# The Dynamics of the Hubbard Model through Stochastic Calculus and Girsanov Transformation

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45/91 slides are pictures or title/cover slides or appendix, motivation has 21 pictures

## 1. Setup and Motivation

### 1. Setup and Motivation

Bose-Hubbard Hamiltonian in d Dimensions (n.n. = nearest neighbors):

$$H = -J \sum_{i,j \atop n.n.} (a_i^+ a_j + a_j^+ a_i) + \frac{U}{2} \sum_j a_j^+ a_j^+ a_j a_j + \sum_j \epsilon_j a_j^+ a_j$$

Bosonic Annihilation and Creation operators:

$$[a_i, a_j^+] = \delta_{i,j}$$

Cubic Lattice T:

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

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### 1. Setup and Motivation: Quantities of Interest

Initial state: N particles at some lattice site  $j_0$ 

$$\psi_0 := rac{(a_{j_0}^+)^N}{\sqrt{N!}} \ket{0}$$

Time evolved state:

$$\psi_t = e^{-itH} \psi_0$$

Number of particles  $\langle n_{j,t} \rangle$  at lattice site j at some time t > 0:

$$\langle n_{j,t} \rangle := \langle \psi_t, a_j^+ a_j \psi_t \rangle$$

Already for just two lattice sites 1 and 2, quite complex behaviour, Example:

### 1. Setup and Motivation: Example Two Site Bose-Hubbard Model

Two Site Bose-Hubbard model:

$$H = \varepsilon \left( a_1^+ a_2^- + a_2^+ a_1^- \right) + u \left( a_1^+ a_1^+ a_1^- a_1^- + a_2^+ a_2^+ a_2^- a_2^- \right)$$

N = 20 particles at lattice site  $j_0 = 1$ :

$$\psi_0 := \frac{(a_1^+)^N}{\sqrt{N!}} |0\rangle$$

Plot 
$$\langle n_{1,t} \rangle = \langle \psi_t, a_1^+ a_1^- \psi_t \rangle$$
 for

$$\varepsilon = 1$$
  

$$t \in [0, 500]$$
  

$$N = 20$$
  

$$u = g/N$$

with interaction strength

$$g \in \left\{ \, 0 \, , \, \frac{1}{16} \, , \, \frac{1}{8} \, , \, \frac{1}{4} \, , \, \frac{1}{2} \, , \, 1 \, , \, 1.5 \, , \, 2.0 \, , \, 2.5 \, , \, 3 \, , \, 4 \, , \, 5 \, , \, 25 \, \right\}$$

$$g=0,~$$
 non interacting case,  $~\langle {\it n}_{1,t}
angle ~=~ N\cos^2arepsilon t$ 



time t in [0,500]

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$$g = 1/16$$



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$$g = 1/8$$

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$$g = 1/4$$

<n1> black , <n2> red , <n1>+<n2> green



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$$g = 1/2$$

<n1> black , <n2> red , <n1>+<n2> green



<n1> black, <n2> red, <n1>+<n2> green



g = 1.5

<n1> black , <n2> red , <n1>+<n2> green



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g = 2.0

<n1> black , <n2> red , <n1>+<n2> green



time t in [0,500]

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$$g = 2.5$$

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$$g = 25$$

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arepsilon=0.5,~g=1/8





arepsilon=0.5, g=1/4





arepsilon=0.5,~g=1/2

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 $\varepsilon = 1$ , g = 1,  $g/\varepsilon = 1$ 

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<n1> black, <n2> red, <n1>+<n2> green



 $\varepsilon = 0.5, \ g = 1, \ g/\varepsilon = 2$ 

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#### <n1> black, <n2> red, <n1>+<n2> green



### $\varepsilon = 0.5, \ g = 1.5, \ g/\varepsilon = 3$

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### Central Problem of Many Body Quantum Mechanics:

#### Calculate Density Matrix Elements or Correlation Functions

 $\langle \psi_t, a_j^+ a_j \psi_t \rangle$ ,  $\langle \psi_t, a_i^+ a_j^+ a_k a_\ell \psi_t \rangle$ , ...

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this talk: new proposal for doing that

### 1. Setup and Motivation: Bargmann-Segal Representation

Bargmann-Segal representation:

$$a_j = \frac{\partial}{\partial z_j}, \quad a_j^+ = z_j$$

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

$$\mathcal{F} \hspace{.1in} := \hspace{.1in} \left\{ \hspace{.1in} f = f\big( \hspace{.1in} \{z_j\} \hspace{.1in} \big) \hspace{.1in} : \hspace{.1in} \mathbb{C}^{|\Gamma|} \rightarrow \mathbb{C} \hspace{.1in} \text{analytic} \hspace{.1in} \left| \hspace{.1in} \|f\|_{\mathcal{F}}^2 = \langle f, f \rangle_{\mathcal{F}} \hspace{.1in} < \infty \hspace{.1in} \right\}$$

with scalar product

$$\langle f,g \rangle_{\mathcal{F}} := \int_{\mathbb{C}^{|\Gamma|} = \mathbb{R}^{2|\Gamma|}} f(z) \overline{g(z)} d\mu(z)$$
  
 $d\mu(z) := \prod_{j} e^{-|z_j|^2} \frac{d\operatorname{Re} z_j d\operatorname{Im} z_j}{\pi}$ 

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### 1. Setup and Motivation: Bargmann-Segal Representation

### Hamiltonian:

$$h = \sum_{i,j} \varepsilon_{ij} z_i \frac{\partial}{\partial z_j} + u \sum_j z_j^2 \frac{\partial^2}{\partial z_j^2} =: h_0 + h_{int}$$

We can allow for a general hopping matrix which should be real and symmetric:

$$\varepsilon := (\varepsilon_{ij})_{i,j\in\Gamma} \in \mathbb{R}^{|\Gamma|\times|\Gamma|}, \quad \varepsilon_{i,j} = \varepsilon_{j,i}$$

For a nearest neighbor hopping J and on-diagonal trapping potentials  $\epsilon_j$ :

$$\varepsilon_{ij} = \begin{cases} -J & \text{if } |i-j| = 1 \\ +\epsilon_j & \text{if } i=j \\ 0 & \text{otherwise} \end{cases}$$

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### 1. Setup and Motivation: Coherent States and Number States

Coherent and Number states,  $\lambda = \{\lambda_j\} \in \mathbb{C}^{|\Gamma|}$  :

$$\psi_{coh}(z) = \psi_{coh}(\{z_j\}) = \prod_j e^{\lambda_j z_j} e^{-\frac{|\lambda_j|^2}{2}} =: e^{\lambda z} e^{-\frac{|\lambda|^2}{2}}$$
  
$$\psi_{num}(z) = \psi_{num}(\{z_j\}) = \frac{1}{\sqrt{N!N^N}} \left(\sum_j \lambda_j z_j\right)^N =: \frac{(\lambda z)^N}{\sqrt{N!N^N}}$$

In both cases: t = 0 expected number of particles at site *j*:

$$\langle \psi_0, a_j^+ a_j \psi_0 \rangle_{\mathcal{F}} = |\lambda_j|^2$$

Thus: Total number of particles N:

$$N = \sum_{j} N_{j} = \sum_{j} |\lambda_{j}|^{2} = |\lambda|^{2}$$



1) Time Evolution of States as Fresnel Expectation Values,  $t = t_k = kdt$ 

$$\psi_t(z) = (e^{-ith}\psi_0)(z) = \mathsf{E}_{\phi}[\psi_0(U_{\phi,t}z)]$$

with unitary evolution matrix

$$U_{kdt}(\phi) = e^{-i dt \varepsilon} e^{-i D_{dt}(\phi_1)} \cdots e^{-i dt \varepsilon} e^{-i D_{dt}(\phi_k)} \in \mathbb{C}^{|\Gamma| \times |\Gamma|}$$

2) Correlation Functions as Fresnel Expectation Values

$$\langle \psi_t, a_i^+ a_j | \psi_t \rangle = \mathsf{E}_{\phi} \bar{\mathsf{E}}_{\theta} \left[ F_{i,j}^{\psi_0} (U_{\phi,t}, \bar{U}_{\theta,t}) \right]$$

3) Stochastic Differential Equation (SDE) for Unitary Evolution Matrix  $U_{\phi,t}$ 

$$dU_t = -i U_t \left( \varepsilon dt + \sqrt{2u} dx_t \right), \qquad dx_{kdt} = \sqrt{dt} \phi_k$$

4) Correlation Functions from SDEs,  $(v_t, \bar{v}_t) := (U_{\phi,t}^T \lambda, \bar{U}_{\theta,t}^T \bar{\lambda})$ 

$$\langle \psi_t, a_i^+ a_j \psi_t \rangle_{coh/num} = \mathsf{E}\bar{\mathsf{E}} \left[ v_{i,t} \bar{v}_{j,t} P_{\psi_0}(v_t \bar{v}_t) \right] / P_{\psi_0}(v_0 \bar{v}_0)$$

with 
$$\begin{aligned} dv_j &= -i \, (\varepsilon v)_j \, dt \, - \, i \, \sqrt{2u} \, v_j \, dx_j \\ d\bar{v}_j &= \, + \, i \, (\varepsilon \bar{v})_j \, dt \, + \, i \, \sqrt{2u} \, \bar{v}_j \, dy_j \, , \qquad \qquad P_{coh/num}(x) = e^x \text{ or } x^{N-1} \end{aligned}$$

5) Correlation Functions from Girsanov-Transformed SDEs

$$\langle \psi_t, a_i^+ a_j \psi_t \rangle_{coh/num} = \mathsf{E}\bar{\mathsf{E}}[v_{i,t} \bar{v}_{j,t}]$$

with  $dv_j = -i(\varepsilon v)_j dt - i2u [\log P_{\psi_0}]'(v\bar{v}) v_j \bar{v}_j v_j dt - i\sqrt{2u} v_j dx_j d\bar{v}_j d\bar{v}_j = +i(\varepsilon \bar{v})_j dt + i2u [\log P_{\psi_0}]'(v\bar{v}) v_j \bar{v}_j \bar{v}_j dt + i\sqrt{2u} \bar{v}_j dy_j$ 

6) Large N Limit: g := uN fixed,  $(w, \bar{w}) := (v, \bar{v})/\sqrt{N}$ , then

$$\langle \psi_t, a_i^+ a_j \psi_t \rangle_{coh/num} = N \times E\overline{E}[w_{i,t} \overline{w}_{j,t}]$$

Large N Limit can be read off:

$$\langle \psi_t, a_i^+ a_j | \psi_t \rangle_{coh/num} = N \times w_i(t) \bar{w}_j(t)$$

with  $w_j, \bar{w}_j$  given by the ODE system ([log  $P_{coh/num}$ ]'  $\rightarrow$  1)

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

which is the time dependent discrete Gross-Pitaevskii equation.

2. Overall Strategy: Additional Results (appendix has more detail)

- Various Exact PDE Representations (confirming stochastic calculus formalism)
- Collapse and Revivals can be obtained from an approximate ODE System Black numbers are from exact diagonalization, the red curve comes from an analytical calculation:



• Equivalence between Mathematical Pendulum and Quartic Double-Well Potential

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Time evolution with Trotter formula,  $t = t_k = k dt$ :

$$e^{-ith} = e^{-ikdt(h_0+h_{int})} \approx (e^{-idth_0}e^{-idth_{int}})^k$$

Let's consider the action of  $e^{-i dt h_0}$  and  $e^{-i dt h_{int}}$ :

Action of  $e^{-ith_0}$ :

$$(e^{-ith_0}f)(z) = f(e^{-it\varepsilon}z)$$

since with  $z_t := e^{-i\varepsilon t} z$ 

$$\frac{\partial}{\partial t} [f(z_t)] = \frac{\partial}{\partial t} [f(e^{-it\varepsilon}z)] = \sum_j \frac{\partial z_{t,j}}{\partial t} \frac{\partial f}{\partial z_j}(z_t) = \sum_j (-i\varepsilon z_t)_j \frac{\partial f}{\partial z_j}(z_t)$$

$$= \left\{ -i\sum_{j,k} \varepsilon_{j,k} z_k \frac{\partial f}{\partial z_j} \right\} (z = z_t) = \left\{ -ih_0 f \right\} (z_t)$$

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Action of  $e^{-it h_{int}}$ :

$$(e^{-it h_{int}} f)(z) = \int_{\mathbb{R}^{|\Gamma|}} f(e^{-iD_t(\phi)}z) \prod_j e^{i\frac{\phi_j^2}{2}} \frac{d\phi_j}{\sqrt{2\pi i}}$$
 (1)

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with  $D_t(\phi)$  the  $|\Gamma| \times |\Gamma|$  diagonal matrix

$$D_t(\phi) = \operatorname{diag}(\{\sqrt{2ut} \phi_j - ut\}_{j \in \Gamma}) \in \mathbb{R}^{|\Gamma| \times |\Gamma|}$$

#### **Proof of (1):**

$$h_{int} \prod_{j} z_{j}^{n_{j}} = \left\{ u \sum_{i} z_{i}^{2} \frac{\partial^{2}}{\partial z_{i}^{2}} \right\} \prod_{j} z_{j}^{n_{j}} = \left\{ u \sum_{i} n_{i}(n_{i}-1) \right\} \prod_{j} z_{j}^{n_{j}}$$

$$e^{-it h_{int}} \prod_{j} z_{j}^{n_{j}} = e^{-iut \sum_{j} n_{j}(n_{j}-1)} \prod_{j} z_{j}^{n_{j}} = \prod_{j} \left( e^{+iut n_{j}} e^{-iut n_{j}^{2}} z_{j}^{n_{j}} \right)$$

Now use Fresnel integral (  $\sqrt{i} := e^{i\frac{\pi}{4}}$  )

$$\int_{\mathbb{R}} e^{-i\lambda\phi} e^{j\frac{\phi^2}{2}} \frac{d\phi}{\sqrt{2\pi i}} = e^{-j\frac{\lambda^2}{2}}$$

to obtain

$$e^{-it h_{int}} \prod_j z_j^{n_j} = \int_{\mathbb{R}^{|\Gamma|}} \prod_j \left( e^{+iut - i\sqrt{2ut} \phi_j} z_j \right)^{n_j} \prod_j e^{j \frac{\phi_j^2}{2}} \frac{d\phi_j}{\sqrt{2\pi i}}$$

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Thus, single Trotter step  $(\phi^2 := \sum_j \phi_j^2)$ :

$$(e^{-i dt h}f)(z) = \left[e^{-i dt h_{int}} \left(e^{-i dt h_0}f\right)\right](z)$$
$$= \int_{\mathbb{R}^{|\Gamma|}} f(e^{-i dt \varepsilon} e^{-i D_{dt}(\phi)}z) e^{i \frac{\phi^2}{2}} \frac{d^{|\Gamma|}\phi}{(2\pi i)^{|\Gamma|/2}}$$

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Iterating,  $t = t_k = kdt$ :

$$(e^{-i\,kdt\,h}f)(z) = \int_{\mathbb{R}^{k|\Gamma|}} f\left(e^{-i\,dt\,\varepsilon}e^{-i\,D_{dt}(\phi_{1})}\cdots e^{-i\,dt\,\varepsilon}e^{-i\,D_{dt}(\phi_{k})}z\right) \prod_{\ell=1}^{k} e^{i\frac{\phi_{\ell}^{2}}{2}} \frac{d^{|\Gamma|}\phi_{\ell}}{(2\pi i)^{|\Gamma|/2}}$$
$$=: \int_{\mathbb{R}^{k|\Gamma|}} f\left(U_{kdt}(\phi)z\right) dF\left(\{\phi_{\ell}\}_{\ell=1}^{k}\right)$$
$$=: \mathsf{E}\left[f\left(U_{\phi,kdt}z\right)\right]$$

with notations (  $k, \ell \in \mathbb{N}$  time indices,  $j = (j_1, \cdots, j_d) \in \Gamma$  lattice site index )

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

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**Theorem 1:** Let  $h = h_0 + h_{int}$  be the *d*-dimensional Bose-Hubbard hamiltonian with cubic lattice  $\Gamma = \{1, ..., L\}^d$ , hopping matrix  $\varepsilon$  and interaction *u*. Then, for t = kdt, the time evolution of some initial state  $\psi_0(z)$  is given by

$$(e^{-i \, k dt \, h} \psi_0)(z) = \int_{\mathbb{R}^{k|\Gamma|}} \psi_0(U_{k dt}(\phi) \, z) \, dF(\{\phi_\ell\}_{\ell=1}^k) = \mathsf{E}[\psi_0(U_{\phi,k dt} \, z)]$$

with unitary evolution matrix

$$U_{kdt}(\phi) = e^{-i dt \varepsilon} e^{-i D_{dt}(\phi_1)} \cdots e^{-i dt \varepsilon} e^{-i D_{dt}(\phi_k)} \in \mathbb{C}^{|\Gamma| \times |\Gamma|}$$
$$D_{dt}(\phi_\ell) = diag(\{\sqrt{2u dt} \phi_{j,\ell} - u dt\}_{j \in \Gamma}) \in \mathbb{R}^{|\Gamma| \times |\Gamma|}$$

and Fresnel measure given by

$$\mathsf{E}\big[\cdot\big] = \int_{\mathbb{R}^{k|\Gamma|}} \cdot d\mathsf{F}\big(\{\phi_\ell\}_{\ell=1}^k\big) = \int_{\mathbb{R}^{k|\Gamma|}} \cdot \prod_{\ell=1}^k e^{j\frac{\phi_\ell^2}{2}} \frac{d^{|\Gamma|}\phi_\ell}{(2\pi i)^{|\Gamma|/2}}$$

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Correlation Functions in Bargmann-Segal Representation:

$$\begin{array}{lll} \langle \psi_t \,, \mathbf{a}_i^+ \mathbf{a}_j \; \psi_t \,\rangle &=& \langle \psi_t \,, [\mathbf{a}_j \; \mathbf{a}_i^+ - \delta_{i,j}] \,\psi_t \,\rangle \\ \\ &=& \int_{\mathbb{C}^{|\Gamma|}} z_j \, \overline{z}_i \; |\psi_t(z)|^2 \, d\mu(z) \; - \; \delta_{i,j} \end{array}$$

From Theorem 1,

$$\psi_{kdt}(z) = \int_{\mathbb{R}^{k|\Gamma|}} \psi_0(U_{\phi,kdt}z) dF(\phi)$$
  
$$\overline{\psi_{kdt}(z)} = \int_{\mathbb{R}^{k|\Gamma|}} \overline{\psi_0(U_{\theta,kdt}z)} d\overline{F}(\theta)$$

with

$$dF(\phi) = \prod_{\ell=1}^{k} e^{+i\frac{\phi_{\ell}^{2}}{2}} \frac{d^{|\Gamma|}\phi_{\ell}}{(2\pi i)^{|\Gamma|/2}} , \quad d\bar{F}(\theta) = \prod_{\ell=1}^{k} e^{-i\frac{\theta_{\ell}^{2}}{2}} \frac{d^{|\Gamma|}\theta_{\ell}}{[2\pi(-i)]^{|\Gamma|/2}}$$

Thus, with t = kdt,

$$\begin{array}{l} \langle \psi_t, a_j a_i^+ \psi_t \rangle &= \int_{\mathbb{C}^{|\Gamma|}} z_j \, \bar{z}_i \, |\psi_t(z)|^2 \, d\mu(z) \\ \\ &= \int_{\mathbb{C}^{|\Gamma|}} z_j \, \bar{z}_i \, \int_{\mathbb{R}^{k|\Gamma|}} \psi_0(U_{\phi,t}z) \, dF(\phi) \, \int_{\mathbb{R}^{k|\Gamma|}} \overline{\psi_0(U_{\theta,t}z)} \, d\bar{F}(\theta) \, d\mu(z) \\ \\ &= \int_{\mathbb{R}^{k|\Gamma|}} \int_{\mathbb{R}^{k|\Gamma|}} \left\{ \int_{\mathbb{C}^{|\Gamma|}} z_j \, \bar{z}_i \, \psi_0(U_{\phi,t}z) \, \overline{\psi_0(U_{\theta,t}z)} \, d\mu(z) \right\} \, dF(\phi) \, d\bar{F}(\theta)$$

The red integral is the expectation over the bosonic Fock space and can be calculated:

The integrand is:

For coherent states:

$$\begin{aligned} z_j \, \bar{z}_i \, \psi_0(U_{\phi,t} z) \, \overline{\psi_0(U_{\theta,t} z)} &= z_j \, \bar{z}_i \, \exp\{\lambda \cdot U_{\phi,t} z\} \, \exp\{\bar{\lambda} \cdot \bar{U}_{\theta,t} \bar{z}\} \, e^{-|\lambda|^2} \\ &= z_j \, \bar{z}_i \, \exp\{U_{\phi,t}^T \lambda \cdot z\} \, \exp\{\bar{U}_{\theta,t}^T \bar{\lambda} \cdot \bar{z}\} \, e^{-|\lambda|^2} \end{aligned}$$

For number states:

$$z_{j} \bar{z}_{i} \psi_{0}(U_{\phi,t}z) \overline{\psi_{0}(U_{\theta,t}z)} = z_{j} \bar{z}_{i} \frac{1}{N!N^{N}} \left(\lambda \cdot U_{\phi,t}z\right)^{N} \left(\bar{\lambda} \cdot \bar{U}_{\theta,t}\bar{z}\right)^{N}$$
$$= z_{j} \bar{z}_{i} \frac{1}{N!N^{N}} \left(U_{\phi,t}^{T}\lambda \cdot z\right)^{N} \left(\bar{U}_{\theta,t}^{T}\bar{\lambda} \cdot \bar{z}\right)^{N}$$

Using  $\left( \begin{array}{c} \text{with} \quad (\lambda, \bar{\lambda}) \to (U_{\phi,t}^T \lambda, \bar{U}_{\theta,t}^T \bar{\lambda}) \quad \text{and recall} \quad d\mu(z) = \prod_j e^{-|z_j|^2} \frac{d\operatorname{Re} z_j d\operatorname{Im} z_j}{\pi} \end{array} \right)$ 

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

and

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

$$\frac{1}{N!} \int_{\mathbb{C}^{|\Gamma|}} z_{j} \bar{z}_{i} (\lambda z)^{N} (\bar{\lambda} \bar{z})^{N} d\mu(z) = \frac{\partial}{\partial \lambda_{j}} \frac{\partial}{\partial \bar{\lambda}_{i}} \frac{(\lambda \bar{\lambda})^{N+1}}{N+1} = N \lambda_{i} \bar{\lambda}_{j} (\lambda \bar{\lambda})^{N-1} + \delta_{i,j} (\lambda \bar{\lambda})^{N}$$

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we find

**Theorem 2:** For t = kdt let  $E\bar{E}[\cdot] = \int_{\mathbb{R}^{k|\Gamma|}} \int_{\mathbb{R}^{k|\Gamma|}} \cdot dF(\phi) d\bar{F}(\theta)$ . Then:

a) For an arbitrary initial state  $\psi_0$ ,

 $\psi_t(z) = (e^{-ith}\psi_0)(z) = \mathsf{E}[\psi_0(U_{\phi,t}z)]$  (reminder, same as Theorem 1)

b) For a coherent state  $\psi_0(z) = e^{\lambda z} e^{-|\lambda|^2/2}$ ,

 $\langle \psi_t, \mathbf{a}_i^+ \mathbf{a}_j \ \psi_t \rangle = \mathsf{E} \mathsf{E} \Big[ \left[ U_{\phi,t}^T \lambda \right]_i \ \left[ \bar{U}_{\theta,t}^T \bar{\lambda} \right]_j \ \exp \Big\{ U_{\phi,t}^T \lambda \cdot \bar{U}_{\theta,t}^T \bar{\lambda} \Big\} \Big] / e^{\lambda \bar{\lambda}}$ 

c) For a number state  $\psi_0(z) = (\lambda z)^N / \sqrt{N! N^N}$ ,  $\langle \psi_t, a_i^+ a_j | \psi_t \rangle = \mathsf{E} \mathsf{E} \Big[ [U_{\phi,t}^T \lambda]_i [\bar{U}_{\theta,t}^T \bar{\lambda}]_j (U_{\phi,t}^T \lambda \cdot \bar{U}_{\theta,t}^T \bar{\lambda})^{N-1} \Big] / (\lambda \bar{\lambda})^{N-1}$ 

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#### 5. SDE Representation: Reminder Brownian Motion and Wiener Measure

Standard Brownian motion in discrete time  $t = t_k = kdt$ :

$$\begin{array}{rcl} x_{t_k} & = & \sqrt{dt} \sum_{\ell=1}^k \phi_\ell & & dx_{t_k} := x_{t_k} - x_{t_{k-1}} = & \sqrt{dt} \phi_k \end{array}$$

Wiener measure in discrete time with fixed time horizon  $T = t_n = ndt$ :

$$dW = \prod_{\ell=1}^{n} e^{-\frac{\phi_{\ell}^{2}}{2}} \frac{d\phi_{\ell}}{\sqrt{2\pi}} = \prod_{\ell=1}^{n} e^{-\frac{(x_{t_{\ell}} - x_{t_{\ell-1}})^{2}}{2dt}} \frac{dx_{t_{\ell}}}{\sqrt{2\pi dt}}$$

Brownian motion calculation rule, basic to stochastic calculus:

$$(dx_t)^2 = dt$$

For more background, see the appendix compact summary stochastic calculus in

https://arxiv.org/pdf/2205.02010.pdf

#### 5. SDE Representation: Fresnel Brownian Motion and Fresnel Measure

Then Fresnel Brownian motion is

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with the  $\phi_\ell$  to be integrated against Fresnel measure,

$$dF = \prod_{\ell=1}^{n} e^{j \frac{\phi_{\ell}^{2}}{2}} \frac{d\phi_{\ell}}{\sqrt{2\pi i}} = \prod_{\ell=1}^{n} e^{j \frac{(x_{t_{\ell}} - x_{t_{\ell-1}})^{2}}{2dt}} \frac{dx_{t_{\ell}}}{\sqrt{2\pi i \, dt}}$$

Fresnel Brownian motion calculation rule:

$$(dx_t)^2 = i dt$$

For more background, see the appendix compact summary stochastic calculus in

https://arxiv.org/pdf/2205.02010.pdf

#### 5. SDE Representation: Unitary Evolution Matrix $U_{kdt}$

Unitary evolution matrix of Theorem 1,

$$U_{kdt} = e^{-i dt \varepsilon} e^{-i D_{dt}(\phi_1)} \cdots e^{-i dt \varepsilon} e^{-i D_{dt}(\phi_k)} = U_{(k-1)dt} e^{-i dt \varepsilon} e^{-i D_{dt}(\phi_k)}$$

with diagonal matrix  $D_{dt}(\phi_k)$  given by

$$D_{dt}(\phi_k) = \operatorname{diag}\left(\left\{\sqrt{2u}\sqrt{dt} \phi_{j,k} - u \, dt\right\}_{j \in \Gamma}\right)$$
  
= 
$$\operatorname{diag}\left(\left\{\sqrt{2u} \, dx_{j,kdt} - u \, dt\right\}_{j \in \Gamma}\right)$$
  
=: 
$$\sqrt{2u} \, dx_{kdt} - u \, dt \, ld$$

and diagonal matrix of Fresnel Brownian motions

$$dx_{kdt} := \operatorname{diag}(\{ dx_{j,kdt} \}_{j \in \Gamma}) \in \mathbb{R}^{|\Gamma| \times |\Gamma|}$$

which satisfies the matrix equation  $(dx_{kdt})^2 = i dt ld$ .

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#### 5. SDE Representation: Unitary Evolution Matrix $U_{kdt}$

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

$$e^{-i D_{dt}(\phi_k)} = 1 - i D_{dt}(\phi_k) - \frac{1}{2} [D_{dt}(\phi_k)]^2$$
  
=  $1 - i [\sqrt{2u} dx_{kdt} - u dt ld] - \frac{1}{2} [\sqrt{2u} dx_{kdt} - u dt ld]^2$   
=  $1 - i \sqrt{2u} dx_{kdt} + i u dt ld - \frac{1}{2} [\sqrt{2u} dx_{kdt}]^2$   
=  $1 - i \sqrt{2u} dx_{kdt} + i u dt ld - i u dt ld$   
=  $1 - i \sqrt{2u} dx_{kdt}$ 

Thus,  $U_{kdt} = U_{(k-1)dt} e^{-i dt \varepsilon} e^{-i D_{dt}(\phi_k)}$   $= U_{(k-1)dt} (1 - i dt \varepsilon) (1 - i \sqrt{2u} dx_{kdt})$   $= U_{(k-1)dt} (1 - i dt \varepsilon - i \sqrt{2u} dx_{kdt})$   $\Rightarrow dU_{t_k} := U_{t_k} - U_{t_{k-1}} = -i U_{t_{k-1}} (dt \varepsilon + \sqrt{2u} dx_{t_k})$ 

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**Theorem 3:** a) The unitary evolution matrix  $U_t$  satisfies the SDE

$$dU_t = -i U_t \left( \varepsilon \, dt + \sqrt{2u} \, dx_t \right)$$

b) The correlation functions have the representations

$$\langle \psi_t, a_i^+ a_j \ \psi_t \rangle_{coh} = \mathsf{E}\bar{\mathsf{E}} \left[ v_i \, \bar{v}_j \ e^{v\bar{v}} \right] / e^{\lambda \bar{\lambda}}$$

$$\langle \psi_t, a_i^+ a_j \ \psi_t \rangle_{num} = \mathsf{E}\bar{\mathsf{E}} \left[ v_i \, \bar{v}_j \ (v\bar{v})^{N-1} \right] / (\lambda \bar{\lambda})^{N-1}$$

with  $v, ar{v} \in \mathbb{C}^{|\Gamma|}$  ,  $v = (v_{j,x,t})$  ,  $ar{v} = (ar{v}_{j,y,t})$  , given by the SDE system

$$dv_j = -i dt (\varepsilon v)_j - i \sqrt{2u} v_j dx_j$$
  
$$d\bar{v}_j = +i dt (\varepsilon \bar{v})_j + i \sqrt{2u} \bar{v}_j dy_j$$

with initial conditions  $(\textit{v}_{x,0},\bar{\textit{v}}_{y,0})=(\lambda,\bar{\lambda})~~\text{and}~~E\bar{E}=E_x\bar{E}_y~$  .

#### Proof 3b) From Theorem 2,

$$\langle \psi_t, a_i^+ a_j \ \psi_t \rangle_{coh} = \mathsf{E}\bar{\mathsf{E}} \left[ \left[ U_{\phi,t}^T \lambda \right]_i \left[ \bar{U}_{\theta,t}^T \bar{\lambda} \right]_j \ \exp\left\{ U_{\phi,t}^T \lambda \cdot \bar{U}_{\theta,t}^T \bar{\lambda} \right\} \right] / e^{\lambda \bar{\lambda}}$$

$$\langle \psi_t, a_i^+ a_j \ \psi_t \rangle_{num} = \mathsf{E}\bar{\mathsf{E}} \left[ \left[ U_{\phi,t}^T \lambda \right]_i \left[ \bar{U}_{\theta,t}^T \bar{\lambda} \right]_j \left( U_{\phi,t}^T \lambda \cdot \bar{U}_{\theta,t}^T \bar{\lambda} \right)^{N-1} \right] / (\lambda \bar{\lambda})^{N-1}$$

With  $(x_{kdt} = \sqrt{dt} \sum_{j=1}^{k} \phi_j, y_{kdt} = \sqrt{dt} \sum_{j=1}^{k} \theta_j)$ 

$$\begin{aligned} v &= v_{x,t} &:= U_{x,t}^T \lambda \in \mathbb{C}^{|\Gamma|} \\ \bar{v} &= \bar{v}_{y,t} &:= \bar{U}_{y,t}^T \bar{\lambda} \in \mathbb{C}^{|\Gamma|} \end{aligned}$$

this looks as follows

$$\langle \psi_t, a_i^+ a_j \ \psi_t \rangle_{coh} = \mathsf{E}\bar{\mathsf{E}} \left[ v_i \ \bar{v}_j \ e^{v\bar{v}} \right] / e^{\lambda \bar{\lambda}} \langle \psi_t, a_i^+ a_j \ \psi_t \rangle_{num} = \mathsf{E}\bar{\mathsf{E}} \left[ v_i \ \bar{v}_j \ (v\bar{v})^{N-1} \right] / (\lambda \bar{\lambda})^{N-1}$$

Since

$$dU_t = -i U_t \left( \varepsilon \, dt + \sqrt{2u} \, dx_t \right)$$

and because of  $\varepsilon^T = \varepsilon$ ,  $dx_t^T = dx_t$ , we obtain

$$\begin{aligned} dU_t^T &= -i\left(\varepsilon \, dt \, + \, \sqrt{2u} \, dx_t\right) \, U_t^T \\ d\bar{U}_t^T &= +i\left(\varepsilon \, dt \, + \, \sqrt{2u} \, dy_t\right) \, \bar{U}_t^T \end{aligned}$$

Thus, with  $v_t = U_t^T \lambda$ ,  $\bar{v}_t = \bar{U}_t^T \bar{\lambda}$ ,

$$dv = -i \left( dt \varepsilon + \sqrt{2u} dx_t \right) v$$
  
$$d\bar{v} = +i \left( dt \varepsilon + \sqrt{2u} dy_t \right) \bar{v}$$

with initial conditions  $v_0 = U_0^T \lambda = \lambda$ ,  $\bar{v}_0 = \bar{U}_0^T \bar{\lambda} = \bar{\lambda}$ .

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## 6. Girsanov Transformed SDE Representation

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6.1 Unitary Time Evolution as a Martingale6.2 Girsanov Transformed SDE System

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As in Theorem 3, one finds just for the norms  $\|\psi_t\|^2$ :

$$\begin{array}{lll} \langle \psi_t, \psi_t \rangle_{coh} &=& \mathsf{E}\bar{\mathsf{E}}[\; e^{v\bar{v}}\;] \; / \; e^{\lambda\lambda} \\ \\ \langle \psi_t, \psi_t \rangle_{num} &=& \mathsf{E}\bar{\mathsf{E}}[\; (v\bar{v})^{N-1}\;] \; / \; (\lambda\bar{\lambda})^{N-1} \end{array}$$

with  $v\bar{v} = \sum_j v_j \bar{v}_j$  and  $v_j, \bar{v}_j$  given by the SDE system

$$dv_j = -i dt (\varepsilon v)_j - i \sqrt{2u} v_j dx_j$$
  
$$d\bar{v}_j = +i dt (\varepsilon \bar{v})_j + i \sqrt{2u} \bar{v}_j dy_j$$

These quantities have to be independent of time, we have to have

$$\begin{split} \mathsf{E}\bar{\mathsf{E}}[\; e^{v\bar{v}}\;] &= \; e^{v_0\bar{v}_0}\; = \; e^{\lambda\bar{\lambda}} \\ \mathsf{E}\bar{\mathsf{E}}[\; (v\bar{v})^{N-1}\;] &= \; (v_0\bar{v}_0)^{N-1}\; = \; (\lambda\bar{\lambda})^{N-1} \end{split}$$

How can this be understood in an SDE context?

From  

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

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

we get 
$$dv^T = -i v^T (\varepsilon dt + \sqrt{2u} dx_t)$$
,

$$d(v\bar{v}) \stackrel{\text{notation}}{=} d(v^T\bar{v}) = dv^T\bar{v} + v^Td\bar{v} + dv^Td\bar{v}$$
$$= -iv^T(\varepsilon dt + \sqrt{2u} dx_t)\bar{v} + iv^T(\varepsilon dt + \sqrt{2u} dy_t)\bar{v} + 0$$
$$= -iv^T\varepsilon \bar{v} dt + iv^T\varepsilon \bar{v} dt - i\sqrt{2u} v^T(dx_t - dy_t)\bar{v}$$
$$= -i\sqrt{2u} \sum_j v_j \bar{v}_j (dx_{j,t} - dy_{j,t})$$

The quantity  $v\bar{v}$  is a martingale, its  $d(v\bar{v})$  has no drift part. Since  $E[d_{x_{j,t}}] = \bar{E}[d_{y_{j,t}}] = 0$ ,

$$\Rightarrow \qquad \mathsf{E}\bar{\mathsf{E}}[(v\bar{v})_{t_k}] = (v\bar{v})_0 + \sum_{\ell=1}^k \mathsf{E}\bar{\mathsf{E}}[d(v\bar{v})_{t_\ell}] = (v\bar{v})_0$$

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Ok, but we need more, we need  $E\bar{E}[f(v_t\bar{v}_t)] = f(v_0\bar{v}_0)$  for arbitrary f. With Ito-Lemma:

$$df(v_t \bar{v}_t) = f'(v \bar{v}) d(v_t \bar{v}_t) + \frac{1}{2} f''(v \bar{v}) [d(v_t \bar{v}_t)]^2$$

Now,

$$\begin{aligned} [d(v_t \bar{v}_t)]^2 &= \left\{ -i\sqrt{2u} \sum_j v_j \bar{v}_j (dx_{j,t} - dy_{j,t}) \right\}^2 \\ &= -2u \sum_{i,j} v_i \bar{v}_i v_j \bar{v}_j (dx_{i,t} - dy_{i,t}) (dx_{j,t} - dy_{j,t}) \\ &= 0 \end{aligned}$$

since  $dx_{i,t}dx_{j,t} = dy_{i,t}dy_{j,t} = dx_{i,t}dy_{j,t} = 0$  for  $i \neq j$  and for i = j:  $(dx_{j,t} - dy_{j,t})^2 = (dx_{j,t})^2 - 2 dx_{j,t}dy_{j,t} + (dy_{j,t})^2$  $= + i dt - 2 \cdot 0 - i dt = 0$ 

Thus,

$$df(v_t \bar{v}_t) = f'(v \bar{v}) d(v_t \bar{v}_t) + \frac{1}{2} f''(v \bar{v}) \underbrace{[d(v_t \bar{v}_t)]^2}_{=0}$$
  
=  $-i\sqrt{2u} f'(v_t \bar{v}_t) \sum_j v_j \bar{v}_j (dx_{j,t} - dy_{j,t})$  (2)

has no drift part which gives  $E\bar{E}[df(v_t\bar{v}_t)] = 0$  and therefore

$$\mathsf{E}\bar{\mathsf{E}}[f(v_t\bar{v}_t)] = f(v_0\bar{v}_0) .$$

Equation (2) allows us in the next section 6.2 to absorb the the quantities  $e^{v\bar{v}}$  or  $(v\bar{v})^{N-1}$  into the Fresnel integration measure and to arrive at the compact expressions

$$\langle \psi_t, a_i^+ a_j \psi_t \rangle_{coh/num} = \mathsf{E}\bar{\mathsf{E}} \left[ v_i \bar{v}_j \right]$$

with new, and initial state coh/num dependent, SDE's for the  $v_i, \bar{v}_i$ . Result is Theorem 4.

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Untransformed representation:

$$\langle \psi_t, a_i^+ a_j \psi_t \rangle_{coh} = \mathsf{E}\bar{\mathsf{E}} \left[ v_i \bar{v}_j e^{v\bar{v}} \right] / e^{\lambda \bar{\lambda}} \langle \psi_t, a_i^+ a_j \psi_t \rangle_{num} = \mathsf{E}\bar{\mathsf{E}} \left[ v_i \bar{v}_j (v\bar{v})^{N-1} \right] / (\lambda \bar{\lambda})^{N-1}$$

We write

$$\langle \psi_t, a_i^+ a_j \psi_t \rangle = \mathsf{E}\bar{\mathsf{E}} \left[ v_{i,t} \bar{v}_{j,t} P(v_t \bar{v}_t) \right] / P(v_0 \bar{v}_0)$$

Now, with  $p := \log P$ ,

$$P(v_{t_{k}}\bar{v}_{t_{k}}) / P(v_{0}\bar{v}_{0}) = \exp\{p(v_{t_{k}}\bar{v}_{t_{k}}) - p(v_{0}\bar{v}_{0})\} = \exp\{\sum_{\ell=1}^{k} dp(v_{t_{\ell}}\bar{v}_{t_{\ell}})\}$$

$$\stackrel{(2)}{=} \exp\{-i\sqrt{2u}\sum_{\ell=1}^{k}\sum_{j}[p'(v\bar{v})(v_{j}\bar{v}_{j})]_{t_{\ell-1}}(dx_{j,t_{\ell}} - dy_{j,t_{\ell}})\}$$

$$= \exp\{-i\sqrt{2u}dt\sum_{\ell=1}^{k}\sum_{j}[p'(v\bar{v})(v_{j}\bar{v}_{j})]_{t_{\ell-1}}(\phi_{j,\ell} - \theta_{j,\ell})\}$$

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#### Since

$$\mathsf{E}\bar{\mathsf{E}}[\,\cdot\,] = \int_{\mathbb{R}^{k|\Gamma|}} \int_{\mathbb{R}^{k|\Gamma|}} \cdot dF(\phi) d\bar{F}(\theta)$$

with

$$dF(\phi) = \prod_{\ell=1}^{k} e^{+i\frac{\phi_{\ell}^{2}}{2}} \frac{d^{|\Gamma|}\phi_{\ell}}{(2\pi i)^{|\Gamma|/2}} , \quad d\bar{F}(\theta) = \prod_{\ell=1}^{k} e^{-i\frac{\theta_{\ell}^{2}}{2}} \frac{d^{|\Gamma|}\theta_{\ell}}{[2\pi(-i)]^{|\Gamma|/2}}$$

the quantity

$$P(v_{t_k}\bar{v}_{t_k}) / P(v_0\bar{v}_0) = \exp \left\{ -i\sqrt{2u \, dt} \sum_{\ell=1}^k \sum_j \left[ p'(v\bar{v})(v_j\bar{v}_j) \right]_{t_{\ell-1}} (\phi_{j,\ell} - \theta_{j,\ell}) \right\}$$

can be absorbed into the Fresnel measure by completing the square. In stochastic calculus, this is called a Girsanov transformation:

$$\begin{split} \tilde{\phi}_{j,\ell} &:= \phi_{j,\ell} - \sqrt{2u \, dt} \left[ p'(v\bar{v}) \, v_j \bar{v}_j \right]_{(\ell-1)dt} \\ \tilde{\theta}_{j,\ell} &:= \theta_{j,\ell} - \sqrt{2u \, dt} \left[ p'(v\bar{v}) \, v_j \bar{v}_j \right]_{(\ell-1)dt} \end{split}$$

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or equivalently

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

We get a new SDE system:

$$dv_j = -i dt (\varepsilon v)_j - i\sqrt{2u} v_j dx_j$$
  
=  $-i dt (\varepsilon v)_j - i\sqrt{2u} v_j [d\tilde{x}_j + \sqrt{2u} dt p' v_j \bar{v}_j]$   
=  $-i dt (\varepsilon v)_j - i 2u dt p' v_j \bar{v}_j v_j - i\sqrt{2u} v_j d\tilde{x}_j$ 

$$d\bar{v}_{j} = + i dt (\varepsilon \bar{v})_{j} + i \sqrt{2u} \bar{v}_{j} dy_{j}$$
  
$$= + i dt (\varepsilon \bar{v})_{j} + i \sqrt{2u} \bar{v}_{j} [d\tilde{y}_{j} + \sqrt{2u} dt p' v_{j} \bar{v}_{j}]$$
  
$$= + i dt (\varepsilon \bar{v})_{j} + i 2u dt p' v_{j} \bar{v}_{j} \bar{v}_{j} + i \sqrt{2u} \bar{v}_{j} d\tilde{y}_{j}$$

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**Theorem 4:** The correlation functions of Theorem 3 have the following equivalent representation:

$$\langle \psi_t, a_i^+ a_j \psi_t \rangle_{coh/num} = E\overline{E}[v_i \overline{v}_j]$$

with the  $v_j$ ,  $\bar{v}_j$  given by the transformed SDE system  $(v_j = v_{j,x,y,t}, \bar{v}_j = \bar{v}_{j,x,y,t})$ 

$$dv_j = -i (\varepsilon v)_j dt - i 2u p' v_j \overline{v}_j v_j dt - i \sqrt{2u} v_j dx_j$$
  
$$d\overline{v}_j = +i (\varepsilon \overline{v})_j dt + i 2u p' v_j \overline{v}_j \overline{v}_j dt + i \sqrt{2u} \overline{v}_j dy_j$$

and

$$p'(v\bar{v}) = [\log P]'(v\bar{v}) = \begin{cases} 1 & \text{for a coherent state} \\ (N-1)/(v\bar{v}) & \text{for a number state} \end{cases}$$

with  $P(x) = e^x$  or  $x^{N-1}$  for coh/num.

# 7. Large N Limit: Gross-Pitaevskii Equation

7.1 GP Equation for the d Dim Bose-Hubbard Model

7.2 GP Equation for the Two Site Bose-Hubbard Model and Numerical Test

#### 7.1 GP Equation for the d Dim Bose-Hubbard Model

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#### 7.1 GP Equation for the d Dim Bose-Hubbard Model

Recall  $|\lambda|^2 = N$ . Define normalized quantities

Then, with  $p' = p'(v\bar{v}) = p'(Nw\bar{w})$ ,

$$dw_j = -i dt (\varepsilon w)_j - i 2uN dt p' w_j \overline{w}_j w_j - i \sqrt{2u} w_j dx_j d\overline{w}_j = +i dt (\varepsilon \overline{w})_j + i 2uN dt p' w_j \overline{w}_j \overline{w}_j + i \sqrt{2u} \overline{w}_j dy_j$$

or, with

$$dw_{j} = -i dt (\varepsilon w)_{j} - i 2g dt p' w_{j} \overline{w}_{j} w_{j} - i \sqrt{2g/N} w_{j} dx_{j}$$
  

$$d\overline{w}_{j} = +i dt (\varepsilon \overline{w})_{j} + i 2g dt p' w_{j} \overline{w}_{j} \overline{w}_{j} + i \sqrt{2g/N} \overline{w}_{j} dy_{j}$$
(3)

The large N limit can be read off:
### 7.1 GP Equation for the d Dim Bose-Hubbard Model

**Theorem 5:** In the limit  $N \to \infty$  with g = uN fixed, Theorem 4 reduces to

$$\langle \psi_t, a_i^+ a_j \psi_t \rangle_{coh/num} = N \times w_i(t) \bar{w}_j(t)$$

with  $w, \bar{w}$  given by the ODE system, in both cases coh/num,

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

$$(4)$$

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with initial conditions

$$w_j(0) = \lambda_j / |\lambda|, \quad \overline{w}_j(0) = \overline{\lambda}_j / |\lambda|$$

The ODE system (4) is the time dependent discrete Gross-Pitaevskii equation.

The first equation of (4) is enough since  $\bar{w}_i$  is the true complex conjugate of  $w_i$  now.

# 7.1 GP Equation for the d Dim Bose-Hubbard Model

**Proof:** For a coherent state p' = 1 and the statement follows immediately from the SDE system (3) since the diffusive part vanishes. For a number state,

$$p' = p'(Nw\bar{w}) = (N-1)/(Nw\bar{w}) \stackrel{N \to \infty}{ o} 1/(w\bar{w})$$

such that we get the following ODE system:

$$\dot{w}_j = -i(\varepsilon w)_j - i 2g \frac{1}{w\bar{w}} w_j \bar{w}_j w_j \dot{\bar{w}}_j = +i(\varepsilon \bar{w})_j + i 2g \frac{1}{w\bar{w}} w_j \bar{w}_j \bar{w}_j$$

However,

$$\frac{d}{dt}(w\bar{w}) = \sum_{j} \left\{ -i(\varepsilon w)_{j}\bar{w}_{j} - i2g \frac{1}{w\bar{w}}(w_{j}\bar{w}_{j})^{2} + iw_{j}(\varepsilon\bar{w})_{j} + i2g \frac{1}{w\bar{w}}(w_{j}\bar{w}_{j})^{2} \right\}$$
$$= -i(\varepsilon w) \cdot \bar{w} + iw \cdot (\varepsilon\bar{w}) \stackrel{\varepsilon = \varepsilon^{T}}{=} 0$$

which results in  $(w\bar{w})_t = (w\bar{w})_0 = 1$ .

### 7.2 GP Equation for the Two Site Bose-Hubbard Model

For just two lattice sites 1 and 2, we get from Theorem 5

$$\langle n_{j,t} \rangle := \langle \psi_t, a_j^+ a_j \psi_t \rangle_{coh/num} \stackrel{N \to \infty}{=} N |w_{j,t}|^2 =: N \varrho_{j,t}$$

with  $w_1, w_2$  given by the GP system

$$\dot{w}_1 = -i\varepsilon w_2 - i2g |w_1|^2 w_1 \dot{w}_2 = -i\varepsilon w_1 - i2g |w_2|^2 w_2$$

Theorem 6 (well known): Introduce the normalized particle imbalance and its integral,

$$arphi_{12} := |w_1|^2 - |w_2|^2$$
  
 $arphi_t := 2g \int_0^t \varrho_{12,s} \, ds$ 

Then  $\varphi_t$  is a solution of

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

and the density of particles at lattice site 1 is obtained as

$$\varrho_{1,t} = |w_{1,t}|^2 = \frac{1}{2} \left( 1 + \frac{\dot{\varphi}_t}{2g} \right)$$

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# 7.2 GP Equation for the Two Site Bose-Hubbard Model

Initial conditions: Put all particles on lattice site 1 at t = 0. Then  $\varphi_0 = 0$ , always, and

$$\dot{\varphi}_0 = 2g \, \varrho_{12,0} = 2g \left( \varrho_{1,0} - \varrho_{2,0} \right) = 2g \left( 1 - 0 \right) = 2g$$

The total energy is

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

The potential energy at  $\varphi = \pi$  is  $E_{pot} = +4\varepsilon^2$ . We have **rollovers** if the total energy is bigger than that:

$$\begin{array}{rcl} 2g^2 - 4\varepsilon^2 &> & +4\varepsilon^2 \\ \Leftrightarrow & \qquad g^2 &> & (2\varepsilon)^2 \end{array}$$

In that case, the velocity  $\dot{\varphi}_t = 2g(\varrho_{1,t} - \varrho_{2,t})$  which is the particle imbalance between the two lattice sites, does not change its sign and this corresponds to the non-oscillatory or self-trapping regime:

# 7.2 GP Equation for the Two Site Bose-Hubbard Model

The mathematical pendulum ODE for  $\varepsilon = 1$  and  $g \in \{1.99, 2.01\}$ :



g = 1.99 (black) and g = 2.01 (red) from ODE system

the quantity  $\varrho_{1,t} = \frac{1}{2} \left( 1 + \frac{\dot{\varphi}_t}{2g} \right)$  with  $\varphi_t$  from ODE,  $\varphi_0 = 0$  and  $\dot{\varphi}_0 = 2g$ 

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Numerical check of the large N limit:  $\varepsilon = 1$  and

$$egin{array}{rcl} N & \in & \left\{ 2500\,,\,5000\,,\,10000\,,\,20000 \,
ight\} & = & \left\{ \, {
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m green}\,,\,{
m light}\,\,{
m blue}\,,\,{
m dark}\,\,{
m blue}\,,\,{
m blue}\,,\,{
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m blue$$

Quantity:

$$\varrho_{1,t} = \begin{cases} \langle \psi_t, a_1^+ a_1 \psi_t \rangle / N & \text{from exact diagonalization} \\ \frac{1}{2} \left( 1 + \frac{\dot{\varphi}_t}{2g} \right) & \text{from ODE mathematical pendulum} \end{cases}$$

The red line below is the ODE solution and the dots come from exact diagonalization:



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# 8. Summary

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# 8. Summary

#### Main Results:

- Simple and Elegant Method to Calculate GP-like Mean Field Equations
- Generic Formalism: Arbitrary Initial State, Arbitrary Hopping Matrix, Arbitrary Dimension
- Various Exact PDE Representations
- o collapse and revivals could be reproduced, proper treatment of diffusive part still missing

#### Outlook:

- Use this for New Numerical or Analytical Calculation Schemes
- Fermi Hubbard Model
- Thermodynamic Quantities

full paper at

https://arxiv.org/abs/2205.02010

# 8. Summary

#### **Theorems:**

Theorem 1: Time Evolution of States as Fresnel Expectation Values, Matrix  $U_{kdt}$ Theorem 2: Correlation Functions as Fresnel Expectation Values Theorem 3: SDE for  $U_{kdt}$  and Correlation Functions as Expectations of Fresnel Diffusions Theorem 4: Girsanov Transformed SDE System: Initial State moves into Drift Part Theorem 5: Large *N*-Limit of Theorem 4: Gross-Pitaevskii Equation Theorem 6: GP Equation for Two Site Bose-Hubbard Model as Mathematical Pendulum

Appendix:

Theorem 7: PDE Representation Correlation Functions, d-dim Bose-Hubbard Model Theorem 8: PDE Representation Correlation Functions, Two Site Bose-Hubbard Model Theorem 9: Equivalence Mathematical Pendulum and Quartic Double-Well Potential Standard Formula Wiener and Fresnel Expectations

# Appendix

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- PDE Representation d Dim Bose-Hubbard Model
- PDE Representation Two Site Bose-Hubbard Model
- Equivalence Mathematical Pendulum and Quartic Double-Well Potential
- Standard Formula Wiener and Fresnel Expectations

## Appendix: PDE Representation d Dim Bose-Hubbard Model

**Theorem 7:** Define the differential operators

$$\mathcal{L}_{0} := \sum_{i,j} \varepsilon_{ij} \left\{ v_{i} \frac{\partial}{\partial v_{j}} - \bar{v}_{i} \frac{\partial}{\partial \bar{v}_{j}} \right\}, \quad \mathcal{L}_{int} := u \sum_{j} \left\{ v_{j}^{2} \frac{\partial^{2}}{\partial v_{j}^{2}} - \bar{v}_{j}^{2} \frac{\partial^{2}}{\partial \bar{v}_{j}^{2}} \right\}$$

and for  $P(x) := \begin{cases} e^x & \text{for coherent state} \\ x^{N-1} & \text{for number state} \end{cases}$ 

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

Then, for the *d*-dimensional Bose-Hubbard model with hopping matrix  $\varepsilon_{ij}$  and interaction *u*,

$$\langle \psi_t, a_i^+ a_j \psi_t \rangle_{coh/num} = e^{-it(\mathcal{L}_0 + \mathcal{L}_{int})} \left\{ v_i \, \bar{v}_j \, P(v\bar{v}) \right\} / P(\lambda\bar{\lambda}) \mid_{v=\lambda, \bar{v}=\bar{\lambda}}$$
$$= e^{-it(\mathcal{L}_0 + \mathcal{L}_{int} + \mathcal{L}_P)} \left\{ v_i \, \bar{v}_j \right\} \mid_{v=\lambda, \bar{v}=\bar{\lambda}} .$$

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# Appendix: PDE Representation Two Site Bose-Hubbard Model

**Theorem 8:** Define the differential operators (with  $p' = [\log P]', P(x) = e^x \text{ or } x^{N-1} \cosh/\text{num}$ )

$$\begin{aligned} \mathcal{L}_{\varepsilon} &:= -\varepsilon \left\{ \left( q - \bar{q} \right) \left( \frac{\partial}{\partial n_{1}} - \frac{\partial}{\partial n_{2}} \right) + \left( n_{1} - n_{2} \right) \left( \frac{\partial}{\partial q} - \frac{\partial}{\partial \bar{q}} \right) \right\} \\ \mathcal{L}_{u} &:= + 2u \left\{ \left( n_{1} \frac{\partial}{\partial n_{1}} - n_{2} \frac{\partial}{\partial n_{2}} \right) \left( q \frac{\partial}{\partial q} - \bar{q} \frac{\partial}{\partial \bar{q}} \right) + p'(n) \left( n_{1} - n_{2} \right) \left( q \frac{\partial}{\partial q} - \bar{q} \frac{\partial}{\partial \bar{q}} \right) \right\} \end{aligned}$$

acting on functions of 4 variables  $F = F(n_1, n_2, q, \bar{q})$ . Then for the two site Bose-Hubbard model

$$\langle \psi_t, a_1^+ a_1 \, \psi_t \rangle_{coh/num} = e^{-it \, (\mathcal{L}_{\varepsilon} + \mathcal{L}_u)} \, n_1 \, \left|_{(n_1, n_2, q, \bar{q}) = (|\lambda_1|^2, |\lambda_2|^2, \lambda_1 \bar{\lambda}_2, \bar{\lambda}_1 \lambda_2)}\right|_{(n_1, n_2, q, \bar{q}) = (|\lambda_1|^2, |\lambda_2|^2, \lambda_1 \bar{\lambda}_2, \bar{\lambda}_1 \lambda_2)}$$

with actions

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

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

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# Appendix: PDE Representation Two Site Bose Hubbard Model

and

$$e^{-it\mathcal{L}_{u}} \left\{ G(n_{1}, n_{2}) q^{b} \bar{q}^{\bar{b}} \right\} = G\left( e^{-i2ut(b-\bar{b})}n_{1}, e^{+i2ut(b-\bar{b})}n_{2} \right) \times \frac{P\left( e^{-i2ut(b-\bar{b})}n_{1} + e^{+i2ut(b-\bar{b})}n_{2} \right)}{P(n_{1} + n_{2})} \times q^{b} \bar{q}^{\bar{b}}$$

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

#### Example, used for Collapse and Revivals:

$$e^{-it\mathcal{L}_{u}} \{ n_{1} \} = n_{1}$$

$$e^{-it\mathcal{L}_{u}} \{ q \} = \frac{P(e^{-i2ut}n_{1} + e^{+i2ut}n_{2})}{P(n_{1} + n_{2})} \times q$$

$$e^{-it\mathcal{L}_{u}} \{ n_{1}q \} = e^{-i2ut}n_{1} \times \frac{P(e^{-i2ut}n_{1} + e^{+i2ut}n_{2})}{P(n_{1} + n_{2})} \times q$$

such that

$$\frac{e^{-it\mathcal{L}_{u}}[n_{1}q]}{e^{-it\mathcal{L}_{u}}[n_{1}]e^{-it\mathcal{L}_{u}}[q]} = e^{-i2ut}, \qquad \frac{e^{-it\mathcal{L}_{\varepsilon}}[n_{1}q]}{e^{-it\mathcal{L}_{\varepsilon}}[n_{1}]e^{-it\mathcal{L}_{\varepsilon}}[q]} = 1.$$

Appendix: Equivalence Mathematical Pendulum and Quartic Double-Well Potential

Theorem 9: The mathematical pendulum

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

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

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

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

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

# Appendix: Standard Formula Wiener and Fresnel Expectations

**Theorem:** Consider *m* times  $0 < t_1 < t_2 < \cdots < t_m \leq T$  and let  $x_{t_j}$  be a standard or Fresnel Brownian motion observed at time  $t_j$ . Let

$$F = F(x_{t_1}, \cdots, x_{t_m}) : \mathbb{R}^m \rightarrow \mathbb{C}$$

be an arbitrary function of *m* variables and let E[F] denote its Wiener or Fresnel expectation value. Then, with  $t_0 := 0$  and  $x_0 := 0$ ,

$$\mathsf{E}[F] = \int_{\mathbb{R}^m} F(x_{t_1}, \cdots, x_{t_m}) \prod_{j=1}^m p_{t_j-t_{j-1}}(x_{t_{j-1}}, x_{t_j}) \, dx_{t_j}$$

with Gaussian or Fresnel kernels given by

$$p_t(x,y) := \begin{cases} rac{1}{\sqrt{2\pi t}} e^{-rac{(x-y)^2}{2t}} & ext{for Wiener expectations} \ rac{1}{\sqrt{2\pi it}} e^{irac{(x-y)^2}{2t}} & ext{for Fresnel expectations} . \end{cases}$$

Basic property:  $\int_{\mathbb{R}} p_t(x, y) p_s(y, z) \, dy = p_{t+s}(x, z)$