi - 1)\} \\
 &= \bar{\lambda} e^{+i(\varepsilon-u)t} \int_{\mathbb{R}} d\xi e^{-i\sqrt{u}t\xi} \delta(\xi + \sqrt{u}t) \times \exp\{|\lambda|^2 (e^{-i\sqrt{4u}t}\xi - 1)\} \\
 &= \bar{\lambda} e^{+i(\varepsilon-u)t} e^{+iut} \times \exp\{|\lambda|^2 (e^{+i2ut} - 1)\} \\
 &= \bar{\lambda} e^{+i\varepsilon t} \times \exp\{|\lambda|^2 (e^{+i2ut} - 1)\} \quad (4.20)
 \end{aligned}$$

and this coincides with the exact result (4.9). Now let's apply Theorem 4. After Girsanov transformation, we have the following representation (we omit the tilde on the transformed Fresnel BMs in the following):

$$(\psi_t, a \psi_t)_{\mathcal{F}} = E_x \bar{E}_y [\bar{v}_t] \quad (4.21)$$

with $v, \bar{v}$ given by

$$\begin{aligned}
 dv_t &= -i dt \varepsilon v_t - i 2u dt v_t \bar{v}_t v_t - i \sqrt{2u} v_t dx_t \\
 d\bar{v}_t &= +i dt \varepsilon \bar{v}_t + i 2u dt v_t \bar{v}_t \bar{v}_t + i \sqrt{2u} \bar{v}_t dy_t \quad (4.22)
 \end{aligned}$$

This SDE system can still be solved in closed form. First we calculate

$$\begin{aligned}
 d(v\bar{v}) &= dv \bar{v} + v d\bar{v} + dv d\bar{v} \\
 &= -i dt \varepsilon v\bar{v} - i 2u dt v\bar{v} v\bar{v} - i \sqrt{2u} v\bar{v} dx_t \\
 &\quad + i dt \varepsilon v\bar{v} + i 2u dt v\bar{v} v\bar{v} + i \sqrt{2u} v\bar{v} dy_t + 0 \\
 &= -i \sqrt{2u} v\bar{v} (dx_t - dy_t) = -i \sqrt{4u} v\bar{v} d\xi_t \quad (4.23)
 \end{aligned}$$

Since

$$(d\xi_t)^2 = \left(\frac{dx_t - dy_t}{\sqrt{2}}\right)^2 = \frac{(dx_t)^2 - 2dx_t dy_t + (dy_t)^2}{2} = \frac{+i dt - 0 - i dt}{2} = 0 \quad (4.24)$$

the solution to (4.23) is

$$(v\bar{v})_t = (v\bar{v})_0 e^{-i\sqrt{4u}\xi_t} = |\lambda|^2 e^{-i\sqrt{4u}\xi_t} \quad (4.25)$$

Thus, the equation for $\bar{v}$ becomes

$$d\bar{v} = \left[+i(\varepsilon + 2u|\lambda|^2 e^{-i\sqrt{4u}\xi_t}) dt + i\sqrt{2u} dy_t \right] \bar{v} \quad (4.26)$$

This is a geometric Fresnel BM with a time dependent and stochastic drift. To solve it, we have to take into account that $(dy_t)^2 = -i dt$ and obtain

$$\begin{aligned}
 \bar{v}_t &= \bar{v}_0 e^{+i \int_0^t (\varepsilon + 2u|\lambda|^2 e^{-i\sqrt{4u}\xi_s}) ds + i\sqrt{2u} y_t - iut} \\
 &= \bar{\lambda} e^{+i(\varepsilon-u)t} e^{+i2u|\lambda|^2 \int_0^t e^{-i\sqrt{4u}\xi_s} ds + i\sqrt{2u} y_t} \\
 &= \bar{\lambda} e^{+i(\varepsilon-u)t} e^{+i2u|\lambda|^2 \int_0^t e^{-i\sqrt{4u}\xi_s} ds + i\sqrt{u}(\eta_t - \xi_t)} \quad (4.27)
 \end{aligned}$$

Since $\bar{v}_t$ is not just a function of the Fresnel BMs at time t , but it depends also through the ds -integral in the exponent on the Fresnel BMs ξ_s at earlier times $s < t$, we can't no longer

make a large step evaluation of the expectation value through a one or two dimensional integral, but we have to write down the full small step path integral. Recall the notations

$$\begin{aligned}x_{t_k} &= \sqrt{dt} \sum_{\ell=1}^k \phi_{\ell} \\y_{t_k} &= \sqrt{dt} \sum_{\ell=1}^k \theta_{\ell}\end{aligned}\quad (4.28)$$

and the Fresnel measure

$$dF d\bar{F} = \prod_{\ell=1}^k e^{i \frac{\phi_{\ell}^2 - \theta_{\ell}^2}{2}} \frac{d\phi_{\ell} d\theta_{\ell}}{2\pi} \quad (4.29)$$

Let us write

$$\begin{aligned}\xi_{t_k} &= \frac{x_{t_k} - y_{t_k}}{\sqrt{2}} = \sqrt{dt} \sum_{\ell=1}^k \frac{\phi_{\ell} - \theta_{\ell}}{\sqrt{2}} =: \sqrt{dt} \sum_{\ell=1}^k \alpha_{\ell} \\ \eta_{t_k} &= \frac{x_{t_k} + y_{t_k}}{\sqrt{2}} = \sqrt{dt} \sum_{\ell=1}^k \frac{\phi_{\ell} + \theta_{\ell}}{\sqrt{2}} =: \sqrt{dt} \sum_{\ell=1}^k \beta_{\ell}\end{aligned}\quad (4.30)$$

such that the Fresnel measure becomes

$$dF d\bar{F} = \prod_{\ell=1}^k e^{i \alpha_{\ell} \beta_{\ell}} \frac{d\alpha_{\ell} d\beta_{\ell}}{2\pi} \quad (4.31)$$

Then in discrete time $t = t_k = kdt$ the $\bar{v}$ is given by

$$\bar{v}_{t_k} = \bar{\lambda} e^{+i(\varepsilon-u)t_k} \exp\left\{ +i 2u|\lambda|^2 \sum_{\ell=1}^k e^{-i\sqrt{4u}\xi_{t_{\ell}}} dt + i\sqrt{udt} \sum_{\ell=1}^k (\beta_{\ell} - \alpha_{\ell}) \right\} \quad (4.32)$$

We have to calculate

$$(\psi_t, a \psi_t)_{\mathcal{F}} = \mathbb{E}_x \bar{\mathbb{E}}_y [\bar{v}_{t_k}] = \int_{\mathbb{R}^{2k}} \bar{v}_{t_k}(\alpha, \beta) \prod_{\ell=1}^k e^{i \alpha_{\ell} \beta_{\ell}} \frac{d\alpha_{\ell} d\beta_{\ell}}{2\pi} \quad (4.33)$$

The β -integrals produce δ -functions,

$$\int_{\mathbb{R}^k} \exp\left\{ +i\sqrt{udt} \sum_{\ell=1}^k \beta_{\ell} \right\} \prod_{\ell=1}^k e^{i \alpha_{\ell} \beta_{\ell}} \frac{d\beta_{\ell}}{2\pi} = \prod_{\ell=1}^k \delta(\sqrt{udt} + \alpha_{\ell}) \quad (4.34)$$

Thus we have $\alpha_{\ell} = -\sqrt{udt}$ for all ℓ and the $\xi_{t_{\ell}}$ in (4.32) becomes

$$\xi_{t_{\ell}} = \sqrt{dt} \sum_{m=1}^{\ell} \alpha_m = -\sqrt{u} dt \ell = -\sqrt{u} t_{\ell} \quad (4.35)$$

We end up with

$$\begin{aligned}\mathbb{E}_x \bar{\mathbb{E}}_y [\bar{v}_{t_k}] &= \bar{\lambda} e^{+i(\varepsilon-u)t_k} \exp\left\{ +i 2u|\lambda|^2 \sum_{\ell=1}^k e^{+i\sqrt{4u}\sqrt{u}t_{\ell}} dt + i\sqrt{udt} \sum_{\ell=1}^k \sqrt{udt} \right\} \\ &= \bar{\lambda} e^{+i(\varepsilon-u)t_k} \exp\left\{ +i 2u|\lambda|^2 \sum_{\ell=1}^k e^{+i 2u t_{\ell}} dt + i u dt k \right\} \\ &\stackrel{dt \rightarrow 0}{=} \bar{\lambda} e^{+i\varepsilon t} \exp\left\{ +i 2u|\lambda|^2 \int_0^t e^{+i 2u s} ds \right\} \\ &= \bar{\lambda} e^{+i\varepsilon t} \exp\left\{ |\lambda|^2 (e^{+i 2u t} - 1) \right\}\end{aligned}\quad (4.36)$$

and this again coincides with the original result (4.9).

Finally, let us check the PDE representations of chapter 3 which are summarized in Theorem 6. There we have the operators $\mathcal{L}_0$, $\mathcal{L}_{\text{int}}$ and $\mathcal{L}_P$ with $P(x) = e^x$ which for the current 0D case reduce to

$$\begin{aligned}\mathcal{L}_0 &= \varepsilon \left\{ v \frac{\partial}{\partial v} - \bar{v} \frac{\partial}{\partial \bar{v}} \right\} \\ \mathcal{L}_{\text{int}} &= u \left\{ v^2 \frac{\partial^2}{\partial v^2} - \bar{v}^2 \frac{\partial^2}{\partial \bar{v}^2} \right\} \\ \mathcal{L}_P &= 2u v \bar{v} \left\{ v \frac{\partial}{\partial v} - \bar{v} \frac{\partial}{\partial \bar{v}} \right\}\end{aligned}\quad (4.37)$$

Theorem 6 makes the following statements:

a) Untransformed Representation:

$$(\psi_t, a \psi_t)_{\mathcal{F}} \stackrel{!}{=} e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}})} \left\{ \bar{v} e^{v\bar{v} - |\lambda|^2} \right\} \Big|_{v=\lambda, \bar{v}=\bar{\lambda}} \quad (4.38)$$

b) Transformed Representation:

$$(\psi_t, a \psi_t)_{\mathcal{F}} \stackrel{!}{=} e^{-it(\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P)} \left\{ \bar{v} \right\} \Big|_{v=\lambda, \bar{v}=\bar{\lambda}} \quad (4.39)$$

In case (b), we have to show that the function

$$F_t(v, \bar{v}) := \bar{v} e^{+i\varepsilon t} \exp\{v\bar{v}(e^{+i2ut} - 1)\} \quad (4.40)$$

this is the original result (4.9) with the $(\lambda, \bar{\lambda})$ replaced by $(v_0, \bar{v}_0) \rightarrow (v, \bar{v})$, is a solution of the PDE

$$i \frac{\partial}{\partial t} F_t = (\mathcal{L}_0 + \mathcal{L}_{\text{int}} + \mathcal{L}_P) F_t \quad (4.41)$$

with initial condition $F_0 = \bar{v}$. The initial condition is obvious, so let's check the derivatives. We have

$$i \frac{\partial}{\partial t} F_t = -\varepsilon F_t - 2u e^{+i2ut} v \bar{v} F_t \quad (4.42)$$

and one calculates

$$\begin{aligned}\mathcal{L}_0 F_t &= -\varepsilon F_t \\ \mathcal{L}_{\text{int}} F_t &= -2u (e^{+i2ut} - 1) v \bar{v} F_t \\ \mathcal{L}_P F_t &= -2u v \bar{v} F_t\end{aligned}\quad (4.43)$$

which validates (4.41) or (4.39).

In case (a), we have to show that the function

$$G_t(v, \bar{v}) := F_t(v, \bar{v}) e^{+v\bar{v}} = \bar{v} e^{+i\varepsilon t} \exp\{v\bar{v} e^{+i2ut}\} \quad (4.44)$$

is a solution of the PDE

$$i \frac{\partial}{\partial t} G_t = (\mathcal{L}_0 + \mathcal{L}_{\text{int}}) G_t \quad (4.45)$$

with initial condition $G_0 = \bar{v} e^{v\bar{v}}$. The initial condition is obvious, so let's check the derivatives. We have

$$i \frac{\partial}{\partial t} G_t = -\varepsilon G_t - 2u e^{+i2ut} v \bar{v} G_t \quad (4.46)$$

and one calculates

$$\begin{aligned}\mathcal{L}_0 G_t &= -\varepsilon G_t \\ \mathcal{L}_{\text{int}} G_t &= -2u e^{+i2ut} v \bar{v} G_t\end{aligned}\quad (4.47)$$

which verifies (4.38) of the untransformed representation (a).

5 The Two Site Bose-Hubbard Model

In this chapter we consider Bose-Hubbard model with just two lattice sites, 1 and 2. Because of its numerical simplicity, everything can be calculated easily with exact diagonalization, but its highly nontrivial physics, the model exhibits collapse and revivals and has a phase transition between an oscillatory and a self trapping regime, it provides an extremely beautiful test case for any calculation scheme which aims at an efficient and reasonable description of quantum many body systems. In fact, about 80 to 90 percent of the research time has been spent within that model, the generalization to arbitrary dimensions in the end then being more or less straightforward.

The Hamiltonian in the Bargmann-Segal representation is

$$\begin{aligned}h &= \sum_{i,j=1}^2 \varepsilon_{ij} a_i^+ a_j + u \sum_{j=1}^2 a_j^+ a_j^+ a_j a_j \\ &= \varepsilon \left(z_1 \frac{\partial}{\partial z_2} + z_2 \frac{\partial}{\partial z_1} \right) + u \left(z_1^2 \frac{\partial^2}{\partial z_1^2} + z_2^2 \frac{\partial^2}{\partial z_2^2} \right)\end{aligned}\quad (5.1)$$

Thus, the connection to the standard notation with hopping J and interaction strength U is made through

$$\varepsilon = -J \quad (5.2)$$

$$u = U/2 \quad (5.3)$$

and we ignore any on-diagonal trapping potentials, that is, we put $\varepsilon_{jj} = \epsilon_j = 0$. Then Theorem 4 of Section 2.2 for coherent states and Theorem 5 of Section 2.3 for number states can be summarized by the following SDE system

$$\begin{aligned}dv_1 &= -i\varepsilon dt v_2 - i2u dt p(v\bar{v}) v_1 \bar{v}_1 v_1 - i\sqrt{2u} v_1 dx_1 \\ dv_2 &= -i\varepsilon dt v_1 - i2u dt p(v\bar{v}) v_2 \bar{v}_2 v_2 - i\sqrt{2u} v_2 dx_2 \\ d\bar{v}_1 &= +i\varepsilon dt \bar{v}_2 + i2u dt p(v\bar{v}) v_1 \bar{v}_1 \bar{v}_1 + i\sqrt{2u} \bar{v}_1 dy_1 \\ d\bar{v}_2 &= +i\varepsilon dt \bar{v}_1 + i2u dt p(v\bar{v}) v_2 \bar{v}_2 \bar{v}_2 + i\sqrt{2u} \bar{v}_2 dy_2\end{aligned}\quad (5.4)$$

with $v\bar{v} = v_1 \bar{v}_1 + v_2 \bar{v}_2$ and

$$p(x) = P'(x)/P(x) = [\log P]'(x) \quad (5.5)$$

with

$$P(x) = \begin{cases} e^x & \text{if the initial state is a coherent state} \\ x^{N-1} & \text{if the initial state is a number state} \end{cases} \quad (5.6)$$

such that

$$p(x) = \begin{cases} 1 & \text{if the initial state is a coherent state} \\ (N-1)/x & \text{if the initial state is a number state} \end{cases} \quad (5.7)$$

Recall that the initial coherent and number states were given by

$$\psi_0(z_1, z_2) = \begin{cases} e^{\lambda_1 z_1 + \lambda_2 z_2} e^{-\frac{|\lambda_1|^2 + |\lambda_2|^2}{2}} = e^{\lambda z} e^{-\frac{|\lambda|^2}{2}} & \text{coherent state} \\ \frac{1}{\sqrt{N!N^N}} (\lambda_1 z_1 + \lambda_2 z_2)^N = \frac{(\lambda z)^N}{\sqrt{N!N^N}} & \text{number state} \end{cases} \quad (5.8)$$

with

$$|\lambda|^2 = |\lambda_1|^2 + |\lambda_2|^2 = N \quad (5.9)$$

being the total number of particles. The density matrix elements are then given by

$$(\psi_t, a_i^+ a_j \psi_t)_{\mathcal{F}} = \mathbb{E}[\bar{v}_i \bar{v}_j] \quad (5.10)$$

with the v_1, v_2 and $\bar{v}_1, \bar{v}_2$ given by (5.4) with initial conditions

$$v_0 = \begin{pmatrix} v_{1,0} \\ v_{2,0} \end{pmatrix} = \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix}, \quad \bar{v}_0 = \begin{pmatrix} \bar{v}_{1,0} \\ \bar{v}_{2,0} \end{pmatrix} = \begin{pmatrix} \bar{\lambda}_1 \\ \bar{\lambda}_2 \end{pmatrix} \quad (5.11)$$

Let's introduce the quadratic quantities

$$\begin{aligned} n_1 &:= v_1 \bar{v}_1 \\ n_2 &:= v_2 \bar{v}_2 \\ q &:= v_1 \bar{v}_2 \\ \bar{q} &:= \bar{v}_1 v_2 \end{aligned} \quad (5.12)$$

where the $\bar{q}$, as long as no expectation values are taken, is not necessarily the complex conjugate of the q . Then, because of $dv_i d\bar{v}_i = 0$, these quantities satisfy the following SDE system. The on-diagonal elements are given by

$$\begin{aligned} dn_1 &= +i \varepsilon dt (q - \bar{q}) - i\sqrt{2u} n_1 (dx_1 - dy_1) \\ dn_2 &= -i \varepsilon dt (q - \bar{q}) - i\sqrt{2u} n_2 (dx_2 - dy_2) \end{aligned} \quad (5.13)$$

and for the off-diagonal elements one obtains, with $n = n_1 + n_2 = v_1 \bar{v}_1 + v_2 \bar{v}_2 = v\bar{v}$,

$$\begin{aligned} dq &= +i \varepsilon dt (n_1 - n_2) - i 2u dt p(n) (n_1 - n_2) q - i\sqrt{2u} q (dx_1 - dy_2) \\ d\bar{q} &= -i \varepsilon dt (n_1 - n_2) + i 2u dt p(n) (n_1 - n_2) \bar{q} - i\sqrt{2u} \bar{q} (dx_2 - dy_1) \end{aligned} \quad (5.14)$$

since for example,

$$\begin{aligned} dq &= dv_1 \bar{v}_2 + v_1 d\bar{v}_2 + dv_1 d\bar{v}_2 \\ &= \{-i \varepsilon dt v_2 - i 2u dt p(v\bar{v}) v_1 \bar{v}_1 v_1 - i\sqrt{2u} v_1 dx_1\} \bar{v}_2 \\ &\quad + v_1 \{i \varepsilon dt \bar{v}_1 + i 2u dt p(v\bar{v}) v_2 \bar{v}_2 \bar{v}_2 + i\sqrt{2u} \bar{v}_2 dy_2\} + 0 \\ &= +i \varepsilon dt (v_1 \bar{v}_1 - v_2 \bar{v}_2) - i 2u dt p(v\bar{v}) (v_1 \bar{v}_1 - v_2 \bar{v}_2) v_1 \bar{v}_2 - i\sqrt{2u} v_1 \bar{v}_2 (dx_1 - dy_2) \end{aligned} \quad (5.15)$$

Let's introduce again, now for $j \in \{1, 2\}$,

$$\begin{aligned} d\xi_j &:= \frac{dx_j - dy_j}{\sqrt{2}} \\ d\eta_j &:= \frac{dx_j + dy_j}{\sqrt{2}} \end{aligned} \quad (5.16)$$

and let's also put

$$\begin{aligned} dv_{12} &:= \sqrt{2} (dx_1 - dy_2) = d\xi_1 + d\xi_2 + d\eta_1 - d\eta_2 \\ dv_{21} &:= \sqrt{2} (dx_2 - dy_1) = d\xi_1 + d\xi_2 - d\eta_1 + d\eta_2 \end{aligned} \quad (5.17)$$

Then, with the abbreviations

$$\begin{aligned} n_{12} &:= n_1 - n_2 \\ n &:= n_1 + n_2 \end{aligned} \quad (5.18)$$

the system (5.13) and (5.14) looks as follows:

$$\begin{aligned} dn &= -i\sqrt{4u} (n_1 d\xi_1 + n_2 d\xi_2) \\ dn_{12} &= +i2\varepsilon dt (q - \bar{q}) - i\sqrt{4u} (n_1 d\xi_1 - n_2 d\xi_2) \\ dq &= +i\varepsilon dt n_{12} - i2u dt p(n) n_{12} q - i\sqrt{u} q dv_{12} \\ d\bar{q} &= -i\varepsilon dt n_{12} + i2u dt p(n) n_{12} \bar{q} - i\sqrt{u} \bar{q} dv_{21} \end{aligned} \quad (5.19)$$

from which we immediately get $\mathbb{E}\bar{\mathbb{E}}[dn_t] = 0$ or

$$\langle n_t \rangle := \mathbb{E}\bar{\mathbb{E}}[n_t] = n_0 = n_{1,0} + n_{2,0} = N \quad \forall t \quad (5.20)$$

Furthermore we have the following exact equations:

$$\begin{aligned} \frac{d}{dt} \langle n_{12,t} \rangle &= +i2\varepsilon (\langle q_t \rangle - \langle \bar{q}_t \rangle) \\ \frac{d}{dt} \langle q_t \rangle &= +i\varepsilon \langle n_{12,t} \rangle - i2u \langle p(n_t) n_{12,t} q_t \rangle \\ \frac{d}{dt} \langle \bar{q}_t \rangle &= -i\varepsilon \langle n_{12,t} \rangle + i2u \langle p(n_t) n_{12,t} \bar{q}_t \rangle \end{aligned} \quad (5.21)$$

Here we reencounter the typical feature of quantum many body systems, namely, the system is non closed and when trying to close it by deriving SDEs for quantities like $n_{12,t} q_t$ or $p(n_t) n_{12,t} q_t$, we generate higher and higher products which basically corresponds to an expansion of the exponential which generates the collapse and revivals.

5.1 Large N Limit

If we introduce the normalized quantities (so the w 's used in this section are different from the w 's used in chapter 2)

$$\begin{aligned} \rho_1 &:= n_1/N, & \rho_2 &:= n_2/N \\ w &:= q/N, & \bar{w} &:= \bar{q}/N \\ g &:= uN \end{aligned} \quad (5.22)$$

and

$$\begin{aligned} \rho_{12} &:= \rho_1 - \rho_2 \\ \rho &:= \rho_1 + \rho_2 \end{aligned} \quad (5.23)$$

the system (5.19) is equivalent to (with $p(n) = p(N\rho)$, we write $p(n)$ for brevity)

$$\begin{aligned} d\rho &= -i\sqrt{4g/N}(\rho_1 d\xi_1 + \rho_2 d\xi_2) \\ d\rho_{12} &= +i2\varepsilon dt(w - \bar{w}) - i\sqrt{4g/N}(\rho_1 d\xi_1 - \rho_2 d\xi_2) \\ dw &= +i\varepsilon dt\rho_{12} - i2g dt p(n)\rho_{12}w - i\sqrt{g/N}w dv_{12} \\ d\bar{w} &= -i\varepsilon dt\rho_{12} + i2g dt p(n)\rho_{12}\bar{w} - i\sqrt{g/N}\bar{w} dv_{21} \end{aligned} \quad (5.24)$$

In the limit $N \rightarrow \infty$ with $g = uN$ held fixed, the diffusive part vanishes and we obtain the ODE system

$$\begin{aligned} \dot{\rho} &= 0 \\ \dot{\rho}_{12} &= +i2\varepsilon(w - \bar{w}) \\ \dot{w} &= +i\varepsilon\rho_{12} - i2g\rho_{12}w \\ \dot{\bar{w}} &= -i\varepsilon\rho_{12} + i2g\rho_{12}\bar{w} \end{aligned} \quad (5.25)$$

Here we can ignore the $p(n_t) = p(N\rho_t)$ also for number states since we have $p(N\rho_t) = (N-1)/(N\rho_t) = (N-1)/N \rightarrow 1$ because of $\rho_t = 1$ for all t . Now let's put all N particles on lattice site 1, that is, we choose the initial conditions

$$(\rho_1, \rho_2, w, \bar{w})_0 = (1, 0, 0, 0) \quad (5.26)$$

The quantity $\bar{w}_t$ is now the true complex conjugate of w_t . We are left with the two equations

$$\dot{\rho}_{12} = -4\varepsilon \operatorname{Im} w \quad (5.27)$$

$$\dot{w} = +i\varepsilon\rho_{12} - i2g\rho_{12}w \quad (5.28)$$

Equation (5.28) is solved by

$$\begin{aligned} w_t &= \frac{\varepsilon}{2g} + \left(w_0 - \frac{\varepsilon}{2g}\right) e^{-2ig \int_0^t \rho_{12,s} ds} \\ &\stackrel{w_0=0}{=} \frac{\varepsilon}{2g} - \frac{\varepsilon}{2g} e^{-2ig \int_0^t \rho_{12,s} ds} \end{aligned} \quad (5.29)$$

We obtain

$$\operatorname{Im} w_t = +\frac{\varepsilon}{2g} \sin\left[2g \int_0^t \rho_{12,s} ds\right] \quad (5.30)$$

Putting this into (5.27) gives

$$\dot{\rho}_{12,t} = -4\varepsilon \operatorname{Im} w_t = -\frac{2\varepsilon^2}{g} \sin\left[2g \int_0^t \rho_{12,s} ds\right] \quad (5.31)$$

Thus, the quantity

$$\varphi_t := 2g \int_0^t \rho_{12,s} ds \quad (5.32)$$

is the solution of the second order equation

$$\ddot{\varphi}_t + 4\varepsilon^2 \sin \varphi_t = 0 \quad (5.33)$$

which is just the equation of motion for the mathematical pendulum. We have the following initial conditions:

$$\begin{aligned}\varphi_0 &= 0 \\ \dot{\varphi}_0 &= 2g \rho_{12,0} = 2g(1-0) = 2g\end{aligned}\quad (5.34)$$

with total energy

$$E = \frac{\dot{\varphi}_t^2}{2} - 4\varepsilon^2 \cos \varphi_t = \frac{\dot{\varphi}_0^2}{2} - 4\varepsilon^2 \cos \varphi_0 = 2g^2 - 4\varepsilon^2 \quad (5.35)$$

The potential energy at $\varphi = \pi$ is $E_{\text{pot}} = +4\varepsilon^2$. We have rollovers if the total energy is bigger than that, that is, if $2g^2 - 4\varepsilon^2 > +4\varepsilon^2$ or

$$g^2 > (2\varepsilon)^2. \quad (5.36)$$

Numerical Test

Let's make a numerical check. We choose the following values: $\varepsilon = 1$ and

$$N \in \{2500, 5000, 10000, 20000\} \quad (5.37)$$

$$g \in \{0.5, 1.0, 1.8, 2.2, 3.0, 6.0\} \quad (5.38)$$

and calculate the quantity

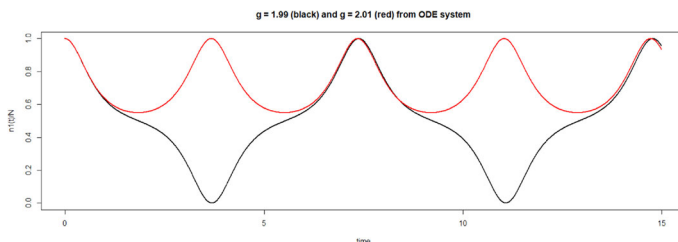
$$\rho_{1,t} = n_{1,t}/N = (\psi_t, a_1^+ a_1 \psi_t)_{\mathcal{F}} / N \quad (5.39)$$

in two different ways: First, by exact diagonalization. There we have to use the different values for N given by (5.37). Second, by simulating the ODE system 5.33 for the mathematical pendulum and calculating $\rho_{1,t}$ through

$$\rho_{1,t} = \frac{1}{2} \left(1 + \frac{\dot{\varphi}_t}{2g} \right) \quad (5.40)$$

This is the large N limit and accordingly no N enters the calculation, but only a value for g . We obtain the following results as displayed in Figs. 1 and 2 below. The red line is the ODE solution and the dots come from exact diagonalization.

The closer the value of g approaches 2, the larger N has to be chosen in order to numerically reach the true $N = +\infty$ limit. The different colors of the dots represent the different values of N , with the obvious ordering of orange, green, light blue and dark blue for increasing values of N . The fact that $g = 2\varepsilon = 2$ marks the transition point is also visualized through the following picture,



which shows the quantity (5.40) for $g = 1.99$ in black and for $g = 2.01$ in red. The fact that the mathematical pendulum shows up in the dynamics of the two site Bose-Hubbard model

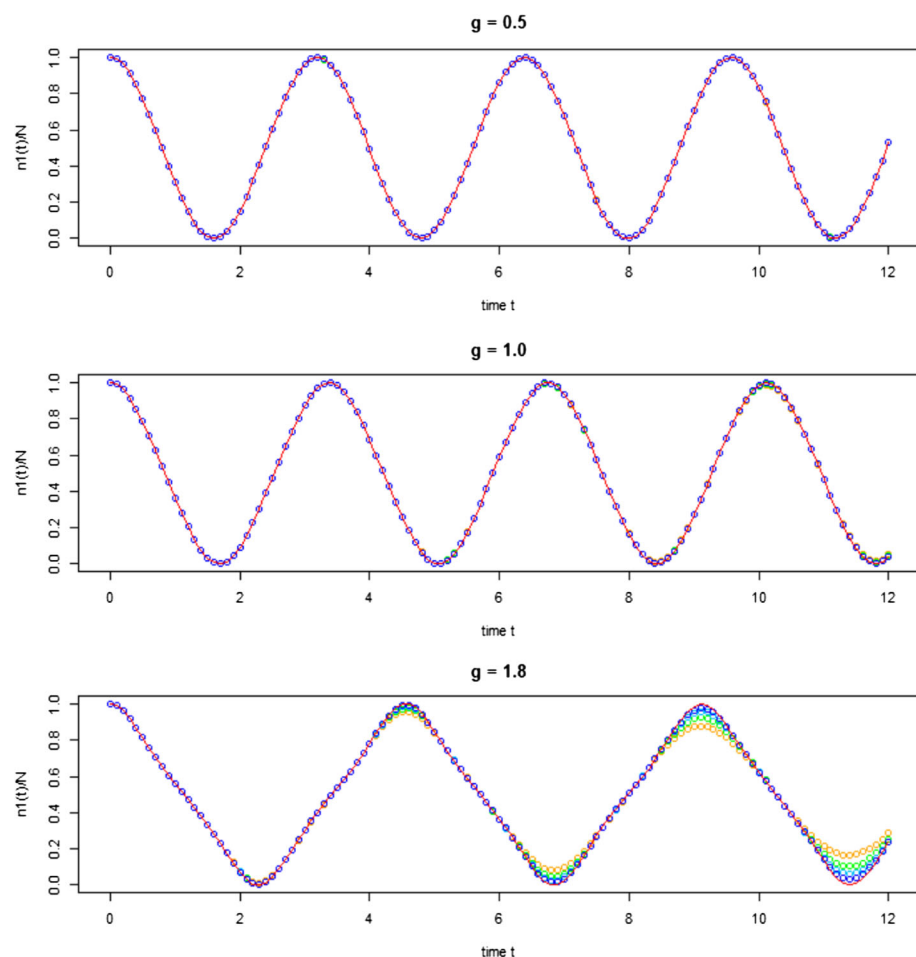


Fig. 1 Exact diagonalization results vs. ODE solution for the quantity $\langle n_{1,t} \rangle / N$

has been observed by several authors, for example in refs [9–12]. The very beautiful thesis of Lena Simon [13] also provides a detailed discussion of the dynamics.

Equivalence to Quartic Double Well Potential

Actually we can obtain $n_{12,t}$ or $\rho_{12,t}$ also as a solution of a classical particle moving in a quartic double well potential. Recall the ODE system (5.27),(5.28),

$$\begin{aligned}\dot{\rho}_{12} &= -4\varepsilon \operatorname{Im} w \\ \dot{w} &= +i\varepsilon \rho_{12} - i2g \rho_{12} w\end{aligned}\quad (5.41)$$

We have

$$\begin{aligned}\ddot{\rho}_{12} &= -4\varepsilon \operatorname{Im} \dot{w} \\ &= -4\varepsilon^2 \rho_{12} + 8g\varepsilon \rho_{12} \operatorname{Re} w\end{aligned}\quad (5.42)$$

and

$$\operatorname{Re} \dot{w} = +2g \rho_{12} \operatorname{Im} w\quad (5.43)$$

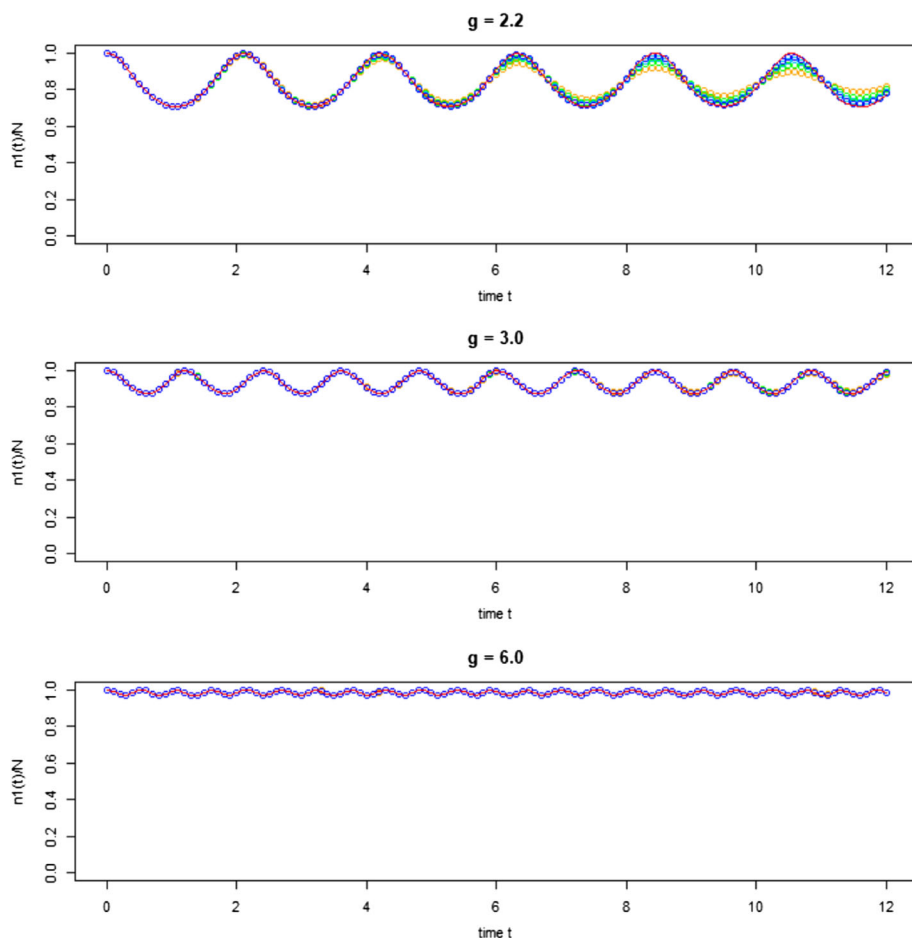


Fig. 2 Exact diagonalization results vs. ODE solution for the quantity $\langle n_{1,t} \rangle / N$

or

$$4\varepsilon \operatorname{Re} \dot{w} = -2g \rho_{12} \dot{\rho}_{12} \quad (5.44)$$

which gives, with initial conditions $w_0 = 0$ and $\rho_{12,0} = 1$,

$$4\varepsilon \operatorname{Re} w_t = g(\rho_{12,0}^2 - \rho_{12,t}^2) = g(1 - \rho_{12,t}^2) \quad (5.45)$$

Thus,

$$\begin{aligned} \ddot{\rho}_{12,t} + 4\varepsilon^2 \rho_{12,t} &= +2g \rho_{12,t} 4\varepsilon \operatorname{Re} w_t \\ &= +2g^2 \rho_{12,t} (1 - \rho_{12,t}^2) \end{aligned} \quad (5.46)$$

or

$$\ddot{\rho}_{12,t} + (4\varepsilon^2 - 2g^2)\rho_{12,t} + 2g^2 \rho_{12,t}^3 = 0 \quad (5.47)$$

with initial conditions $\rho_{12,0} = 1$ and $\dot{\rho}_{12,0} = 0$. Let's summarize in the following

Theorem 7 *The mathematical pendulum*

$$\ddot{\varphi}_t + 4\varepsilon^2 \sin \varphi_t = 0 \quad (5.48)$$

with $\varphi_0 = 0$ and $\dot{\varphi}_0 = 2g$ is equivalent to the cubic equation

$$\ddot{x}_t + (4\varepsilon^2 - 2g^2)x_t + 2g^2x_t^3 = 0 \quad (5.49)$$

with $x_0 = 1$ and $\dot{x}_0 = 0$ through the transformation

$$\varphi_t = 2g \int_0^t x_s ds \quad \Leftrightarrow \quad x_t = \frac{1}{2g} \dot{\varphi}_t \quad (5.50)$$

Proof Since this is a stand-alone result independent of the rest of the paper, let us also write down a stand-alone proof independent of the earlier derivations. We have

$$\begin{aligned} 2g [\ddot{x}_t + (4\varepsilon^2 - 2g^2)x_t + 2g^2x_t^3] &= \frac{d}{dt} \ddot{\varphi}_t + (4\varepsilon^2 - 2g^2)\dot{\varphi}_t + \frac{\dot{\varphi}_t^3}{2} \\ &= \frac{d}{dt} [\ddot{\varphi}_t + 4\varepsilon^2 \sin \varphi_t] + \dot{\varphi}_t \left[\frac{\dot{\varphi}_t^2}{2} - 4\varepsilon^2 \cos \varphi_t - (2g^2 - 4\varepsilon^2) \right] \\ &= \frac{d}{dt} [\ddot{\varphi}_t + 4\varepsilon^2 \sin \varphi_t] + \dot{\varphi}_t \int_0^t \frac{d}{ds} \left[\frac{\dot{\varphi}_s^2}{2} - 4\varepsilon^2 \cos \varphi_s \right] ds \\ &= \frac{d}{dt} [\ddot{\varphi}_t + 4\varepsilon^2 \sin \varphi_t] + \dot{\varphi}_t \int_0^t [\ddot{\varphi}_s + 4\varepsilon^2 \sin \varphi_s] \dot{\varphi}_s ds \end{aligned}$$

Thus, if (5.48) holds, then also (5.49) is fulfilled. On the other hand, if (5.49) holds, then the quantity $F_t := \ddot{\varphi}_t + 4\varepsilon^2 \sin \varphi_t$ satisfies the equation

$$\dot{F}_t + 4g^2x_t \int_0^t F_s x_s ds = 0$$

or

$$x_t \ddot{F}_t - \dot{x}_t \dot{F}_t + 4g^2x_t^3 F_t = 0$$

which is a linear homogeneous second order equation. Since we have the initial conditions $F_0 = 0$ and, using (5.49) again, also $\dot{F}_0 = 0$, F_t has to vanish identically. $\square$

The transition between the oscillatory and the self trapping regime is intuitive for the mathematical pendulum, let's try to understand this also by using the cubic equation. The total energy for (5.49) is

$$E = \frac{\dot{\rho}_{12,t}^2}{2} + (2\varepsilon^2 - g^2)\rho_{12,t}^2 + \frac{g^2}{2}\rho_{12,t}^4 = \frac{4\varepsilon^2 - g^2}{2} \quad (5.51)$$

The potential energy is

$$E_{\text{pot}}(\rho_{12}) = (2\varepsilon^2 - g^2)\rho_{12,t}^2 + \frac{g^2}{2}\rho_{12,t}^4 \quad (5.52)$$

and has stationary points at $\rho_{12} = 0$ and

$$4\varepsilon^2 - 2g^2 + 2g^2\rho_{12,t}^2 = 0 \quad (5.53)$$

or

$$\rho_{12,t}^2 = 1 - \frac{2\varepsilon^2}{g^2} < 1 \quad (5.54)$$

Thus, for $g^2 > 2\varepsilon^2$ we have a double well potential which, for $E < 0$ or $g^2 > 4\varepsilon^2$, is sufficiently deep such that $\rho_{12,t}$ cannot escape the right well when starting at $\rho_{12,0} = 1$ with $\dot{\rho}_{12,0} = 0$. Since, $\rho_{12,t}$ starts at 1 with a negative energy and the potential energy at $\rho_{12} = 0$ is zero such that the energy required to cross this point is $\dot{\rho}_{12,t}^2/2 > 0$ which is not available.

Obviously, the mathematical pendulum has no collapse and revivals, so in order to see these, we have to take the diffusive part of the SDE system into account. Before we do this, let's have a look at PDE representations.

5.2 PDE Representations

In chapter 3, we used the $v_j, \bar{v}_j$ as the basic variables to obtain PDE representations for the density matrix elements. Now, it is very instructive to see the corresponding PDE representations if the quadratic quantities

$$(n_1, n_2, q, \bar{q}) = (v_1 \bar{v}_1, v_2 \bar{v}_2, v_1 \bar{v}_2, v_2 \bar{v}_1) \quad (5.55)$$

are used directly as variables. To this end recall the SDE system (5.13) and (5.14) for the quadratic quantities from the last section,

$$\begin{aligned} dn_1 &= +i\varepsilon(q - \bar{q})dt - i\sqrt{4u}n_1 d\xi_1 \\ dn_2 &= -i\varepsilon(q - \bar{q})dt - i\sqrt{4u}n_2 d\xi_2 \\ dq &= +i\varepsilon n_{12}dt - i2u p(n)n_{12}qdt - i\sqrt{u}q dv_{12} \\ d\bar{q} &= -i\varepsilon n_{12}dt + i2u p(n)n_{12}\bar{q}dt - i\sqrt{u}\bar{q} dv_{21} \end{aligned} \quad (5.56)$$

with $n = n_1 + n_2 = v\bar{v}$, $n_{12} = n_1 - n_2$ and

$$p(x) = P'(x)/P(x) = [\log P]'(x) \quad (5.57)$$

with

$$P(x) = \begin{cases} e^x & \text{if the initial state is a coherent state} \\ x^{N-1} & \text{if the initial state is a number state} \end{cases} \quad (5.58)$$

such that

$$p(x) = \begin{cases} 1 & \text{if the initial state is a coherent state} \\ (N-1)/x & \text{if the initial state is a number state} \end{cases} \quad (5.59)$$

Recall the abbreviations

$$\begin{aligned} d\xi_1 &= (dx_1 - dy_1)/\sqrt{2} \\ d\xi_2 &= (dx_2 - dy_2)/\sqrt{2} \\ dv_{12} &= \sqrt{2}(dx_1 - dy_2) \\ dv_{21} &= \sqrt{2}(dx_2 - dy_1) \end{aligned} \quad (5.60)$$

To write down a PDE representation which is again obtained as a Kolmogorov backward equation, recall the logic of Appendices A.3 and A.4, we need to determine the differential operator A which is associated to the SDE system (5.56). To do this, we need the following identities which determine the second order part of A :

$$(d\xi_1)^2 = (d\xi_2)^2 = (dv_{12})^2 = (dv_{21})^2 = d\xi_1 d\xi_2 = dv_{12} dv_{21} = 0 \quad (5.61)$$

and

$$\begin{aligned}d\xi_1 dv_{12} &= (dx_1)^2 = +i dt \\d\xi_1 dv_{21} &= (dy_1)^2 = -i dt \\d\xi_2 dv_{12} &= (dy_2)^2 = -i dt \\d\xi_2 dv_{21} &= (dx_2)^2 = +i dt\end{aligned}\quad (5.62)$$

Now let

$$F = F(n_1, n_2, q, \bar{q})$$

by any function. We plug in the $n_{1,t}$, $n_{2,t}$ and q_t , $\bar{q}_t$ from the SDE system above and calculate the dF with the Ito lemma:

$$\begin{aligned}dF &= \frac{\partial F}{\partial n_1} dn_1 + \frac{\partial F}{\partial n_2} dn_2 + \frac{\partial F}{\partial q} dq + \frac{\partial F}{\partial \bar{q}} d\bar{q} \\&+ \frac{\partial^2 F}{\partial n_1 \partial q} dn_1 dq + \frac{\partial^2 F}{\partial n_1 \partial \bar{q}} dn_1 d\bar{q} + \frac{\partial^2 F}{\partial n_2 \partial q} dn_2 dq + \frac{\partial^2 F}{\partial n_2 \partial \bar{q}} dn_2 d\bar{q} \\&= +i\varepsilon dt (q - \bar{q}) \frac{\partial F}{\partial n_1} - i\varepsilon dt (q - \bar{q}) \frac{\partial F}{\partial n_2} \\&+ \left\{ idt \varepsilon n_{12,t} - idt 2u p(n) n_{12,t} q_t \right\} \frac{\partial F}{\partial q} - \left\{ idt \varepsilon n_{12,t} - idt 2u p(n) n_{12,t} \bar{q}_t \right\} \frac{\partial F}{\partial \bar{q}} \\&- 2u \left\{ \frac{\partial^2 F}{\partial n_1 \partial q} n_1 q d\xi_1 dv_{12} + \frac{\partial^2 F}{\partial n_1 \partial \bar{q}} n_1 \bar{q} d\xi_1 dv_{21} \right. \\&\left. + \frac{\partial^2 F}{\partial n_2 \partial q} n_2 q d\xi_2 dv_{12} + \frac{\partial^2 F}{\partial n_2 \partial \bar{q}} n_2 \bar{q} d\xi_2 dv_{21} \right\} + \text{diffusive}\end{aligned}\quad (5.63)$$

or, using (5.62),

$$\begin{aligned}dF &= +i\varepsilon (q - \bar{q}) \left(\frac{\partial F}{\partial n_1} - \frac{\partial F}{\partial n_2} \right) dt + i\varepsilon (n_1 - n_2) \left(\frac{\partial F}{\partial q} - \frac{\partial F}{\partial \bar{q}} \right) dt \\&- i2u p(n) (n_1 - n_2) \left(q \frac{\partial F}{\partial q} - \bar{q} \frac{\partial F}{\partial \bar{q}} \right) dt \\&- i2u \left(\frac{\partial^2 F}{\partial n_1 \partial q} n_1 q - \frac{\partial^2 F}{\partial n_1 \partial \bar{q}} n_1 \bar{q} - \frac{\partial^2 F}{\partial n_2 \partial q} n_2 q + \frac{\partial^2 F}{\partial n_2 \partial \bar{q}} n_2 \bar{q} \right) dt + \text{diffusive} \\&=: AF dt + \text{diffusive}\end{aligned}\quad (5.64)$$

Thus, any expectation

$$F := \mathbb{E}_0^t[f(n_{1,t}, n_{2,t}, q_t, \bar{q}_t)] = F_t(n_{1,0}, n_{2,0}, q_0, \bar{q}_0) \quad (5.66)$$

considered as a function of its initial values, has to be a solution of (again, we drop the zero subscripts on the right hand side of (5.66))

$$\begin{aligned}\frac{\partial F}{\partial t} &= AF = +i\varepsilon (q - \bar{q}) \left(\frac{\partial F}{\partial n_1} - \frac{\partial F}{\partial n_2} \right) + i\varepsilon (n_1 - n_2) \left(\frac{\partial F}{\partial q} - \frac{\partial F}{\partial \bar{q}} \right) \\&- i2u p(n) (n_1 - n_2) \left(q \frac{\partial F}{\partial q} - \bar{q} \frac{\partial F}{\partial \bar{q}} \right) \\&- i2u \left(\frac{\partial^2 F}{\partial n_1 \partial q} n_1 q - \frac{\partial^2 F}{\partial n_1 \partial \bar{q}} n_1 \bar{q} - \frac{\partial^2 F}{\partial n_2 \partial q} n_2 q + \frac{\partial^2 F}{\partial n_2 \partial \bar{q}} n_2 \bar{q} \right) \\&=: -i(\mathcal{L}_\varepsilon + \mathcal{L}_u)F\end{aligned}\quad (5.67)$$

with initial condition $F_0 = f$ and differential operators

$$\mathcal{L}_\varepsilon := -\varepsilon \left\{ (q - \bar{q}) \left(\frac{\partial}{\partial n_1} - \frac{\partial}{\partial n_2} \right) + (n_1 - n_2) \left(\frac{\partial}{\partial q} - \frac{\partial}{\partial \bar{q}} \right) \right\} \quad (5.68)$$

$$\mathcal{L}_u := +2u \left\{ \left(n_1 \frac{\partial}{\partial n_1} - n_2 \frac{\partial}{\partial n_2} \right) \left(q \frac{\partial}{\partial q} - \bar{q} \frac{\partial}{\partial \bar{q}} \right) + p(n) (n_1 - n_2) \left(q \frac{\partial}{\partial q} - \bar{q} \frac{\partial}{\partial \bar{q}} \right) \right\} \quad (5.69)$$

This proves part (a) of the following

Theorem 8 Consider the two site Bose-Hubbard model with Hamiltonian

$$\begin{aligned} h &= \varepsilon (a_1^\dagger a_2 + a_2^\dagger a_1) + u (a_1^\dagger a_1^\dagger a_1 a_1 + a_2^\dagger a_2^\dagger a_2 a_2) \\ &= \varepsilon \left(z_1 \frac{\partial}{\partial z_2} + z_2 \frac{\partial}{\partial z_1} \right) + u \left(z_1^2 \frac{\partial^2}{\partial z_1^2} + z_2^2 \frac{\partial^2}{\partial z_2^2} \right) \end{aligned} \quad (5.70)$$

and initial state

$$\psi_0(z_1, z_2) = \begin{cases} e^{\lambda_1 z_1 + \lambda_2 z_2} e^{-\frac{|\lambda_1|^2 + |\lambda_2|^2}{2}} & \text{if coherent is chosen} \\ \frac{1}{\sqrt{N!N!}} (\lambda_1 z_1 + \lambda_2 z_2)^N & \text{if number is chosen} \end{cases} \quad (5.71)$$

with a total number of $N = |\lambda_1|^2 + |\lambda_2|^2$ particles. Let P be the function of one variable given by

$$P(x) = \begin{cases} e^x & \text{if coherent is chosen} \\ x^{N-1} & \text{if number is chosen} \end{cases} \quad (5.72)$$

and let $p(x) = P'(x)/P(x)$. Then the following statements hold:

a) The expected number of particles $\langle n_{1,t} \rangle = \mathbb{E}\bar{\mathbb{E}}[n_{1,t}] = (\psi_t, a_1^\dagger a_1 \psi_t)_{\mathcal{F}}$ at lattice site 1 can be written as

$$\langle n_{1,t} \rangle = e^{-it(\mathcal{L}_\varepsilon + \mathcal{L}_u)} n_1 \Big|_{(n_1, n_2, q, \bar{q}) = (|\lambda_1|^2, |\lambda_2|^2, \lambda_1 \bar{\lambda}_2, \bar{\lambda}_1 \lambda_2)} \quad (5.73)$$

with the differential operators $\mathcal{L}_\varepsilon$ and $\mathcal{L}_u$ given by (5.68) and (5.69) above.

b) The actions of $e^{-it\mathcal{L}_\varepsilon}$ and $e^{-it\mathcal{L}_u}$ are as follows: For $e^{-it\mathcal{L}_\varepsilon}$ we obtain

$$(e^{-it\mathcal{L}_\varepsilon} F)(n_1, n_2, q, \bar{q}) = F(R_t(n_1, n_2, q, \bar{q})^T) \quad (5.74)$$

where $F = F(n_1, n_2, q, \bar{q})$ is an arbitrary function and R_t is the 4×4 matrix

$$R_t = \begin{pmatrix} \cos^2 \varepsilon t & \sin^2 \varepsilon t & +i \sin \varepsilon t \cos \varepsilon t & -i \sin \varepsilon t \cos \varepsilon t \\ \sin^2 \varepsilon t & \cos^2 \varepsilon t & -i \sin \varepsilon t \cos \varepsilon t & +i \sin \varepsilon t \cos \varepsilon t \\ +i \sin \varepsilon t \cos \varepsilon t & -i \sin \varepsilon t \cos \varepsilon t & \cos^2 \varepsilon t & \sin^2 \varepsilon t \\ -i \sin \varepsilon t \cos \varepsilon t & +i \sin \varepsilon t \cos \varepsilon t & \sin^2 \varepsilon t & \cos^2 \varepsilon t \end{pmatrix} \quad (5.75)$$

For $e^{-it\mathcal{L}_u}$ we find:

$$e^{-it\mathcal{L}_u} \{ G(n_1, n_2) q^b \bar{q}^{\bar{b}} \} = \quad (5.76)$$

$$G(e^{-i2ut(b-\bar{b})} n_1, e^{+i2ut(b-\bar{b})} n_2) \times \frac{P(e^{-i2ut(b-\bar{b})} n_1 + e^{+i2ut(b-\bar{b})} n_2)}{P(n_1 + n_2)} \times q^b \bar{q}^{\bar{b}}$$

where $G = G(n_1, n_2)$ is an arbitrary function and $b, \bar{b}$ are arbitrary natural numbers.

Proof It remains to prove part (b). If we make the Ansatz

$$(e^{-it\mathcal{L}_\varepsilon} F)(n_1, n_2, q, \bar{q}) = F(e^{-itA}(n_1, n_2, q, \bar{q})^T) \quad (5.77)$$

and take the time derivative, we find

$$A = -\varepsilon \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \in \mathbb{R}^{4 \times 4} \quad (5.78)$$

with

$$\sigma := \begin{pmatrix} +1 & -1 \\ -1 & +1 \end{pmatrix} \in \mathbb{R}^{2 \times 2} \quad (5.79)$$

Since

$$A^{2k} = (-\varepsilon)^{2k} \begin{pmatrix} \sigma^{2k} & 0 \\ 0 & \sigma^{2k} \end{pmatrix}, \quad A^{2k+1} = (-\varepsilon)^{2k+1} \begin{pmatrix} 0 & \sigma^{2k+1} \\ \sigma^{2k+1} & 0 \end{pmatrix} \quad (5.80)$$

and because of $\sigma^n = 2^{n-1}\sigma = 2^n \frac{\sigma}{2}$ for $n \geq 1$, we obtain

$$\begin{aligned} e^{-itA} &= Id + \sum_{k=1}^{\infty} \frac{(+2it\varepsilon)^{2k}}{(2k)!} \frac{1}{2} \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix} + \sum_{k=0}^{\infty} \frac{(+2it\varepsilon)^{2k+1}}{(2k+1)!} \frac{1}{2} \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \\ &= \begin{pmatrix} Id & 0 \\ 0 & Id \end{pmatrix} + \frac{\cos(2\varepsilon t) - 1}{2} \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix} + i \frac{\sin(2\varepsilon t)}{2} \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \end{aligned} \quad (5.81)$$

which coincides with R_t since $\cos^2 \varepsilon t = (1 + \cos 2\varepsilon t)/2$ and $\sin^2 \varepsilon t = (1 - \cos 2\varepsilon t)/2$.

The action of $e^{-it\mathcal{L}_u}$ we calculate by evaluating the Fresnel expectation directly. That is, we write down the $\varepsilon = 0$ SDE system

$$\begin{aligned} dn_1 &= -i\sqrt{4u} n_1 d\xi_1 \\ dn_2 &= -i\sqrt{4u} n_2 d\xi_2 \\ dq &= -i2u dt p(n) n_{12} q - i\sqrt{u} q dv_{12} \\ d\bar{q} &= +i2u dt p(n) n_{12} \bar{q} - i\sqrt{u} \bar{q} dv_{21} \end{aligned} \quad (5.82)$$

which is solved by

$$\begin{aligned} n_{1,t} &= n_1 e^{-i\sqrt{4u} \int_0^t d\xi_{1,s}} \\ n_{2,t} &= n_2 e^{-i\sqrt{4u} \int_0^t d\xi_{2,s}} \end{aligned} \quad (5.83)$$

and

$$\begin{aligned} q_t &= q e^{-i2u \int_0^t p(n_s) n_{12,s} ds - i\sqrt{u} \int_0^t dv_{12,s}} \\ \bar{q}_t &= \bar{q} e^{+i2u \int_0^t p(n_s) n_{12,s} ds - i\sqrt{u} \int_0^t dv_{21,s}} \end{aligned} \quad (5.84)$$

We have to evaluate

$$\begin{aligned} e^{-it\mathcal{L}_u} \{ G(n_1, n_2) q^b \bar{q}^{\bar{b}} \} &= \mathbb{E}\bar{\mathbb{E}}[G(n_{1,t}, n_{2,t}) q_t^b \bar{q}_t^{\bar{b}}] \\ &= \mathbb{E}\bar{\mathbb{E}} \left[G(n_{1,t}, n_{2,t}) e^{-i2u(b-\bar{b}) \int_0^t p(n_s) n_{12,s} ds} e^{-i\sqrt{u} \int_0^t [b dv_{12,s} + \bar{b} dv_{21,s}] } \right] q^b \bar{q}^{\bar{b}} \\ &=: \mathbb{E}\bar{\mathbb{E}} \left[\tilde{G}(\xi_1, \xi_2) e^{-i\sqrt{u} \int_0^t [b dv_{12,s} + \bar{b} dv_{21,s}] } \right] q^b \bar{q}^{\bar{b}} \end{aligned} \quad (5.85)$$

where we abbreviated the quantity

$$\tilde{G}(\xi_1, \xi_2) := [G(n_{1,t}, n_{2,t}) e^{-i2u(b-\bar{b}) \int_0^t p(n_s) n_{12,s} ds}](\xi_1, \xi_2) \quad (5.86)$$

which depends only on the ξ -variables, but is independent of the η -variables which only show up in the last exponential in (5.85). This means that as in chapter 4 the η -integrals can be performed and give δ -functions for the ξ -variables. With Fresnel BMs given by, for $j \in \{1, 2\}$ and $t = t_k = kdt$,

$$\begin{aligned} x_{j,t_k} &= \sqrt{dt} \sum_{\ell=1}^k \phi_{j,\ell} \\ y_{j,t_k} &= \sqrt{dt} \sum_{\ell=1}^k \theta_{j,\ell} \end{aligned} \quad (5.87)$$

the Fresnel measure is

$$dF d\bar{F} = \prod_{\ell=1}^k e^{i \sum_{j=1}^2 \frac{\phi_{j,\ell}^2 - \theta_{j,\ell}^2}{2}} \frac{d^2\phi_\ell d^2\theta_\ell}{(2\pi)^2} \quad (5.88)$$

We write again

$$\begin{aligned} \xi_{j,t_k} &= \frac{x_{j,t_k} - y_{j,t_k}}{\sqrt{2}} = \sqrt{dt} \sum_{\ell=1}^k \frac{\phi_{j,\ell} - \theta_{j,\ell}}{\sqrt{2}} =: \sqrt{dt} \sum_{\ell=1}^k \alpha_{j,\ell} \\ \eta_{j,t_k} &= \frac{x_{j,t_k} + y_{j,t_k}}{\sqrt{2}} = \sqrt{dt} \sum_{\ell=1}^k \frac{\phi_{j,\ell} + \theta_{j,\ell}}{\sqrt{2}} =: \sqrt{dt} \sum_{\ell=1}^k \beta_{j,\ell} \end{aligned} \quad (5.89)$$

such that the Fresnel measure becomes

$$dF d\bar{F}(\alpha, \beta) = \prod_{\ell=1}^k e^{i(\alpha_{1,\ell}\beta_{1,\ell} + \alpha_{2,\ell}\beta_{2,\ell})} \frac{d^2\alpha_\ell d^2\beta_\ell}{(2\pi)^2} \quad (5.90)$$

We have to calculate

$$\begin{aligned} \mathbb{E}\bar{\mathbb{E}} \left[\tilde{G}(\xi_1, \xi_2) e^{-i\sqrt{u} \int_0^t [b dv_{12,s} + \bar{b} dv_{21,s}] } \right] &= \\ \int_{\mathbb{R}^{4k}} \tilde{G}(\xi_1, \xi_2) \exp \{ -i\sqrt{u} b \int_0^t dv_{12} - i\sqrt{u} \bar{b} \int_0^t dv_{21} \} dF d\bar{F}(\alpha, \beta) \end{aligned} \quad (5.91)$$

with the discrete time expressions

$$\begin{aligned} \int_0^t dv_{12} &= \int_0^t (d\xi_1 + d\xi_2 + d\eta_1 - d\eta_2) = \sqrt{dt} \sum_{\ell=1}^k (\alpha_{1,\ell} + \alpha_{2,\ell} + \beta_{1,\ell} - \beta_{2,\ell}) \\ \int_0^t dv_{21} &= \int_0^t (d\xi_1 + d\xi_2 - d\eta_1 + d\eta_2) = \sqrt{dt} \sum_{\ell=1}^k (\alpha_{1,\ell} + \alpha_{2,\ell} - \beta_{1,\ell} + \beta_{2,\ell}) \end{aligned} \quad (5.92)$$

The β -integrals can be performed and produce δ -functions:

$$\begin{aligned} \int_{\mathbb{R}^{2k}} \exp \left\{ -i\sqrt{udt} \sum_{\ell=1}^k (b - \bar{b}) [\beta_{1,\ell} - \beta_{2,\ell}] \right\} \prod_{\ell=1}^k e^{i(\alpha_{1,\ell}\beta_{1,\ell} + \alpha_{2,\ell}\beta_{2,\ell})} \frac{d\beta_{1,\ell} d\beta_{2,\ell}}{(2\pi)^2} \\ = \prod_{\ell=1}^k \delta(\alpha_{1,\ell} - [b - \bar{b}]\sqrt{udt}) \delta(\alpha_{2,\ell} + [b - \bar{b}]\sqrt{udt}) \end{aligned} \quad (5.93)$$

Thus,

$$\begin{aligned}\alpha_{1,\ell} &= +(b-\bar{b})\sqrt{udt} \\ \alpha_{2,\ell} &= -(b-\bar{b})\sqrt{udt}\end{aligned}\quad (5.94)$$

such that $n_{1,t}$ and $n_{2,t}$ become, with $t = t_k = kdt$,

$$\begin{aligned}n_{1,t} &= n_1 e^{-i\sqrt{4udt}\sum_{\ell=1}^k \alpha_{1,\ell}} = n_1 e^{-i2u(b-\bar{b})t} \\ n_{2,t} &= n_2 e^{-i\sqrt{4udt}\sum_{\ell=1}^k \alpha_{2,\ell}} = n_2 e^{+i2u(b-\bar{b})t}\end{aligned}\quad (5.95)$$

and therefore

$$\begin{aligned}& -i2u(b-\bar{b}) \int_0^t p(n_s) n_{12,s} ds \\ &= -i2u(b-\bar{b}) \int_0^t p(n_1 e^{-i2u(b-\bar{b})s} + n_2 e^{+i2u(b-\bar{b})s}) (n_1 e^{-i2u(b-\bar{b})s} - n_2 e^{+i2u(b-\bar{b})s}) ds \\ &= + \int_0^t p(n_1 e^{-i2u(b-\bar{b})s} + n_2 e^{+i2u(b-\bar{b})s}) \frac{d}{ds} (n_1 e^{-i2u(b-\bar{b})s} + n_2 e^{+i2u(b-\bar{b})s}) ds \\ &= + \int_0^t \frac{d}{ds} [\log P(n_1 e^{-i2u(b-\bar{b})s} + n_2 e^{+i2u(b-\bar{b})s})] ds \\ &= \log P(n_1 e^{-i2u(b-\bar{b})t} + n_2 e^{+i2u(b-\bar{b})t}) - \log P(n_1 + n_2)\end{aligned}\quad (5.96)$$

Hence we arrive at

$$\begin{aligned}\mathbb{E}\mathbb{E}\left[G(n_{1,t}, n_{2,t}) e^{-i2u(b-\bar{b}) \int_0^t p(n_s) n_{12,s} ds} e^{-i\sqrt{u} \int_0^t [b dv_{12,s} + \bar{b} dv_{21,s}]} \right] &= \\ G(e^{-i2ut(b-\bar{b})} n_1, e^{+i2ut(b-\bar{b})} n_2) &\times \frac{P(n_1 e^{-i2u(b-\bar{b})t} + n_2 e^{+i2u(b-\bar{b})t})}{P(n_1 + n_2)}\end{aligned}\quad (5.97)$$

and this proves part (b) of the theorem. $\square$

5.3 Collapse and Revivals

For small u , the two site Bose-Hubbard model shows the intriguing phenomenon of collapse and revivals. In two very beautiful papers, Fishman and Veksler [14] and Bakman, Fishman and Veksler [15] gave a very precise quantitative description of this phenomenon not only for the two site Bose-Hubbard model, but also, to emphasize the general mechanism, for a quantum mechanical oscillator with a small anharmonic perturbation. The main technical tool there was a careful semiclassical analysis of the energy spectrum. Lena Simon and Walter Strunz also used semiclassical methods in their article [16].

Here in our setting we have SDEs and ODEs and of course we want to use them in order to demonstrate the phenomenon. In this paper, we do not aim at the most sophisticated version of doing that, solving this problem would basically mean to solve the quantum mechanical many body problem, but here we just want to give a ‘proof of concept’, namely, to show that

the formalism is able to do that at all. To this end, recall the exact equations (5.20) and (5.21) which in the coherent state case read as follows:

$$\begin{aligned}\langle n_t \rangle &= N \quad \forall t \\ \frac{d}{dt} \langle n_{12,t} \rangle &= +i2\varepsilon (\langle q_t \rangle - \langle \bar{q}_t \rangle) \\ \frac{d}{dt} \langle q_t \rangle &= +i\varepsilon \langle n_{12,t} \rangle - i2u \langle n_{12,t} q_t \rangle \\ \frac{d}{dt} \langle \bar{q}_t \rangle &= -i\varepsilon \langle n_{12,t} \rangle + i2u \langle n_{12,t} \bar{q}_t \rangle\end{aligned}\quad (5.98)$$

If we would simply factorize $\langle n_{12} q \rangle \approx \langle n_{12} \rangle \langle q \rangle$, we would recover the mathematical pendulum which does not have collapse and revivals. From part (b) of Theorem 8 of the previous section, we have

$$\begin{aligned}\langle n_{1,t} q_t \rangle_u &:= e^{-it\mathcal{L}_u} \{ n_1 q \} = e^{-i2ut} n_1 \times \frac{P(e^{-i2ut} n_1 + e^{+i2ut} n_2)}{P(n_1 + n_2)} q \\ \langle n_{2,t} q_t \rangle_u &:= e^{-it\mathcal{L}_u} \{ n_2 q \} = e^{+i2ut} n_2 \times \frac{P(e^{-i2ut} n_1 + e^{+i2ut} n_2)}{P(n_1 + n_2)} q\end{aligned}\quad (5.99)$$

or, since we are considering the coherent state case with $P(x) = e^x$,

$$\begin{aligned}\langle n_{1,t} q_t \rangle_u &= e^{-i2ut} n_1 \times \exp\{ (e^{-i2ut} - 1)n_1 + (e^{+i2ut} - 1)n_2 \} \times q \\ \langle n_{2,t} q_t \rangle_u &= e^{+i2ut} n_2 \times \exp\{ (e^{-i2ut} - 1)n_1 + (e^{+i2ut} - 1)n_2 \} \times q\end{aligned}\quad (5.100)$$

We also have

$$\begin{aligned}\langle n_{1,t} \rangle_u &= e^{-it\mathcal{L}_u} n_1 = n_1 \\ \langle n_{2,t} \rangle_u &= e^{-it\mathcal{L}_u} n_2 = n_2\end{aligned}\quad (5.101)$$

and

$$\langle q_t \rangle_u = e^{-it\mathcal{L}_u} q = \exp\{ (e^{-i2ut} - 1)n_1 + (e^{+i2ut} - 1)n_2 \} \times q \quad (5.102)$$

Thus, for the dynamics under $\varepsilon = 0$, we can write

$$\begin{aligned}\frac{\langle n_{1,t} q_t \rangle_u}{\langle n_{1,t} \rangle_u \langle q_t \rangle_u} &= e^{-i2ut} \\ \frac{\langle n_{2,t} q_t \rangle_u}{\langle n_{2,t} \rangle_u \langle q_t \rangle_u} &= e^{+i2ut}\end{aligned}\quad (5.103)$$

Now consider the dynamics under $u = 0$. Since $e^{-it\mathcal{L}_\varepsilon}$ simply rotates the argument when applied to an arbitrary function F ,

$$\left\langle F(n_{1,t}, n_{2,t}, q_t, \bar{q}_t) \right\rangle_\varepsilon := (e^{-it\mathcal{L}_\varepsilon} F)(n_1, n_2, q, \bar{q}) = F(R_t(n_1, n_2, q, \bar{q})^T) \quad (5.104)$$

the action of $e^{-it\mathcal{L}_\varepsilon}$ factorizes when applied to an arbitrary product,

$$e^{-it\mathcal{L}_\varepsilon} (FG) = e^{-it\mathcal{L}_\varepsilon} F \times e^{-it\mathcal{L}_\varepsilon} G \quad (5.105)$$

Thus, under $u = 0$,

$$\begin{aligned}\frac{\langle n_{1,t} q_t \rangle_\varepsilon}{\langle n_{1,t} \rangle_\varepsilon \langle q_t \rangle_\varepsilon} &= 1 \\ \frac{\langle n_{2,t} q_t \rangle_\varepsilon}{\langle n_{2,t} \rangle_\varepsilon \langle q_t \rangle_\varepsilon} &= 1\end{aligned}\quad (5.106)$$

Then, for the full dynamics with both ε and u being nonzero, one may try the approximation

$$\begin{aligned}\frac{\langle n_{1,t} q_t \rangle}{\langle n_{1,t} \rangle \langle q_t \rangle} &\approx \frac{1}{2} \left(1 + e^{-i2ut} \right) \\ \frac{\langle n_{2,t} q_t \rangle}{\langle n_{2,t} \rangle \langle q_t \rangle} &\approx \frac{1}{2} \left(1 + e^{+i2ut} \right)\end{aligned}\quad (5.107)$$

and this in fact generates collapse and revivals. That is, we modify the exact system (5.98) to the following approximate system (recall the abbreviation $n_{12} := n_1 - n_2$)

$$\begin{aligned}\langle n_t \rangle &= N \quad \forall t \\ \frac{d}{dt} \langle n_{12,t} \rangle &= +i2\varepsilon (\langle q_t \rangle - \langle \bar{q}_t \rangle) \\ \frac{d}{dt} \langle q_t \rangle &\approx +i\varepsilon \langle n_{12,t} \rangle - iu \left\{ (1 + e^{-i2ut}) \langle n_{1,t} \rangle \langle q_t \rangle - (1 + e^{+i2ut}) \langle n_{2,t} \rangle \langle q_t \rangle \right\} \\ \frac{d}{dt} \langle \bar{q}_t \rangle &\approx -i\varepsilon \langle n_{12,t} \rangle + iu \left\{ (1 + e^{+i2ut}) \langle n_{1,t} \rangle \langle \bar{q}_t \rangle - (1 + e^{-i2ut}) \langle n_{2,t} \rangle \langle \bar{q}_t \rangle \right\}\end{aligned}\quad (5.108)$$

which then reduces to the following two equations (since $\langle n_t \rangle = \langle n_{1,t} + n_{2,t} \rangle = N$)

$$\begin{aligned}\frac{d}{dt} \langle n_{12,t} \rangle &= -4\varepsilon \operatorname{Im} \langle q_t \rangle \\ \frac{d}{dt} \langle q_t \rangle &\approx +i\varepsilon \langle n_{12,t} \rangle - iu (1 + \cos 2ut) \langle n_{12,t} \rangle \langle q_t \rangle - uN \sin 2ut \langle q_t \rangle\end{aligned}\quad (5.109)$$

Before we look at the numerical results, let's make some quick analytical considerations. Since from now on we are purely in the ODE framework, let's omit the angular brackets and summarize the system as follows:

$$\begin{aligned}\dot{n}_{12,t} &= -4\varepsilon \operatorname{Im} q_t \\ \dot{q}_t &= +i\varepsilon n_{12,t} - iu (1 + \cos 2\tilde{u}t) n_{12,t} q_t - uN \sin 2\tilde{u}t q_t\end{aligned}\quad (5.110)$$

Here the $\tilde{u}$ on the right hand side of (5.110) is actually a u , we put this in since for $\tilde{u} = 0$ this reduces to the system (5.27), (5.28) of Section 5.1 where we have shown that this is actually the mathematical pendulum. Thus, by switching the $\tilde{u}$ from 0 to u we can interpolate between the mathematical pendulum without collapse and revivals and the actual case under consideration. We write

$$\begin{aligned}\ddot{n}_{12,t} &= -4\varepsilon \operatorname{Im} \dot{q}_t \\ &= -4\varepsilon^2 n_{12,t} + 4\varepsilon u (1 + \cos 2\tilde{u}t) n_{12,t} \operatorname{Re} q_t + 4\varepsilon u N \sin 2\tilde{u}t \operatorname{Im} q_t \\ &= -4\varepsilon^2 n_{12,t} + 4\varepsilon u (1 + \cos 2\tilde{u}t) n_{12,t} \operatorname{Re} q_t - uN \sin 2\tilde{u}t \dot{n}_{12,t}\end{aligned}\quad (5.111)$$

or

$$\ddot{n}_{12,t} + uN \sin 2\tilde{u}t \dot{n}_{12,t} + 4\varepsilon^2 n_{12,t} = +4\varepsilon u (1 + \cos 2\tilde{u}t) n_{12,t} \operatorname{Re} q_t \quad (5.112)$$

For $\tilde{u} = 0$, the case without collapse and revivals, this reduces to

$$\ddot{n}_{12,t} + 0 + 4\varepsilon^2 n_{12,t} = +4\varepsilon u(1+1)n_{12,t} \operatorname{Re} q_t \quad (5.113)$$

That is, the right hand side of (5.112) is basically responsible for the difference between a harmonic pendulum and the mathematical pendulum and it generates the effect of self trapping or rollovers for $g > 2\varepsilon$. Since collapse and revivals do already show up for very small g where surely the harmonic approximation should be valid, we should be able to see them already in the following equation

$$\ddot{n}_{12,t} + uN \sin 2\tilde{u}t \dot{n}_{12,t} + 4\varepsilon^2 n_{12,t} = 0 \quad (5.114)$$

This is simply a harmonic oscillator with a time dependent friction

$$\gamma_t := uN \sin 2\tilde{u}t \quad (5.115)$$

which can be transformed away with the Ansatz

$$n_{12,t} = e^{-\frac{1}{2} \int_0^t \gamma_s ds} y_t \quad (5.116)$$

which then produces the following equation for y_t ,

$$\ddot{y}_t + \omega_t^2 y_t = 0 \quad (5.117)$$

with a time dependent frequency

$$\omega_t^2 = 4\varepsilon^2 - \frac{\gamma_t^2}{4} - \frac{\dot{\gamma}_t}{2} = 4\varepsilon^2 - \frac{(uN)^2 \sin^2 2\tilde{u}t}{4} - \tilde{u} uN \cos 2\tilde{u}t \quad (5.118)$$

For small $g = uN$, one may put this roughly to $4\varepsilon^2$ such that y_t is identical to the exact $u = 0$ solution which is

$$y_t \approx N \cos 2\varepsilon t \quad (5.119)$$

Thus, collapse and revivals arise from the damping factor

$$e^{-\frac{1}{2} \int_0^t \gamma_s ds} = \exp\left\{-\frac{uN}{2} \int_0^t \sin 2\tilde{u}s ds\right\} \stackrel{\tilde{u} \equiv u}{=} \exp\left\{-\frac{N}{4} (1 - \cos 2ut)\right\} \quad (5.120)$$

and we arrive at the approximate small g solution

$$n_{12,t} \approx \exp\left\{-\frac{N}{4} (1 - \cos 2ut)\right\} \times N \cos 2\varepsilon t \quad (5.121)$$

In the following Fig. 3 and 4, the quantity $n_{12,t}/N$ obtained from exact diagonalization, in black, is plotted together with the analytical collapse factor (5.120), in red. We chose $N = 50$, $\varepsilon = 1$ and g as displayed on the plots and all 50 particles were put onto lattice site 1 at time $t = 0$:

However, now we have to remark that the exact diagonalization numbers were produced with a number state, not with a coherent state. While in the large N limit the dynamics of coherent

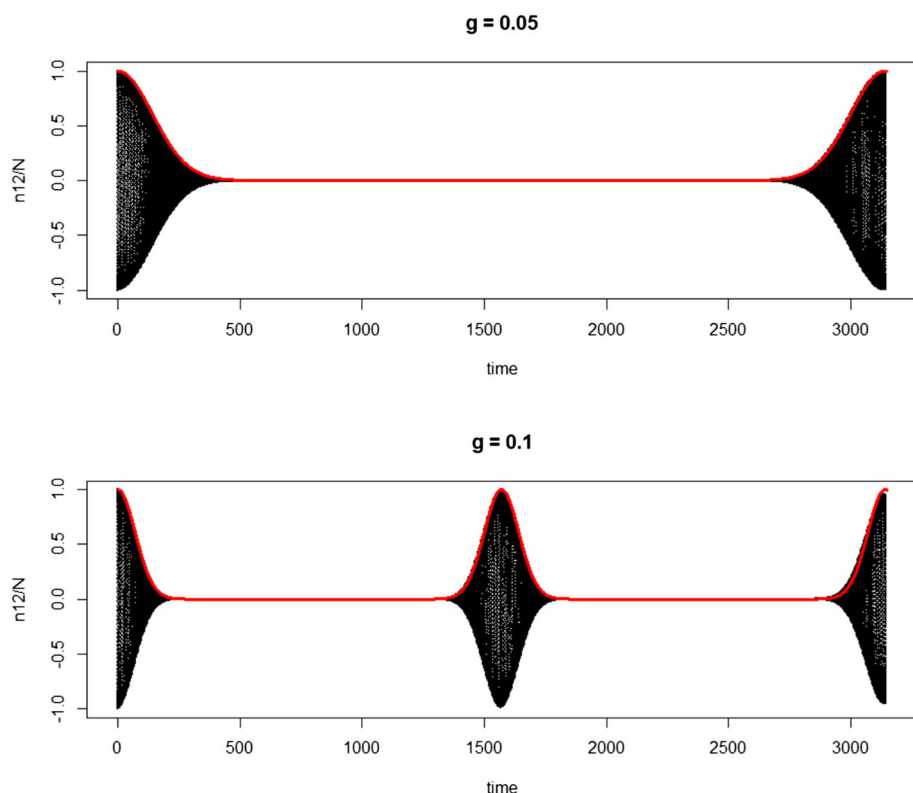


Fig. 3 Exact diagonalization vs. analytical collapse factor $\exp\left\{-\frac{N}{4}(1 - \cos 2ut)\right\}$

states and number states are identical, this no longer holds in the revival region after the first collapse has occurred. In the large N limit, this region moves to infinity and hence is not visible there. For example, if we put $g = 0.02$ and choose a time horizon of $T = 10000\pi$ instead of $T = 1000\pi$ as above, a comparison of number state and coherent state dynamics looks as displayed in Fig. 5.

This clearly demonstrates that the problem is subtle and a more careful analysis is required. For example, in the approximation (5.107) we could have equally well have said, we use e^{-i2ut} instead of an average $(1 + e^{-i2ut})/2$, and then this would have had the effect that the analytical collapse factor in (5.120) would have come with an $N/2$ in the exponent instead of an $N/4$ and the revival blobs were too small. So, this really should be considered as some kind of a ‘teaser’, some kind of a motivational argument, but nothing more. A proper and systematic treatment of the diffusive part is basically equivalent to solving the quantum mechanical many body problem and this still needs to be developed. But to do so, we believe indeed that the formalism presented in this paper is a very useful tool.

Let us remark that the qualitative behaviour seen in Fig. 5 below, number states have twice the number of revivals than coherent states, actually can be made plausible by comparing

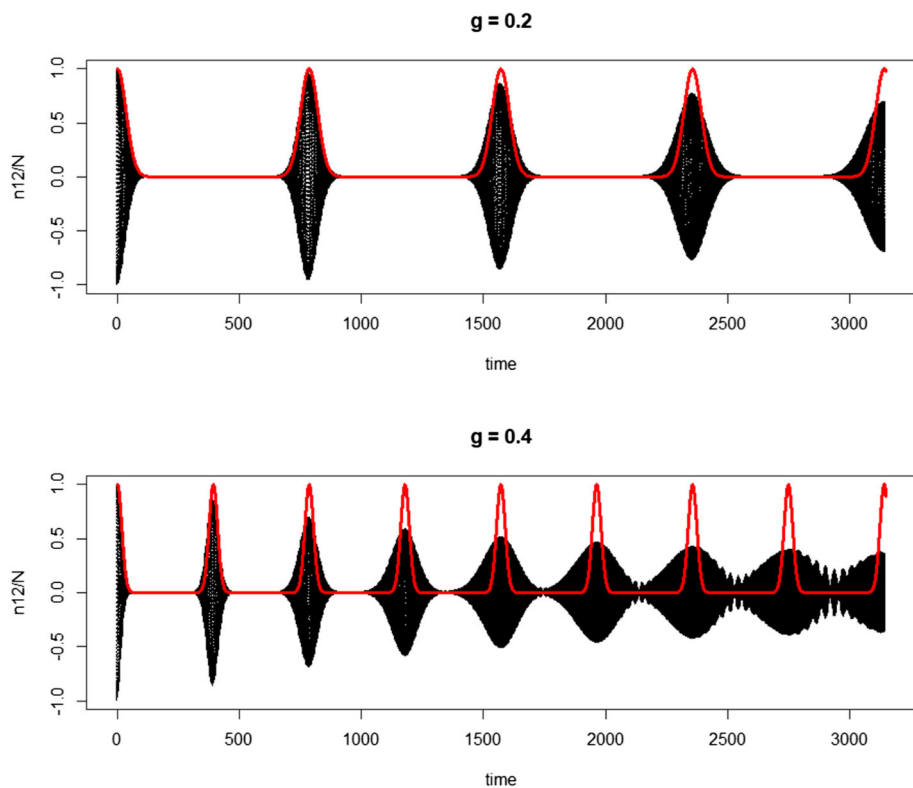
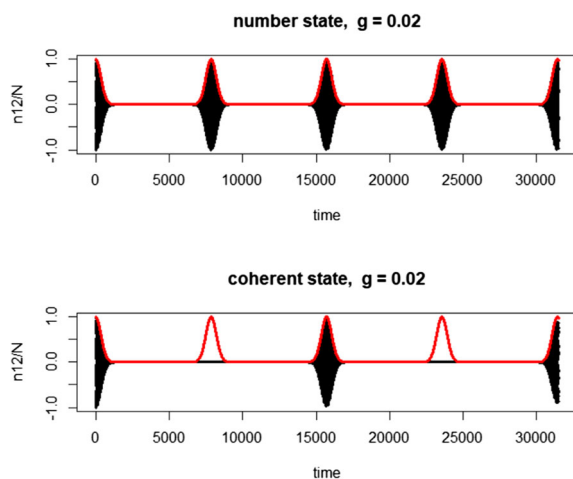


Fig. 4 Exact diagonalization vs. analytical collapse factor $\exp\{-\frac{N}{4}(1 - \cos 2ut)\}$, other g 's

Fig. 5 Coherent state vs. number state dynamics



their respective collapse factors: for coherent states, there is basically a factor of $\exp\{-N[1 - \cos(2ut)]\}$ (ignoring the width of the revival blobs for the moment) while for number states there is a factor $[\cos(2ut)]^N$. In the first case, we have revivals at $\cos(2ut) = +1$ while in the second case, we have revivals at $\cos(2ut) = +1$ but also for $\cos(2ut) = -1$, so just twice as much, as seen in the numerical simulation.

We also implemented the full approximate ODE system (5.109) and compared with exact diagonalization numbers, again using a number state, not a coherent state. We used a fourth order Runge-Kutta method and separated off the collapse factor to obtain a stable implementation ($N = 50$ and $\varepsilon = 1$ as above, g fixed to 0.1 and zoomed in on different time windows), the exact diagonalization numbers are in black and the ODE solution is in red in the following Figs. 6:

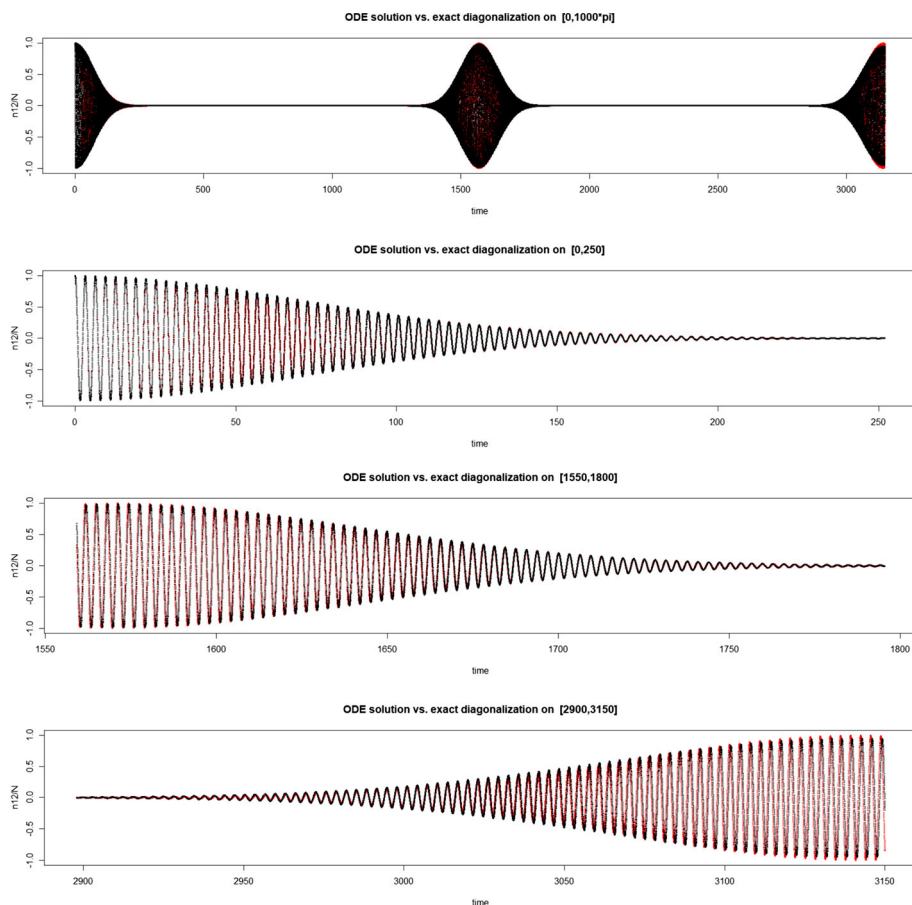


Fig. 6 Exact diagonalization (black) and ODE solution (red) on different time windows

6 Summary

The paper has demonstrated that the formalism of stochastic calculus is very useful to address the dynamics of the Bose-Hubbard model. The fact that in the large N limit the exact quantum dynamics can be obtained from an ODE system, the time dependent discrete GP equation, has been derived in a conceptually very pure and clean and transparent way. For finite N , the dynamics is given by the SDE systems of Theorems 4 and 5 of chapter 2 and the diffusive parts of those systems vanish in the large N limit. More generally, the paper provides a technique to obtain GP-like mean field equations for an arbitrary given initial state, in arbitrary dimension and for an arbitrary hopping matrix. For the two site Bose-Hubbard model, the diffusive part has been taken into account with an approximation and collapse and revivals could be reproduced, numerically and also through an analytic calculation. A proper systematic treatment of the diffusive part is still missing and needs to be developed. It has also been shown that density matrix elements can be obtained from various exact parabolic second order PDEs.

7 Additional Remarks

By the end of 2016, the mathematics department of Hochschule RheinMain joined the Faculty of Engineering and the author was asked by Klaus Michael Indlekofer from Electrical Engineering whether there would be some interest in joining a project on quantum dynamics. After 9 years as a financial engineer at a bank, the author found that this would be a good opportunity to reenter the field and it didn't took long until it was realized that the Hubbard model is more relevant than ever due to some major experimental breakthroughs in the ultracold atoms area [17–21]. Working purely on the theoretical side, we can only humbly take notice of what is doable there [22].

First attention then was drawn to phase space methods and the truncated Wigner approximation because of the very attractive idea to get the quantum dynamics from suitably weighted ODE trajectories. In particular, the beautiful papers of Polkovnikov [23–25], Polkovnikov, Sachdev and Girvin [26] and Davidson, Sels and Polkovnikov [27] served as a major motivation and inspiration for the current work.

With a theoretical and practical background in stochastic calculus from 9 years of option pricing, then it was natural to take a closer look to the long history of stochastic methods applied to the quantum many body problem [28, 29]. In particular, the formalism of the Husimi Q-Function and the Positive P-Representation [30–34] was considered more closely and this, combined with the background of the author [35, 36], then lead to the approach which is taken in this paper.

Nowadays nearly taken for granted, but the almost unlimited and instantaneous access to the science knowledge of the planet and the people who provide it also has been critical for the completion of this work. There have been numerous papers, the majority of them probably not being cited here, where just a particular item was looked up and then the conclusion was, okay, for our purposes this does not lead in the right direction. Those references may not seem directly relevant to the now final version of this paper, but they have been critical in order to get there. In this class fall for example references for BCH like formulas and time ordered exponentials [37–40] ([39] derives very interesting formulae which are in the same spirit but more general than a formula derived by the author in chapter 10 of [36]), Carleman Linearization Technique and Kroenecker products of matrices (Kowalski and Steeb [41]

wrote a very beautiful book on that) or references which relate to the author's attempt to evaluate the Fresnel integrals directly.

With the presented formalism, the paper opens up the possibility to address a range of very interesting topics like fermionic models or thermodynamic quantities with an $e^{-\beta H}$ in it instead of an e^{-itH} , and the author looks very much forward to consider these issues, but with a teaching load of 18 hours per week at a German University of Applied Sciences, research basically has to be restricted to the off-term periods which are March and August and September each year.

Appendix: Compact Summary Stochastic Calculus

A.1 Standard Brownian Motion and Wiener Measure

A standard Brownian motion $x_t = x_{t_k}$ in discretized time $t = t_k = k\Delta t$ is the combination of integration variables

$$x_{t_k} = \sqrt{\Delta t} \sum_{\ell=1}^k \phi_\ell \quad (\text{A.1})$$

where the ϕ_ℓ are to be integrated against Wiener measure which is simply a product of independent standard Gaussian distributions,

$$dW := \prod_{\ell=1}^N e^{-\frac{\phi_\ell^2}{2}} \frac{d\phi_\ell}{\sqrt{2\pi}} = \prod_{\ell=1}^N e^{-\frac{(x_{t_\ell} - x_{t_{\ell-1}})^2}{2\Delta t}} \frac{dx_{t_\ell}}{\sqrt{2\pi \Delta t}} \quad (\text{A.2})$$

where $T = N\Delta t$ is a fixed time horizon. Basic to stochastic calculus, in particular for the Ito formula in the next section, is the Brownian motion calculation rule

$$(dx_t)^2 = dt \quad (\text{A.3})$$

which can be motivated in several ways. Consider the discretized version of the quantity $\int_0^T f(t) (dx_t)^2$ which is

$$I_{\Delta t}(f) := \sum_{k=1}^N f(t_k) (x_{t_k} - x_{t_{k-1}})^2 = \Delta t \sum_{k=1}^N f(t_k) \phi_k^2 \quad (\text{A.4})$$

where f is an arbitrary function of one variable. Its expectation value and variance are given by

$$\mathbb{E}[I_{\Delta t}(f)] = \Delta t \sum_{k=1}^{N_t} f(t_k) \xrightarrow{\Delta t \rightarrow 0} \int_0^T f(t) dt \quad (\text{A.5})$$

$$\mathbb{V}[I_{\Delta t}(f)] = 2(\Delta t)^2 \sum_{k=1}^{N_t} f(t_k)^2 \approx 2\Delta t \int_0^T f(t)^2 dt \xrightarrow{\Delta t \rightarrow 0} 0 \quad (\text{A.6})$$

Thus, with Chebyshev's inequality we get for any $\varepsilon > 0$

$$\lim_{\Delta t \rightarrow 0} \text{Prob}\left[\left|I_{\Delta t}(f) - \int_0^T f(t) dt\right| \geq \varepsilon\right] = 0 \quad (\text{A.7})$$

or more intuitively

$$\int_0^T f(t) (dx_t)^2 = \lim_{\Delta t \rightarrow 0} \sum_{k=1}^N f(t_k) (x_{t_k} - x_{t_{k-1}})^2 = \int_0^T f(t) dt \quad (\text{A.8})$$

for arbitrary f . The validity of this equation is usually more compactly written as

$$(dx_t)^2 = dt \quad (\text{A.9})$$

although the last equation on its own is not correct, in discretized form we have

$$(\Delta x_{t_k})^2 = (x_{t_k} - x_{t_{k-1}})^2 = (\sqrt{\Delta t} \phi_k)^2 = \Delta t \phi_k^2 \neq \Delta t \quad (\text{A.10})$$

and only after applying the operation

$$\int_0^T f(t) \cdots = \lim_{\Delta t \rightarrow 0} \sum_{k=1}^N f(t_k) \cdots \quad (\text{A.11})$$

to the left and right hand side of (A.10) we get a valid equation. Since we cannot use Chebyshev's inequality in the complex Fresnel case, let us motivate the basic Brownian motion calculation rule (A.3) in a different way which directly generalizes to the Fresnel case:

Theorem A1 Let $I_{\Delta t}(f)$ be defined as in (A.4) and let $E[\cdot]$ denote the expectation with respect to the Wiener measure (A.2). Then

$$\lim_{\Delta t \rightarrow 0} E[e^{iq I_{\Delta t}(f)}] = e^{iq \int_0^T f(t) dt} \quad (\text{A.12})$$

such that for any $F(x) = \int_{\mathbb{R}} \hat{F}(q) e^{iqx} dq / (2\pi)$ we obtain

$$\lim_{\Delta t \rightarrow 0} E[F(I_{\Delta t}(f))] = F\left(\int_0^T f(t) dt\right) \quad (\text{A.13})$$

Proof We have

$$\begin{aligned} E[e^{iq I_{\Delta t}(f)}] &= \int_{\mathbb{R}^N} \prod_{k=1}^N e^{-\frac{1}{2}(1-2iq\Delta t f(t_k))\phi_k^2} \frac{d\phi_k}{\sqrt{2\pi}} \\ &= \prod_{k=1}^N \frac{1}{\sqrt{1-2iq\Delta t f(t_k)}} \\ &= \exp\left\{-\frac{1}{2} \sum_{k=1}^N \log[1-2iq\Delta t f(t_k)]\right\} \\ &= \exp\left\{+\frac{1}{2} \sum_{k=1}^N 2iq\Delta t f(t_k) + O(\Delta t)\right\} \\ &\xrightarrow{\Delta t \rightarrow 0} \exp\left\{+iq \int_0^T f(t) dt\right\} \end{aligned} \quad (\text{A.14})$$

which coincides with (A.12). $\square$

Let us close this section by recalling that the calculation rule $(dx_t)^2 = dt$ is accompanied by the rules

$$dx_t dt = dt dt = 0 \quad (\text{A.15})$$

which also will be used in the next section.

A.2 Ito Formula and Stochastic Integrals

For some arbitrary function $f = f(x)$ and x_t a Brownian motion we can write

$$\begin{aligned} f(x_T) - f(x_0) &= \sum_{k=1}^N \{ f(x_{t_k}) - f(x_{t_{k-1}}) \} \\ &= \sum_{k=1}^N \{ f(x_{t_{k-1}} + dx_{t_k}) - f(x_{t_{k-1}}) \} \end{aligned} \quad (\text{A.16})$$

with

$$dx_{t_k} = x_{t_k} - x_{t_{k-1}} \quad (\text{A.17})$$

Using a standard Taylor expansion,

$$\begin{aligned} f(x_{t_k}) &= f(x_{t_{k-1}} + dx_{t_k}) \\ &= f(x_{t_{k-1}}) + f'(x_{t_{k-1}}) dx_{t_k} + \frac{1}{2} f''(x_{t_{k-1}}) (dx_{t_k})^2 + \frac{1}{3!} f'''(x_{t_{k-1}}) (dx_{t_k})^3 + \dots \end{aligned} \quad (\text{A.18})$$

and the calculation rules of a Brownian motion,

$$(dx_{t_k})^2 = dt \quad (\text{A.19})$$

and $(dx_{t_k})^3 = (dx_{t_k})^2 dx_{t_k} = dt dx_{t_k} = 0$, we obtain in the limit $\Delta t \rightarrow 0$:

$$f(x_{t_k}) = f(x_{t_{k-1}}) + f'(x_{t_{k-1}}) dx_{t_k} + \frac{1}{2} f''(x_{t_{k-1}}) dt + \frac{1}{3!} f'''(x_{t_{k-1}}) \times 0 \quad (\text{A.20})$$

or

$$df(x_{t_k}) := f(x_{t_k}) - f(x_{t_{k-1}}) = f'(x_{t_{k-1}}) dx_{t_k} + \frac{1}{2} f''(x_{t_{k-1}}) dt \quad (\text{A.21})$$

which is the differential version of the Ito formula. If we sum this up,

$$\begin{aligned} f(x_T) - f(x_0) &= \sum_{k=1}^N \{ f(x_{t_k}) - f(x_{t_{k-1}}) \} \\ &= \sum_{k=1}^N \left\{ f'(x_{t_{k-1}}) dx_{t_k} + \frac{1}{2} f''(x_{t_{k-1}}) dt \right\} \\ &\stackrel{\Delta t \rightarrow 0}{=} \int_0^T f'(x_t) dx_t + \frac{1}{2} \int_0^T f''(x_t) dt \end{aligned} \quad (\text{A.22})$$

where the first integral is referred to as an Ito integral. Thus, its definition is, we replace the f' by an f ,

$$\int_0^T f(x_t) dx_t := \lim_{\Delta t \rightarrow 0} \sum_{k=1}^N f(x_{t_{k-1}}) dx_{t_k} \quad (\text{A.23})$$

What on a first sight looks a bit odd is the fact that if we replace the $x_{t_{k-1}}$ on the right hand side of (A.23) in the f by, say, $(x_{t_{k-1}} + x_{t_k})/2$, we actually get a different limit. This is a consequence of the fact that $(dx_t)^2$ is nonzero. The following definition is referred to as a Stratonovich integral:

$$\int_0^T f(x_t) \circ dx_t := \lim_{\Delta t \rightarrow 0} \sum_{k=1}^N f\left(\frac{x_{t_{k-1}} + x_{t_k}}{2}\right) dx_{t_k} \quad (\text{A.24})$$

Then there is the following relation:

$$\int_0^T f(x_t) \circ dx_t = \int_0^T f(x_t) dx_t + \frac{1}{2} \int_0^T f'(x_t) dt \quad (\text{A.25})$$

Namely, because of

$$\frac{x_{t_{k-1}} + x_{t_k}}{2} = x_{t_{k-1}} + \frac{x_{t_k} - x_{t_{k-1}}}{2} = x_{t_{k-1}} + \frac{dx_{t_k}}{2} \quad (\text{A.26})$$

we have, using $(dx_t)^2 = dt$ and $dx_t dt = 0$ in the third line,

$$\begin{aligned} f\left(\frac{x_{t_{k-1}} + x_{t_k}}{2}\right) dx_{t_k} &= f\left(x_{t_{k-1}} + \frac{dx_{t_k}}{2}\right) dx_{t_k} \\ &= \left\{ f(x_{t_{k-1}}) + f'(x_{t_{k-1}}) \frac{dx_{t_k}}{2} + \frac{1}{2} f''(x_{t_{k-1}}) \left(\frac{dx_{t_k}}{2}\right)^2 \right\} dx_{t_k} \\ &= f(x_{t_{k-1}}) dx_{t_k} + f'(x_{t_{k-1}}) \frac{dt}{2} + \frac{1}{2} f''(x_{t_{k-1}}) \times 0 \end{aligned} \quad (\text{A.27})$$

and (A.25) follows. We summarize in the following

Theorem A2 Let $f = f(x)$ be an arbitrary function and $\{x_t\}_{t \geq 0}$ be a Brownian motion. Then:

$$f(x_T) - f(x_0) = \int_0^T df = \int_0^T f'(x_t) dx_t + \frac{1}{2} \int_0^T f''(x_t) dt \quad (\text{A.28})$$

$$= \int_0^T f'(x_t) \circ dx_t \quad (\text{A.29})$$

where the first integral in (A.28) is a stochastic Ito integral and the integral in (A.29) is a Stratonovich integral. Equation (A.28) is referred to as Ito formula or the Ito lemma.

Finally we want to recall a very practical property of Ito integrals, namely, that their expectation value always vanishes,

$$\mathbb{E} \left[\int_0^T f(x_t) dx_t \right] = 0 \quad (\text{A.30})$$

for arbitrary f . This follows from the fact that

$$dx_{t_k} = x_{t_k} - x_{t_{k-1}} = \sqrt{dt} \phi_k \quad (\text{A.31})$$

while

$$f(x_{t_{k-1}}) = f\left(\sqrt{dt} \sum_{\ell=1}^{k-1} \phi_\ell\right) \quad (\text{A.32})$$

does not depend on ϕ_k . Thus, $f(x_{t_{k-1}})$ and dx_{t_k} are independent quantities and we obtain

$$\mathbb{E} [f(x_{t_{k-1}}) dx_{t_k}] = \mathbb{E} [f(x_{t_{k-1}})] \times \sqrt{dt} \mathbb{E} [\phi_k] = 0 \quad (\text{A.33})$$

It is exactly this property which makes Ito integrals a preferable choice over Stratonovich integrals, at least in the context of this paper, although just concerning the optics one may consider the Ito formula (A.28) as more complicated than the Stratonovich formula (A.29) which looks more like the standard calculus formula.

A.3 Kolmogorov Backward Equation and Feynman-Kac Formula

A, let's say, one dimensional Ito diffusion X_t is a stochastic quantity which is given by the recursion

$$X_{t_k} = X_{t_{k-1}} + a(X_{t_{k-1}}, t_{k-1}) dt + b(X_{t_{k-1}}, t_{k-1}) \sqrt{dt} \phi_k \quad (\text{A.34})$$

where the $\{\phi_k\}_{k=1}^N$ are to be integrated against standard Wiener measure. In continuous time, this reads

$$dX_t = a(X_t, t) dt + b(X_t, t) dx_t \quad (\text{A.35})$$

with x_t a Brownian motion. To each Ito diffusion we can assign a second order differential operator A defined by the following equation: Let $f = f(x, t)$ be an arbitrary function of two variables. Then, using $(dx_t)^2 = dt$ and $dx_t dt = (dt)^2 = 0$ in the fourth line,

$$\begin{aligned} df(X_t, t) &= f(X_t, t) - f(X_{t-dt}, t-dt) \\ &= \frac{\partial f}{\partial x} dX_t + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} (dX_t)^2 + \frac{\partial f}{\partial t} dt \\ &= \frac{\partial f}{\partial x} [a dt + b dx_t] + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} [a dt + b dx_t]^2 + \frac{\partial f}{\partial t} dt \\ &= \frac{\partial f}{\partial x} [a dt + b dx_t] + \frac{b^2}{2} \frac{\partial^2 f}{\partial x^2} dt + \frac{\partial f}{\partial t} dt \\ &= \left\{ a \frac{\partial f}{\partial x} + \frac{b^2}{2} \frac{\partial^2 f}{\partial x^2} + \frac{\partial f}{\partial t} \right\} dt + b \frac{\partial f}{\partial x} dx_t \\ &=: \{Af + \frac{\partial f}{\partial t}\} dt + \text{diffusive} \end{aligned} \quad (\text{A.36})$$

That is,

$$(Af)(x, t) := a(x, t) \frac{\partial f}{\partial x}(x, t) + \frac{b^2(x, t)}{2} \frac{\partial^2 f}{\partial x^2}(x, t) \quad (\text{A.37})$$

Now let $g = g(x)$ be another arbitrary function of one variable. We fix a start time t and an end time $T > t$ and consider the expectation (the f below also depends on end time T , but this dependency we do not make explicit in the notation)

$$f(x, t) := E_t^T [g(X_T^{t,x})] \quad (\text{A.38})$$

which in discrete time $t = t_k = kdt$ and $T = t_N = Ndt$ is given by

$$f(x, t_k) = E_{t_k}^{t_N} [g(X_{t_N}^{t_k,x})] := \int_{\mathbb{R}^{N-k}} g(X_{t_N}^{t_k,x}(\{\phi_\ell\}_{\ell=k+1}^N)) \prod_{\ell=k+1}^N e^{-\frac{\phi_\ell^2}{2}} \frac{d\phi_\ell}{\sqrt{2\pi}} \quad (\text{A.39})$$

Here we used the notation $X_T^{t,x}$ with superscripts (t, x) to indicate that the diffusion X starts at time t with initial value x ,

$$X_t^{t,x} = x \quad (\text{A.40})$$

In particular, there is the identity

$$X_{t_N}^{t_k, X_{t_k}^{t_j, x_j}} = X_{t_N}^{t_j, x_j} \quad (\text{A.41})$$

for arbitrary times $t_j \leq t_k \leq t_N$. Thus, if we define for some fixed initial values (t_0, x_0) the stochastic quantity

$$M_{t_k} := f(X_{t_k}^{t_0, x_0}, t_k) = \mathbb{E}_{t_k}^T \left[g(X_{t_N}^{t_k, X_{t_k}^{t_0, x_0}}) \right] = \mathbb{E}_{t_k}^T \left[g(X_{t_N}^{t_0, x_0}) \right] \quad (\text{A.42})$$

then this quantity is a martingale since we have for arbitrary time $t_j < t_k$

$$\mathbb{E}_{t_j}^T [M_{t_k}] = \mathbb{E}_{t_j}^T \left[\mathbb{E}_{t_k}^T \left[g(X_{t_N}^{t_0, x_0}) \right] \right] = \mathbb{E}_{t_j}^T \left[g(X_{t_N}^{t_0, x_0}) \right] = M_{t_j} \quad (\text{A.43})$$

In particular, we have $\mathbb{E}_{t_{k-1}}^T [M_{t_k}] = M_{t_{k-1}}$ which means that we have to have

$$\begin{aligned} 0 &\stackrel{!}{=} \mathbb{E}_{t_{k-1}}^T [M_{t_k}] - M_{t_{k-1}} = \mathbb{E}_{t_{k-1}}^T [M_{t_k} - M_{t_{k-1}}] = \mathbb{E}_{t_{k-1}}^T [df(X_{t_k}^{t_0, x_0}, t_k)] \\ &\stackrel{(\text{A.36})}{=} \mathbb{E}_{t_{k-1}}^T \left[\left\{ Af + \frac{\partial f}{\partial t} \right\} (X_{t_{k-1}}^{t_0, x_0}, t_{k-1}) dt + \text{diffusive} \right] \\ &= \left\{ Af + \frac{\partial f}{\partial t} \right\} (X_{t_{k-1}}^{t_0, x_0}, t_{k-1}) dt + \mathbb{E}_{t_{k-1}}^T [\text{diffusive}] \\ &= \left\{ Af + \frac{\partial f}{\partial t} \right\} dt + 0 \end{aligned} \quad (\text{A.44})$$

That is, the expectation $f(x, t) = \mathbb{E}_t^T [g(X_T^{t, x})]$ has to satisfy the second order PDE

$$\frac{\partial f}{\partial t} + Af = 0 \quad (\text{A.45})$$

We summarize in the following

Theorem A3 a) Let X_t be an Ito diffusion given by

$$dX_t = a(X_t, t) dt + b(X_t, t) dx_t \quad (\text{A.46})$$

and for some initial values (t, x) define the Wiener expectation

$$f(x, t) := \mathbb{E}_t^T [g(X_T^{t, x})] \quad (\text{A.47})$$

Then f can be obtained as the solution of the parabolic second order PDE

$$\frac{\partial f}{\partial t} + Af = 0 \quad (\text{A.48})$$

with final condition $f(x, T) = g(x)$ and A given by (A.37) above.

b) Let X_t be a time-homogenous Ito diffusion given by

$$dX_t = a(X_t) dt + b(X_t) dx_t \quad (\text{A.49})$$

with coefficients $a = a(X_t)$ and $b = b(X_t)$ which do not explicitly depend on time. Then there is the identity

$$\mathbb{E}_t^T [g(X_T^{t, x})] = \mathbb{E}_0^{T-t} [g(X_{T-t}^{0, x})] \quad (\text{A.50})$$

In particular, the expectation

$$f(x, t) := \mathbb{E}_0^t [g(X_t^{0, x})] \quad (\text{A.51})$$

now considered as a function of the end time t (start time is 0), is a solution of the PDE

$$-\frac{\partial f}{\partial t} + Af = 0 \quad (\text{A.52})$$

with initial condition $f(x, 0) = g(x)$ and A given by

$$(Af)(x, t) := a(x) \frac{\partial f}{\partial x}(x, t) + \frac{b^2(x)}{2} \frac{\partial^2 f}{\partial x^2}(x, t) . \quad (\text{A.53})$$

Equation (A.52) is then usually referred to as Kolmogorov's backward equation, see for example Theorem 8.1.1 in the book of Oksendal [42]. By a slight variation of the above argument one also obtains a PDE representation for the quantity

$$u(x, t) := \mathbb{E}_0^t [e^{-\int_0^t r(X_s^{0,x}) ds} g(X_t^{0,x})] \quad (\text{A.54})$$

which is then the Wiener measure version of the Feynman-Kac formula, this is Theorem 8.2.1 in Oksendal [42], and it reads

$$-\frac{\partial u}{\partial t} + Au - ru = 0 \quad (\text{A.55})$$

$$u(x, 0) = g(x)$$

In this paper we do not use it, neither the Wiener nor the Fresnel version, we only use the Fresnel version of part (b) of the theorem above and this version we write down in the next section.

A.4 Stochastic Calculus with Respect to Fresnel Measure

Fresnel Brownian Motion and Fresnel Measure

A Fresnel Brownian motion or Fresnel BM in discretized time $t = t_k = k\Delta t$ we define as the combination of integration variables

$$x_{t_k} = \sqrt{\Delta t} \sum_{\ell=1}^k \phi_\ell \quad (\text{A.56})$$

where the ϕ_ℓ are to be integrated against Fresnel measure which is given by

$$dF := \prod_{\ell=1}^N e^{i \frac{\phi_\ell^2}{2}} \frac{d\phi_\ell}{\sqrt{2\pi i}} = \prod_{\ell=1}^N e^{i \frac{(x_{t_\ell} - x_{t_{\ell-1}})^2}{2\Delta t}} \frac{dx_{t_\ell}}{\sqrt{2\pi i \Delta t}} \quad (\text{A.57})$$

Let's consider again the discretized version of the quantity $\int_0^T f(t) (dx_t)^2$ which is

$$I_{\Delta t}(f) := \sum_{k=1}^N f(t_k) (x_{t_k} - x_{t_{k-1}})^2 = \Delta t \sum_{k=1}^{N_t} f(t_k) \phi_k^2 \quad (\text{A.58})$$

Then the Fresnel analog of (A.12) is

$$\lim_{\Delta t \rightarrow 0} \mathbb{E} [e^{iq I_{\Delta t}(f)}] = e^{-q \int_0^T f(t) dt} \quad (\text{A.59})$$

which then leads to the following basic calculation rule for Fresnel Brownian motions:

$$(dx_t)^2 = i dt \quad (\text{A.60})$$

and $dx_t dt = dt dt = 0$. The proof of (A.59) is as follows:

$$\begin{aligned}
 \mathbb{E} \left[e^{iq I_{\Delta t}(f)} \right] &= \int_{\mathbb{R}^N} \prod_{k=1}^N e^{\frac{i}{2} (1 + 2q \Delta t f(t_k)) \phi_k^2} \frac{d\phi_k}{\sqrt{2\pi i}} \\
 &= \prod_{k=1}^N \frac{1}{\sqrt{1 + 2q \Delta t f(t_k)}} \\
 &= \exp \left\{ -\frac{1}{2} \sum_{k=1}^N \log [1 + 2q \Delta t f(t_k)] \right\} \\
 &= \exp \left\{ -\frac{1}{2} \sum_{k=1}^N 2q \Delta t f(t_k) + O(\Delta t) \right\} \\
 &\xrightarrow{\Delta t \rightarrow 0} \exp \left\{ -q \int_0^T f(t) dt \right\}
 \end{aligned} \tag{A.61}$$

and this coincides with (A.59).

The Fresnel Version of the Ito Formula

As in Section A.2, we can write for some arbitrary function $f = f(x)$ and x_t now being a Fresnel BM

$$f(x_T) - f(x_0) = \sum_{k=1}^N \{ f(x_{t_k}) - f(x_{t_{k-1}}) \} \tag{A.62}$$

with

$$\begin{aligned}
 df(x_{t_k}) &:= f(x_{t_k}) - f(x_{t_{k-1}}) = f'(x_{t_{k-1}}) dx_{t_k} + \frac{1}{2} f''(x_{t_{k-1}}) (dx_{t_k})^2 \\
 &\stackrel{(A.60)}{=} f'(x_{t_{k-1}}) dx_{t_k} + \frac{i}{2} f''(x_{t_{k-1}}) dt
 \end{aligned} \tag{A.63}$$

Summing this up,

$$\begin{aligned}
 f(x_T) - f(x_0) &= \sum_{k=1}^N \left\{ f'(x_{t_{k-1}}) dx_{t_k} + \frac{i}{2} f''(x_{t_{k-1}}) dt \right\} \\
 &\stackrel{dt \rightarrow 0}{=} \int_0^T f'(x_t) dx_t + \frac{i}{2} \int_0^T f''(x_t) dt
 \end{aligned} \tag{A.64}$$

where the first integral again has the property that its expectation value always vanishes,

$$\mathbb{E} \left[\int_0^T f(x_t) dx_t \right] = 0 \tag{A.65}$$

since as in the Wiener case the quantities $f(x_{t_{k-1}})$ and dx_{t_k} are independent and we obtain

$$\mathbb{E} [f(x_{t_{k-1}}) dx_{t_k}] = \mathbb{E} [f(x_{t_{k-1}})] \times \sqrt{dt} \mathbb{E} [\phi_k] = 0 \tag{A.66}$$

Concerning the last equality, one probably should make the definition

$$\mathbb{E} [\phi] = \int_{-\infty}^{+\infty} \phi e^{i \frac{\phi^2}{2}} \frac{d\phi}{\sqrt{2\pi i}} := \lim_{R \rightarrow \infty} \int_{-R}^{+R} \phi e^{i \frac{\phi^2}{2}} \frac{d\phi}{\sqrt{2\pi i}} = 0 \tag{A.67}$$

Fresnel Version of Kolmogorov's Backward Equation

We proceed as in Section A.3 and define a Fresnel diffusion X_t as a stochastic quantity which is given by the recursion

$$X_{t_k} = X_{t_{k-1}} + a(X_{t_{k-1}}, t_{k-1}) dt + b(X_{t_{k-1}}, t_{k-1}) \sqrt{dt} \phi_k \quad (\text{A.68})$$

where the $\{\phi_k\}_{k=1}^N$ are to be integrated against Fresnel measure. In continuous time, we write

$$dX_t = a(X_t, t) dt + b(X_t, t) dx_t \quad (\text{A.69})$$

To each Fresnel diffusion, we assign the second order operator A through (f again denotes an arbitrary function of two variables)

$$\begin{aligned} df(X_t, t) &= \frac{\partial f}{\partial x} dX_t + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} (dX_t)^2 + \frac{\partial f}{\partial t} dt \\ &= \frac{\partial f}{\partial x} [a dt + b dx_t] + \frac{1}{2} \frac{\partial^2 f}{\partial x^2} [a dt + b dx_t]^2 + \frac{\partial f}{\partial t} dt \\ &= \frac{\partial f}{\partial x} [a dt + b dx_t] + i \frac{b^2}{2} \frac{\partial^2 f}{\partial x^2} dt + \frac{\partial f}{\partial t} dt \\ &= \left\{ a \frac{\partial f}{\partial x} + i \frac{b^2}{2} \frac{\partial^2 f}{\partial x^2} + \frac{\partial f}{\partial t} \right\} dt + b \frac{\partial f}{\partial x} dx_t \\ &=: \{ Af + \frac{\partial f}{\partial t} \} dt + \text{diffusive} \end{aligned} \quad (\text{A.70})$$

That is,

$$(Af)(x, t) := a(x, t) \frac{\partial f}{\partial x}(x, t) + i \frac{b^2(x, t)}{2} \frac{\partial^2 f}{\partial x^2}(x, t) \quad (\text{A.71})$$

and we still have

$$\mathbb{E}[\text{diffusive}] = 0 \quad (\text{A.72})$$

We consider the Fresnel expectation

$$f(x, t) := \mathbb{E}_t^T [g(X_T^{t,x})] \quad (\text{A.73})$$

which in discrete time $t = t_k = kdt$ and $T = t_N = Ndt$ is given by

$$f(x, t_k) = \mathbb{E}_{t_N}^{t_N} [g(X_{t_N}^{t_k, x})] := \int_{\mathbb{R}^{N-k}} g(X_{t_N}^{t_k, x}(\{\phi_\ell\}_{\ell=k+1}^N)) \prod_{\ell=k+1}^N e^{i \frac{\phi_\ell^2}{2}} \frac{d\phi_\ell}{\sqrt{2\pi i}} \quad (\text{A.74})$$

For some fixed initial values (t_0, x_0) , we define the stochastic quantity

$$M_{t_k} := f(X_{t_k}^{t_0, x_0}, t_k) = \mathbb{E}_{t_k}^T \left[g(X_{t_N}^{t_k, X_{t_k}^{t_0, x_0}}) \right] = \mathbb{E}_{t_k}^T [g(X_{t_N}^{t_0, x_0})] \quad (\text{A.75})$$

which again is a martingale since for $t_j < t_k$

$$\mathbb{E}_{t_j}^T [M_{t_k}] = \mathbb{E}_{t_j}^T \left[\mathbb{E}_{t_k}^T [g(X_{t_N}^{t_0, x_0})] \right] = \mathbb{E}_{t_j}^T [g(X_{t_N}^{t_0, x_0})] = M_{t_j} \quad (\text{A.76})$$

In particular, we have $E_{t_{k-1}}^T[M_{t_k}] = M_{t_{k-1}}$ which means that we have to have

$$\begin{aligned} 0 &\stackrel{!}{=} E_{t_{k-1}}^T[M_{t_k}] - M_{t_{k-1}} = E_{t_{k-1}}^T[M_{t_k} - M_{t_{k-1}}] = E_{t_{k-1}}^T[df(X_{t_k}^{t_0, x_0}, t_k)] \\ &\stackrel{(A.70)}{=} E_{t_{k-1}}^T\left[\left\{Af + \frac{\partial f}{\partial t}\right\}(X_{t_{k-1}}^{t_0, x_0}, t_{k-1}) dt + \text{diffusive}\right] \\ &= \left\{Af + \frac{\partial f}{\partial t}\right\}(X_{t_{k-1}}^{t_0, x_0}, t_{k-1}) dt + E_{t_{k-1}}^T[\text{diffusive}] \\ &= \left\{Af + \frac{\partial f}{\partial t}\right\} dt + 0 \end{aligned} \quad (A.77)$$

That is, the Fresnel expectation $f(x, t) = E_t^T[g(X_T^{t, x})]$ has to satisfy the PDE

$$\frac{\partial f}{\partial t} + Af = 0 \quad (A.78)$$

with final condition $f(x, T) = g(x)$ and second order operator A given by (A.71).

The time-homogenous case, the analog of part (b) of Theorem A3, then reads as follows: Let X_t be a time-homogenous Fresnel diffusion given by

$$dX_t = a(X_t) dt + b(X_t) dx_t \quad (A.79)$$

with coefficients $a = a(X_t)$ and $b = b(X_t)$ which do not explicitly depend on time and let $g = g(x)$ be an arbitrary function of one variable. Then the Fresnel expectation

$$f(x, t) := E_0^t[g(X_t^{0, x})] \quad (A.80)$$

is a solution of the PDE

$$\frac{\partial f}{\partial t} = Af = a(x) \frac{\partial f}{\partial x} + i \frac{b^2(x)}{2} \frac{\partial^2 f}{\partial x^2} \quad (A.81)$$

with initial condition

$$f(x, 0) = g(x) \quad (A.82)$$

Finally, let us recall that in general Wiener or Fresnel expectations can be calculated through the following

Theorem A4 Consider m times $0 < t_1 < t_2 < \dots < t_m \leq T$ and let x_{t_j} be a standard or Fresnel BM observed at time t_j . Let

$$F = F(x_{t_1}, \dots, x_{t_m}) \quad (A.83)$$

be an arbitrary function of m variables and let $E[F] = E_0^T[F]$ denote its Wiener or Fresnel expectation value. Then, with $t_0 := 0$ and $x_0 := 0$,

$$E[F] = \int_{\mathbb{R}^m} F(x_{t_1}, \dots, x_{t_m}) \prod_{j=1}^m p_{t_j - t_{j-1}}(x_{t_{j-1}}, x_{t_j}) dx_{t_j} \quad (A.84)$$

with Gaussian or Fresnel kernels given by

$$p_\tau(x, y) := \begin{cases} \frac{1}{\sqrt{2\pi\tau}} e^{-\frac{(x-y)^2}{2\tau}} & \text{for Wiener expectations} \\ \frac{1}{\sqrt{2\pi i\tau}} e^{i\frac{(x-y)^2}{2\tau}} & \text{for Fresnel expectations.} \end{cases} \quad (A.85)$$

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