# Chapter 5

# The gauge P representation

The gauge P representation, which will be used in subsequent chapters, is explained and its properties investigated here. It is based on the positive P representation of quantum optics, which uses an off-diagonal coherent state kernel, but due to the inclusion of a global phase can be used to introduce weighting and drift gauges. The original distribution concept is due to P. D. Drummond, and its basic derivation is given in published work by Drummond and Deuar[66, 56, 61].

The positive P distribution is a promising starting point because it has already been successfully used in some many-body problems in quantum optics (e.g. squeezing in optical solitons [12, 13]) and with Bose atoms as well (evaporative cooling[14, 15, 46]). The coherent-state mode-based approach gives simple equations similar to the mean-field Gross-Pitaevskii (GP) equations, and automatically applies to open systems. However, stability and systematic error problems can occur[70, 71, 64, 66] with these simulations, which hinders effective use of the method. The gauge P representation inherits all the useful features of the positive P but allows drift gauges, which can be used to tailor the equations so that stability problems and systematic (boundary term) errors are removed. Weighting gauges allow one to also perform thermodynamic simulations of grand canonical ensembles by including an evolving trajectory weight.

Stochastic equations for the interacting Bose gas model are found in Sections 5.3, and 5.6. Extension to non-local interparticle interactions is derived in Section 5.5.

## 5.1 Properties of the representation

The representation uses an un-normalized (Bargmann) coherent state basis. On a subsystem $j$ this basis is

$$||\alpha_j\rangle_j = \exp\left(\alpha_j \widehat{a}_j^\dagger\right)|0\rangle = \exp\left(\frac{|\alpha_j|^2}{2}\right)|\alpha_j\rangle_j, \tag{5.1}$$

with the complex amplitude $\alpha_j$, and mean particle occupation $\langle \widehat{n}_j\rangle = |\alpha_j|^2$. As usual, the boson annihilation operators at subsystem $j$ are $\widehat{a}_j$, and obey the commutation relations

$$\left[\widehat{a}_j\,,\,\widehat{a}_k^\dagger\right] = \delta_{jk}. \tag{5.2}$$

The basis states are mutually non-orthogonal

$$\langle\beta_j^*||_j||\alpha_k\rangle_k = \delta_{jk}e^{\alpha_j\beta_j}, \tag{5.3}$$

(from (3.30)) and overcomplete (from (3.31)).

The kernel (on $N$ separable subsystems) is chosen to be

$$\begin{aligned} \widehat{\Lambda} &= e^{z_0}\otimes_{j=1}^N \widehat{\Lambda}_j, \\ \widehat{\Lambda}_j &= ||\alpha_j\rangle_j\langle\beta_j^*||_j\,\exp\left(-\alpha_j\beta_j\right). \end{aligned} \tag{5.4}$$

If one defines coherent amplitude vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ to contain all $N$ elements $\alpha_j$ and $\beta_j$, respectively, then the full variable set is $C = \{z_0, \boldsymbol{\alpha}, \boldsymbol{\beta}\}$, containing $2N+1$ complex variables. The non-orthogonality of the basis coherent states allows normalization $\mathrm{Tr}\left[\widehat{\Lambda}\right] = e^{z_0}$ apart from the complex global weight $\Omega = e^{z_0}$. The kernel is also seen to be analytic in all complex variables $\alpha_j$, $\beta_j$, and $z_0$, so the procedure of Section 3.4.3 can be used to ensure a stochastic realization for any FPE.

As per expression (3.1), the density matrix (possibly un-normalized) is expanded as

$$\widehat{\rho}_u = \int P_G(C)\widehat{\Lambda}(C)\,d^{2N}\boldsymbol{\alpha}\,d^{2N}\boldsymbol{\beta}\,d^2z_0 \tag{5.5}$$

with the gauge P distribution $P_G(C)$.

Now, it can be verified by expansion that

$$\widehat{a}_k||\alpha_j\rangle_j = \delta_{jk}\alpha_j||\alpha_j\rangle_j \tag{5.6a}$$

$$\widehat{a}_k^\dagger||\alpha_j\rangle_j = \frac{\partial}{\partial\alpha_k}||\alpha_j\rangle_j. \tag{5.6b}$$

This then leads to the basic kernel operator correspondences

$$\widehat{a}_j\widehat{\Lambda} = \alpha_j\widehat{\Lambda}, \tag{5.7a}$$

$$\widehat{a}_j^\dagger\widehat{\Lambda} = \left(\beta_j + \frac{\partial}{\partial\alpha_j}\right)\widehat{\Lambda}, \tag{5.7b}$$

$$\widehat{\Lambda}\widehat{a}_j = \left(\alpha_j + \frac{\partial}{\partial\beta_j}\right)\widehat{\Lambda}, \tag{5.7c}$$

$$\widehat{\Lambda}\widehat{a}_j^\dagger = \beta_j\widehat{\Lambda} \tag{5.7d}$$

in the form (3.39) Together with

$$\frac{\partial}{\partial z_0}\widehat{\Lambda} = \widehat{\Lambda}, \tag{5.8}$$

which is seen to apply by inspection of (5.4), these operator equations can be used to obtain observable moment estimates and stochastic equations using the procedures of Sections 3.3.1, 3.4.1, 3.4.3.

The similarity of the gauge P to the positive P representation allows one to adopt some exact results obtained for the latter. Any state that has the positive P representation $P_+(\boldsymbol{\alpha},\boldsymbol{\beta})$ can be represented by the gauge P representation

$$P_G(z_0,\boldsymbol{\alpha},\boldsymbol{\beta}) = \delta^2(z_0)\,P_+(\boldsymbol{\alpha},\boldsymbol{\beta}), \tag{5.9}$$

by inspection of the kernels (5.4) and (3.6). (This is not a unique correspondence, but the simplest of many.)

Since it has been shown that any quantum state $\widehat{\rho}$ has a positive P representation[11], it follows from (5.9) that all quantum states must also have gauge P representations. The constructive expression (3.10) for a positive P representation of arbitrary $\widehat{\rho}$ can be substituted into (5.9) to obtain a similar expression for the gauge P.

## 5.2 Observables

Calculation of observables proceeds in a very similar manner to the positive P representation in Section 3.3.5. All operators on supported states can be written as linear combinations of the moments of the local annihilation and creation operators $\widehat{a}_j$, $\widehat{a}_j^\dagger$. Thus, to evaluate any observable it suffices to know how to evaluate an expectation

value of a Hermitian operator with two adjoint separable terms of the form

$$\widehat{Q}(\{L_j, L'_k\}, \theta) = \frac{e^{i\theta}}{2} \otimes_j \widehat{a}^\dagger_{L_j} \otimes_k \widehat{a}_{L'_k} + \frac{e^{-i\theta}}{2} \otimes_k \widehat{a}^\dagger_{L'_k} \otimes_j \widehat{a}_{L_j}. \tag{5.10}$$

$\theta$ is a phase, the $L_j$ and $L'_k$ are subsystem labels (not necessarily unique), while the $j$ and $k$ are "subsystem label counters". For example the particle number operator for subsystem $p$ has $j = k = \{1\}$, $L_1 = L'_1 = p$, $\theta = 0$; while a quadrature operator $\widehat{q}(\theta) = \frac{1}{2}(\widehat{a}^\dagger e^{i\theta} + \widehat{a} e^{-i\theta})$ on subsystem $p$ has $j = \{1\}$, $k = \{\,\}$, $L_1 = p$.

Using (5.7) and $\mathrm{Tr}\left[\widehat{\Lambda}\right] = e^{z_0}$, one then obtains

$$\begin{aligned} \mathrm{Tr}\left[\widehat{Q}\widehat{\Lambda}\right] &= \frac{e^{i\theta}}{2} \prod_k \alpha_{L'_k} \prod_j \left(\beta_{L_j} + \frac{\partial}{\partial \alpha_{L_j}}\right) \mathrm{Tr}\left[\widehat{\Lambda}\right] + \frac{e^{-i\theta}}{2} \prod_j \alpha_{L_j} \prod_k \left(\beta_{L'_k} + \frac{\partial}{\partial \alpha_{L'_k}}\right) \mathrm{Tr}\left[\widehat{\Lambda}\right] \\ &= \frac{e^{i\theta+z_0}}{2} \prod_j \beta_{L_j} \prod_k \alpha_{L'_k} + \frac{e^{-i\theta+z_0}}{2} \prod_k \beta_{L'_k} \prod_j \alpha_{L_j}. \end{aligned} \tag{5.11}$$

Similarly,

$$\mathrm{Tr}\left[\widehat{Q}\widehat{\Lambda}^\dagger\right] = \frac{e^{i\theta+z_0^*}}{2} \prod_j \alpha^*_{L_j} \prod_k \beta^*_{L'_k} + \frac{e^{-i\theta+z_0^*}}{2} \prod_k \alpha^*_{L'_k} \prod_j \beta^*_{L_j}. \tag{5.12}$$

These can be entered directly into the general observable estimate expression (3.14) giving

$$\begin{aligned} \overline{Q}(\{L_j, L'_k\}, \theta) &= \frac{\left\langle \mathrm{Re}\left\{ \frac{1}{2} e^{z_0} \left( e^{i\theta} \prod_{jk} \beta_{L_j} \alpha_{L'_k} + e^{-i\theta} \prod_{jk} \beta_{L'_k} \alpha_{L_j} \right) \right\} \right\rangle_{\mathrm{stoch}}}{\langle \mathrm{Re}\{e^{z_0}\} \rangle_{\mathrm{stoch}}} \\ \langle \widehat{Q}(\{L_j, L'_k\}, \theta) \rangle &= \lim_{\mathcal{S}\to\infty} \overline{Q}(\{L_j, L'_k\}, \theta). \end{aligned} \tag{5.13}$$

Comparing (5.10) and (5.13), one sees that the same form appears in both, and so an algorithm to determine the finite-sample estimate of the expectation value of an arbitrary observable $\langle \widehat{O} \rangle$ can be given:

1. Normally-order $\widehat{O}$, using (5.2) by placing all annihilation operators to the right.

2. The numerator of the stochastic estimate $\overline{O}$ is formed by replacing $\widehat{a}_k$, $\widehat{a}^\dagger_j$, and $\otimes$ in the normally-ordered expression for $\widehat{O}$ by $\alpha_k$, $\beta_j$, and $\prod$, respectively, and finally multiplying by the global weight $e^{z_0} = \Omega$.

3. Take the average of the real part of the numerator terms, and divide by the average of the real part of the weight $\langle \mathrm{Re}\,\{e^{z_0}\} \rangle_{\mathrm{stoch}}$.

In cases where the normalization of $\widehat{\rho}$ is known to be conserved (e.g. dynamical master equations (2.20), but not thermodynamic (2.29)), the average in the denominator can be dropped, because it is known to always be equal to one in the limit of many trajectories. Its variations about unity are an indication of the sampling error in the calculation, but are not necessary to obtain expectation values.

The above algorithm applies also when $\widehat{O}$ is an infinite sum of moments, such as for example the parity operator at subsystem $k$, which can be written as

$$\widehat{\pi}_k = \sum_{n=0}^{\infty} (-1)^n \left|n\right\rangle_k \left\langle n\right|_k \tag{5.14}$$

in terms of Fock number states $\left|n\right\rangle_k$ with occupation $n$ at subsystem $k$. Since $\left|n\right\rangle_k = (1/\sqrt{n!})(\widehat{a}_k^\dagger)^n \left|0\right\rangle$, the one obtains

$$\langle \widehat{\pi}_k \rangle = \lim_{\mathcal{S}\to\infty} \frac{\langle \mathrm{Re}\left\{\exp\left(z_0 - 2\alpha_k\beta_k\right)\right\}\rangle_{\mathrm{stoch}}}{\langle \mathrm{Re}\left\{e^{z_0}\right\}\rangle_{\mathrm{stoch}}}. \tag{5.15}$$

With such operators of infinite order in annihilation and creation operators, one should, however, be wary of boundary term errors (of the second kind), as explained in Section 6.2.1.

Finally, for estimates of fidelity using expression (3.22), one requires the trace of kernel products. Using (5.4) and the properties of Bargmann states (5.3), one obtains

$$\mathrm{Tr}\left[\widehat{\Lambda}(\boldsymbol{\alpha}_1,\boldsymbol{\beta}_1,\Omega_1)\widehat{\Lambda}(\boldsymbol{\alpha}_2,\boldsymbol{\beta}_2,\Omega_2)\right] = \Omega_1\Omega_2 \exp\left[-(\boldsymbol{\alpha}_1-\boldsymbol{\alpha}_2)\cdot(\boldsymbol{\beta}_1-\boldsymbol{\beta}_2)\right] \tag{5.16a}$$

$$\mathrm{Tr}\left[\widehat{\Lambda}(\boldsymbol{\alpha}_1,\boldsymbol{\beta}_1,\Omega_1)\widehat{\Lambda}^\dagger(\boldsymbol{\alpha}_2^*,\boldsymbol{\beta}_2^*,\Omega_2^*)\right] = \Omega_1\Omega_2^* \exp\left[-(\boldsymbol{\alpha}_1-\boldsymbol{\beta}_2^*)\cdot(\boldsymbol{\beta}_1-\boldsymbol{\alpha}_2^*)\right] \tag{5.16b}$$

## 5.3 Dynamics of locally-interacting Bose gas

The master equation for the dynamics of a locally interacting Bose gas on a lattice is (2.20) with the Hamiltonian given by (2.17). Using the operator correspondences (5.7), and the methods of Sections 3.4.1, 3.4.3, one can obtain an FPE for this system. Subsequently using the methods of Section 3.4.2, the square root form of the noise matrix $\underline{B} = \underline{B}_0 = \sqrt{\underline{D}}$, and standard drift gauges, the stochastic equations given below are obtained from (4.25) and (4.26) (or more directly, from

(4.90), setting $g_{jk} = 0$). Diffusion gauges have been omitted at this stage (so, $O(g_{jk}) = I$) for clarity. Note that the $M$ spatial modes are now labeled by the lattice labels $\mathbf{n}$, or $\mathbf{m}$ as defined in Section 2.3. Each mode is a "subsystem".

It was chosen to separate the noise contributions from each process, as discussed in Section 4.4.7. This is done so that the noise terms take on a simple form.

With no environment interactions, the purely Hamiltonian evolution is found to lead to the Ito stochastic equations

$$d\alpha_{\mathbf{n}} = -i\sum_{\mathbf{m}}\omega_{\mathbf{nm}}\alpha_{\mathbf{m}}dt - 2i\chi\alpha_{\mathbf{n}}^2\beta_{\mathbf{n}}dt + i\alpha_{\mathbf{n}}\sqrt{2i\chi}(dW_{\mathbf{n}} - \mathcal{G}_{\mathbf{n}}), \tag{5.17a}$$

$$d\beta_{\mathbf{n}} = i\sum_{\mathbf{m}}\omega_{\mathbf{mn}}\beta_{\mathbf{m}}dt + 2i\chi\alpha_{\mathbf{n}}\beta_{\mathbf{n}}^2dt + \beta_{\mathbf{n}}\sqrt{2i\chi}(d\widetilde{W}_{\mathbf{n}} - \widetilde{\mathcal{G}}_{\mathbf{n}}), \tag{5.17b}$$

$$d\Omega = \Omega\sum_{\mathbf{n}}\left[\mathcal{G}_{\mathbf{n}}dW_{\mathbf{n}} + \widetilde{\mathcal{G}}_{\mathbf{n}}d\widetilde{W}_{\mathbf{n}}\right], \tag{5.17c}$$

with $2M$ independent real Wiener increments $dW_{\mathbf{n}}$ and $d\widetilde{W}_{\mathbf{n}}$. The corresponding complex drift gauges are $\mathcal{G}_{\mathbf{n}}$ and $\widetilde{\mathcal{G}}_{\mathbf{n}}$.

Addition of a heat bath at temperature $T$ results in the following additions:

$$d\alpha_{\mathbf{n}} = \cdots - \frac{\gamma_{\mathbf{n}}}{2}\alpha_{\mathbf{n}}dt + \sqrt{\gamma_{\mathbf{n}}\overline{n}_{\mathrm{bath}}(T)}(d\eta_{\mathbf{n}} - \mathcal{G}_{\mathbf{n}}^{(1)}) \tag{5.18a}$$

$$d\beta_{\mathbf{n}} = \cdots - \frac{\gamma_{\mathbf{n}}}{2}\beta_{\mathbf{n}}dt + \sqrt{\gamma_{\mathbf{n}}\overline{n}_{\mathrm{bath}}(T)}(d\eta_{\mathbf{n}}^* - \widetilde{\mathcal{G}}_{\mathbf{n}}^{(1)}) \tag{5.18b}$$

$$d\Omega = \cdots + \Omega\sum_{\mathbf{n}}\left[d\eta_{\mathbf{n}}\widetilde{\mathcal{G}}_{\mathbf{n}}^{(1)} + d\eta^*\mathcal{G}_{\mathbf{n}}^{(1)}\right], \tag{5.18c}$$

where $\overline{n}_{\mathrm{bath}}$ is given by the Bose-Einstein distribution (2.23). Here the *complex* noises $d\eta_{\mathbf{n}}$ are independent, and satisfy

$$\langle d\eta_{\mathbf{n}}d\eta_{\mathbf{m}}^*\rangle_{\mathrm{stoch}} = \delta_{\mathbf{nm}}dt, \tag{5.19a}$$

$$\langle d\eta_{\mathbf{n}}d\eta_{\mathbf{m}}\rangle_{\mathrm{stoch}} = 0, \tag{5.19b}$$

$$\langle d\eta_{\mathbf{n}}\rangle_{\mathrm{stoch}} = 0. \tag{5.19c}$$

The drift gauges $\mathcal{G}_{\mathbf{n}}^{(1)}$ and $\widetilde{\mathcal{G}}_{\mathbf{n}}^{(1)}$ are also complex.

Two-particle losses to a zero temperature heat bath result in the following addi-

tions to the dynamical equations:

$$d\alpha_{\mathbf{n}} = \cdots - \gamma_{\mathbf{n}}^{(2)}\alpha_{\mathbf{n}}^2\beta_{\mathbf{n}}dt + i\alpha_{\mathbf{n}}\sqrt{\gamma_{\mathbf{n}}^{(2)}}\left(dW_{\mathbf{n}}^{(2)} - \mathcal{G}_{\mathbf{n}}^{(2)}\right), \tag{5.20a}$$

$$d\beta_{\mathbf{n}} = \cdots - \gamma_{\mathbf{n}}^{(2)}\alpha_{\mathbf{n}}\beta_{\mathbf{n}}^2dt + i\beta_{\mathbf{n}}\sqrt{\gamma_{\mathbf{n}}^{(2)}}\left(d\widetilde{W}_{\mathbf{n}}^{(2)} - \widetilde{\mathcal{G}}_{\mathbf{n}}^{(2)}\right), \tag{5.20b}$$

$$d\Omega = \cdots + \Omega\sum_{\mathbf{n}}\left[\mathcal{G}_{\mathbf{n}}^{(2)}dW_{\mathbf{n}}^{(2)} + \widetilde{\mathcal{G}}_{\mathbf{n}}^{(2)}d\widetilde{W}_{\mathbf{n}}^{(2)}\right]. \tag{5.20c}$$

Here, again, the noises $dW_{\mathbf{n}}^{(2)}$ and $d\widetilde{W}_{\mathbf{n}}^{(2)}$ are independent Wiener increments, and the drift gauges $\mathcal{G}_{\mathbf{n}}^{(2)}$ and $\widetilde{\mathcal{G}}_{\mathbf{n}}^{(2)}$ are complex.

Lastly, A coherent driving field leads to the deterministic corrections

$$d\alpha_{\mathbf{n}} = \cdots + \varepsilon dt, \tag{5.21a}$$

$$d\beta_{\mathbf{n}} = \cdots + \varepsilon^* dt. \tag{5.21b}$$

The numerical simulation strategy is (briefly)

1. Sample a trajectory according to the known initial condition $P_G(0) = P_G(\,\widehat{\rho}(0)\,)$
2. Evolve according to the stochastic equations, calculating moments of interest, and accumulating appropriate sums of them.
3. Repeat for $\mathcal{S} \gg 1$ independent trajectories.

One could equally well remain with $2M \times 2M$ complex noise matrix, which would use only $2M$ real noises and $2M$ drift gauges, instead of the $6M$ real noises and $6M$ complex drift gauges above. In general, however, the stochastic terms would then have a complicated dependence on the parameters $\chi, \overline{n}_{\text{bath}}, \gamma_{\mathbf{n}}$, and $\gamma_{\mathbf{n}}^{(2)}$ — possibly undesirable. On the other hand, the amount of noise in the simulation might be reduced, because the effects of one process may partly cancel the effects of another. This may be particularly so if both scattering $\propto \chi$ and two-boson heat bath interactions $\propto \gamma_{\mathbf{n}}^{(2)}$ are present. These two processes lead to similar terms in the equations (apart from factors of $i$, etc.), and may be expected to cancel some noise without causing excessively complicated equations.

Some brief comments about the behavior of the above equations:

- The (un-gauged) equations for $d\beta_{\mathbf{n}}$ are simply the complex conjugates of $d\alpha_{\mathbf{n}}$, apart from possessing independent noises.

- The Hamiltonian evolution (5.17) leads to a nonlinear equation in the coherent amplitudes, with obligatory noise.
- All interactions with a heat bath (irrespective of the temperature) cause a deterministic exponential loss of particles.
- Finite temperature thermal interactions cause a directionless randomization of the coherent amplitudes $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, leading also to a mean growth of boson numbers.
- Two-particle losses also lead to nonlinear equations and noise.
- The noise from scattering and two-particle losses is directional in phase space, as opposed to thermal noise.
- Coherent gain causes no noise in the equations.

## 5.4 Comparison to Gross-Pitaevskii semiclassical equations

The lossless equations (5.17) are similar in form to the Gross-Pitaevskii (GP) semiclassical equations ubiquitous in calculations on Bose-Einstein Condensates at temperatures well below condensation. (For details of these gases and results that are obtained with the GP equations see e.g. the review by Dalfovo *et al*[31].) Derivation of the GP equations basically assumes the particles all coherently occupy a single orbital, and can be described by its wavefunction.

In fact, if one

1. Ignores stochastic and drift gauge terms in (5.17).
2. Makes the assumption that the field is coherent — i.e. the local kernels are coherent state projectors $\widehat{\Lambda}_{\mathbf{n}} \to |\alpha_{\mathbf{n}}\rangle_{\mathbf{n}} \langle\alpha_{\mathbf{n}}|_{\mathbf{n}}$, implying

$$\boldsymbol{\beta} \to \boldsymbol{\alpha}^*. \tag{5.22}$$

Note that this is consistent with the first assumption of no stochastic terms, since $d\beta_{\mathbf{n}}$ differs from $d\alpha^*_{\mathbf{n}}$ only by having independent noises.

3. Makes a variable change

$$\psi_{\mathbf{n}} = \psi(\mathbf{x_n}) = \frac{\alpha_{\mathbf{n}}}{\sqrt{\prod_d \Delta x_d}} = \frac{\beta^*_{\mathbf{n}}}{\sqrt{\prod_d \Delta x_d}}, \tag{5.23}$$

such that $\psi$ is the order parameter (i.e. the wavefunction normalized to $\overline{N} = \int \psi(\mathbf{x})\, d^{\mathcal{D}}\mathbf{x}$, where $\overline{N}$ is the mean particle number):

then precisely the (lattice) GP equations for $\psi(\mathbf{x_n})$ are obtained. From this, it can be surmised that in regimes where the GP equations are a reasonably good approximation, the noise will be relatively small and calculations precise.

It is quite remarkable that just by the addition of simple stochastic terms, full first-principles quantum evolution is recovered from a mean field theory. This convenient property suggests that full quantum simulations using this method have the potential to remain numerically tractable.

## 5.5 Extended interparticle interactions

Equations for the case of extended interparticle interactions as in the Hamiltonian (2.12) will be derived here. Proceeding as in Section 5.3, the complex diffusion matrix (before introducing any drift gauges) in the FPE can now be written

$$\underline{D} = \begin{bmatrix} D^{(\alpha)} & 0 \\ 0 & D^{(\beta)} \end{bmatrix}, \tag{5.24}$$

where $D^{(\alpha)}$ appears in the FPE as $\frac{1}{2}D^{(\alpha)}_{\mathbf{nm}}\partial^2/\partial\alpha_{\mathbf{n}}\partial\alpha_{\mathbf{m}}$, and $D^{(\beta)}$ as $\frac{1}{2}D^{(\beta)}_{\mathbf{nm}}\partial^2/\partial\beta_{\mathbf{n}}\partial\beta_{\mathbf{m}}$. Their matrix elements are given by

$$D^{(\alpha)}_{\mathbf{nm}} = -i\frac{u_{\mathbf{nm}}}{\hbar}\alpha_{\mathbf{n}}\alpha_{\mathbf{m}}, \tag{5.25a}$$

$$D^{(\beta)}_{\mathbf{nm}} = i\frac{u_{\mathbf{nm}}}{\hbar}\beta_{\mathbf{n}}\beta_{\mathbf{m}}. \tag{5.25b}$$

Since the interaction potential $u_{\mathbf{nm}}$ is symmetric, then it could be orthogonally decomposed by its matrix square root $\upsilon$, which satisfies

$$\upsilon\upsilon = u = \upsilon\upsilon^T. \tag{5.26}$$

The matrix $\upsilon$ could be calculated at the beginning of a simulation and subsequently used in noise matrices satisfying $B^{(z)}[B^{(z)}]^T = D^{(z)}$ (with $z$ taking on the labels $\alpha$ or $\beta$), where

$$B^{(\alpha)}_{\mathbf{nm}} = \sqrt{\frac{-i}{\hbar}}\alpha_{\mathbf{n}}\,\upsilon_{\mathbf{nm}} \tag{5.27a}$$

$$B^{(\beta)}_{\mathbf{nm}} = \sqrt{\frac{i}{\hbar}}\beta_{\mathbf{n}}\,\upsilon_{\mathbf{nm}}. \tag{5.27b}$$

Unfortunately finding the matrix square root would usually need to be done numerically, which would require storing $\mathcal{O}\left(M^2\right)$ matrix elements $\upsilon_{\mathbf{nm}}$ and take a time $\mathcal{O}\left(M^4\right)$ to compute — not efficient for large lattices.

A much more efficient, though involved, approach is possible. One would like to obtain some orthogonal decomposition of $\underline{D}$ dependent directly on $U_{\mathbf{n}}$ that depends only on the interparticle spacing. This potential has $M$ elements, rather than the $M \times M$ of $u_{\mathbf{nm}}$. Writing the Langevin equations in terms of stochastic increments $dX^{(z)}_{\mathbf{n}}$ (See Section 3.4.2) as

$$dz_{\mathbf{n}} = A^{(z)}_{\mathbf{n}}\,dt + dX^{(z)}_{\mathbf{n}}, \tag{5.28}$$

the stochastic increments must obey

$$\left\langle dX^{(z)}_{\mathbf{n}}\right\rangle_{\text{stoch}} = 0 \tag{5.29a}$$

$$\left\langle dX^{(z)}_{\mathbf{n}} dX^{(z)}_{\mathbf{m}}\right\rangle_{\text{stoch}} = D^{(z)}_{\mathbf{nm}}\,dt \tag{5.29b}$$

$$\left\langle dX^{(\alpha)}_{\mathbf{n}} dX^{(\beta)}_{\mathbf{m}}\right\rangle_{\text{stoch}} = 0. \tag{5.29c}$$

Firstly, we can define new stochastic increments $dY^{(\alpha)}_{\mathbf{n}}$ and $dY^{(\beta)}_{\mathbf{n}}$, such that

$$dX^{(\alpha)}_{\mathbf{n}} = \alpha_{\mathbf{n}}\sqrt{\frac{-i}{\hbar}}\,dY^{(\alpha)}_{\mathbf{n}} \tag{5.30a}$$

$$dX^{(\beta)}_{\mathbf{n}} = \beta_{\mathbf{n}}\sqrt{\frac{i}{\hbar}}\,dY^{(\beta)}_{\mathbf{n}}, \tag{5.30b}$$

and these must obey relationships (Remembering from (2.15) that $u_{\mathbf{nm}} = u_{\mathbf{mn}} = U_{|\mathbf{n}-\mathbf{m}|}$),

$$\left\langle dY^{(z)}_{\mathbf{n}}\right\rangle_{\text{stoch}} = 0 \tag{5.31a}$$

$$\left\langle dY^{(z)}_{\mathbf{n}} dY^{(z)}_{\mathbf{m}}\right\rangle_{\text{stoch}} = U_{|\mathbf{n}-\mathbf{m}|}\,dt, \tag{5.31b}$$

which now depend only on the *a-priori* potential $U_{\mathbf{n}}$, not on the dynamically evolving mode amplitudes. Note that while the variances of the $dY_{\mathbf{n}}^{(z)}$ are the same for both choices of $z$, the actual realizations of the increments must be independent.

It is useful to now consider the $\mathcal{D}$-dimensional discrete Fourier transform of the interparticle potential:

$$\widetilde{U}_{\tilde{\mathbf{n}}} = \widetilde{U}'_{\tilde{\mathbf{n}}} + i\widetilde{U}''_{\tilde{\mathbf{n}}} = \frac{1}{C_{\text{norm}}} \sum_{\mathbf{n}} U_{\mathbf{n}} e^{-i\mathbf{k}_{\tilde{\mathbf{n}}}\cdot\mathbf{x}_{\mathbf{n}}}, \tag{5.32}$$

with the normalization constant $C_{\text{norm}} = (2\pi)^{\mathcal{D}/2}/\prod_d \Delta x_d$. All the lattice notation used from here on has been defined in Section 2.3. Note now that since $U_{\mathbf{n}}$ is real, and $\mathbf{k}_{-\tilde{\mathbf{n}}} = -\mathbf{k}_{\tilde{\mathbf{n}}}$, then (5.32) implies

$$\widetilde{U}'_{\tilde{\mathbf{n}}} = \widetilde{U}'_{-\tilde{\mathbf{n}}} \tag{5.33a}$$

$$\widetilde{U}''_{\tilde{\mathbf{n}}} = -\widetilde{U}''_{-\tilde{\mathbf{n}}}. \tag{5.33b}$$

The inverse transform is

$$U_{\mathbf{n}} = \frac{C_{\text{norm}}}{M} \sum_{\tilde{\mathbf{n}}} \widetilde{U}_{\tilde{\mathbf{n}}} e^{i\mathbf{k}_{\tilde{\mathbf{n}}}\cdot\mathbf{x}_{\mathbf{n}}}. \tag{5.34}$$

Expanding out the elements of lattice coordinate vectors, one can write $|\mathbf{x_n} - \mathbf{x_m}| = \{\vartheta_1 \Delta x_1 (n_1 - m_1), \ldots, \vartheta_{\mathcal{D}} \Delta x_{\mathcal{D}} (n_{\mathcal{D}} - m_{\mathcal{D}})\}$, where the quantities $\vartheta_d$ can take on the values $+1$ or $-1$, depending on what is required to take the modulus. Recalling the symmetry property of the interparticle potential that was assumed in Section 2.3 ($U_{\{n_1,\ldots,n_d,\ldots\}} = U_{\{n_1,\ldots,M_d-n_d,\ldots\}}$ for any dimension $d$), one obtains

$$\begin{aligned} U_{\{n_1,\ldots,n_d,\ldots\}} &= \frac{C_{\text{norm}}}{M} \sum_{\tilde{\mathbf{n}}} \widetilde{U}_{\tilde{\mathbf{n}}} \prod_d e^{ik_d(\tilde{n}_d)x_d(n_d)} \\ &= \frac{C_{\text{norm}}}{M} \sum_{\tilde{\mathbf{n}}} \widetilde{U}_{\tilde{\mathbf{n}}} e^{-ik_d(\tilde{n}_d)x_d(n_d)} \prod_{d' \neq d} e^{ik_{d'}(\tilde{n}_{d'})x_{d'}(n_{d'})}, \end{aligned} \tag{5.35}$$

since $\exp[ik_d M_d \Delta x_d] = 1$ for any $k_d$. So, the phase for dimension $d$ can have either sign. This result can then be applied to each dimension where $\vartheta_d = -1$ to obtain (using also $\mathbf{x_{n-m}} = \mathbf{x_n} - \mathbf{x_m}$) the expression (subtly different from (5.34))

$$U_{|\mathbf{n}-\mathbf{m}|} = \frac{C_{\text{norm}}}{M} \sum_{\tilde{\mathbf{n}}} \widetilde{U}_{\tilde{\mathbf{n}}} e^{i\mathbf{k}_{\tilde{\mathbf{n}}}\cdot(\mathbf{x_n}-\mathbf{x_m})}. \tag{5.36}$$

If one introduces new stochastic increments $dZ_{\mathbf{n}}^{(v)}$, then using (5.36), condition (5.31b) is equivalent to

$$\left\langle dY_{\mathbf{n}}^{(z)} dY_{\mathbf{m}}^{(z)} \right\rangle_{\text{stoch}} = \frac{C_{\text{norm}}}{M} \sum_{\widetilde{\mathbf{n}}\widetilde{\mathbf{m}}} e^{i\mathbf{k}_{\widetilde{\mathbf{n}}}\cdot\mathbf{x}_{\mathbf{n}}} e^{-i\mathbf{k}_{\widetilde{\mathbf{m}}}\cdot\mathbf{x}_{\mathbf{m}}} \sqrt{\widetilde{U}_{\widetilde{\mathbf{n}}}\widetilde{U}_{\widetilde{\mathbf{m}}}} \left\langle dZ_{\widetilde{\mathbf{n}}}^{(v)} dZ_{\widetilde{\mathbf{m}}}^{(v)} \right\rangle_{\text{stoch}} \tag{5.37}$$

provided that

$$\left\langle dZ_{\widetilde{\mathbf{n}}}^{(z)} \right\rangle_{\text{stoch}} = 0 \tag{5.38a}$$

$$\left\langle dZ_{\widetilde{\mathbf{n}}}^{(z)} dZ_{\widetilde{\mathbf{m}}}^{(z)} \right\rangle_{\text{stoch}} = \delta_{\widetilde{\mathbf{n}}\widetilde{\mathbf{m}}}\, dt. \tag{5.38b}$$

This can be checked by substitution. This is not yet quite what one wants to be able to decompose into $dY_{\mathbf{n}}^{(z)}$ because the second phase in (5.37) has the wrong sign. Again using $-\mathbf{k}_{\widetilde{\mathbf{n}}} = \mathbf{k}_{-\widetilde{\mathbf{n}}}$, to relabel $\widetilde{\mathbf{m}} \to -\widetilde{\mathbf{m}}$, and applying (5.33) one has

$$\left\langle dY_{\mathbf{n}}^{(z)} dY_{\mathbf{m}}^{(z)} \right\rangle_{\text{stoch}} = \frac{C_{\text{norm}}}{M} \sum_{\widetilde{\mathbf{n}}\widetilde{\mathbf{m}}} e^{i\mathbf{k}_{\widetilde{\mathbf{n}}}\cdot\mathbf{x}_{\mathbf{n}}} e^{i\mathbf{k}_{\widetilde{\mathbf{m}}}\cdot\mathbf{x}_{\mathbf{m}}} \sqrt{\widetilde{U}_{\widetilde{\mathbf{n}}}\widetilde{U}^{*}_{\widetilde{\mathbf{m}}}}\, \delta_{\mathbf{n},-\mathbf{m}} dt. \tag{5.39}$$

The phase factor is now fine, but the complex conjugate $U^{*}_{\widetilde{\mathbf{m}}}$ spoils the potential decomposition. What is needed are some stochastic increments $d\widetilde{Z}_{\widetilde{\mathbf{n}}}^{(z)}$ that will satisfy

$$\left\langle d\widetilde{Z}_{\widetilde{\mathbf{n}}}^{(z)} \right\rangle_{\text{stoch}} = 0 \tag{5.40a}$$

$$\left\langle d\widetilde{Z}_{\widetilde{\mathbf{n}}}^{(z)} d\widetilde{Z}_{\widetilde{\mathbf{m}}}^{(z)} \right\rangle_{\text{stoch}} = \delta_{\widetilde{\mathbf{n}},-\widetilde{\mathbf{m}}} \widetilde{U}_{\widetilde{\mathbf{n}}}\, dt, \tag{5.40b}$$

to allow then a decomposition

$$dY_{\mathbf{n}}^{(z)} = \sqrt{\frac{C_{\text{norm}}}{M}} \sum_{\widetilde{\mathbf{n}}} e^{i\mathbf{k}_{\widetilde{\mathbf{n}}}\cdot\mathbf{x}_{\mathbf{n}}}\, d\widetilde{Z}_{\widetilde{\mathbf{n}}}^{(z)}. \tag{5.41}$$

This can be achieved by separating out the real and imaginary parts of $\widetilde{U}$ as

$$d\widetilde{Z}_{\widetilde{\mathbf{n}}}^{(z)} = \sqrt{\widetilde{U}'_{\widetilde{\mathbf{n}}}}\, d\zeta_{\widetilde{\mathbf{n}}}^{(z)} + \sqrt{\widetilde{U}''_{\widetilde{\mathbf{n}}}}\, d\widetilde{\zeta}_{\widetilde{\mathbf{n}}}^{(z)}, \tag{5.42}$$

with the new stochastic increments

$$\left\langle d\zeta_{\widetilde{\mathbf{n}}}^{(z)} \right\rangle_{\text{stoch}} = \left\langle d\widetilde{\zeta}_{\widetilde{\mathbf{n}}}^{(z)} \right\rangle_{\text{stoch}} = 0 \tag{5.43a}$$

$$\left\langle d\zeta_{\widetilde{\mathbf{n}}}^{(z)} d\zeta_{\widetilde{\mathbf{m}}}^{(z)} \right\rangle_{\text{stoch}} = \delta_{\widetilde{\mathbf{n}},-\widetilde{\mathbf{m}}}\, dt \tag{5.43b}$$

$$\left\langle d\widetilde{\zeta}_{\widetilde{\mathbf{n}}}^{(z)} d\widetilde{\zeta}_{\widetilde{\mathbf{m}}}^{(z)} \right\rangle_{\text{stoch}} = \delta_{\widetilde{\mathbf{n}},-\widetilde{\mathbf{m}}}\, dt \tag{5.43c}$$

$$\left\langle d\zeta_{\widetilde{\mathbf{n}}}^{(z)} d\widetilde{\zeta}_{\widetilde{\mathbf{m}}}^{(z)} \right\rangle_{\text{stoch}} = 0. \tag{5.43d}$$

Note that $\sqrt{\widetilde{U}''_{\tilde{\mathbf{n}}}\widetilde{U}''_{-\tilde{\mathbf{n}}}} = i\widetilde{U}''_{\tilde{\mathbf{n}}}$ by (5.33). Let us divide the $\tilde{\mathbf{n}} \neq 0$ momentum mode space into two symmetric halves $\mathcal{R}$ and $\widetilde{\mathcal{R}}$, such that e.g. when $\mathcal{D} = 3$:

$$\tilde{\mathbf{n}} \in \mathcal{R} \text{ if } \begin{cases} \widetilde{n}_1 > 0 \\ \text{or,} \quad \widetilde{n}_1 = 0 \qquad \text{and} \quad \widetilde{n}_2 > 0 \\ \text{or,} \quad \widetilde{n}_1 = \widetilde{n}_2 = 0 \quad \text{and} \quad \widetilde{n}_3 > 0 \end{cases} \tag{5.44}$$

while $\tilde{\mathbf{n}} \in \widetilde{\mathcal{R}}$ if $\tilde{\mathbf{n}} \notin \{\mathcal{R}, \mathbf{0}\}$. The $d\zeta^{(z)}_{\tilde{\mathbf{n}}}$ noises can now be realized by the construction

$$d\zeta^{(z)}_{\tilde{\mathbf{n}}} = \begin{cases} (dW_{\tilde{\mathbf{n}},1} + i dW_{\tilde{\mathbf{n}},2})/\sqrt{2} & \text{if } \tilde{\mathbf{n}} \in \mathcal{R} \\ dW_{\mathbf{0},1} & \text{if } \tilde{\mathbf{n}} = \mathbf{0} \\ (dW_{-\tilde{\mathbf{n}},1} - i dW_{-\tilde{\mathbf{n}},2})/\sqrt{2} & \text{if } \tilde{\mathbf{n}} \in \widetilde{\mathcal{R}}. \end{cases} \tag{5.45}$$

in terms of real independent Wiener increments $dW_{\tilde{\mathbf{n}},j}$, for all $\tilde{\mathbf{n}} \in \{\mathcal{R}, \mathbf{0}\}$, numbering $M$ in total[1]. $d\widetilde{\zeta}^{(z)}_{\tilde{\mathbf{n}}}$ requires separate $M$ independent noises $dW_{\tilde{\mathbf{n}},3}$ and $dW_{\tilde{\mathbf{n}},4}$.

Collecting all this together, one obtains

$$dX^{(\alpha)}_{\mathbf{n}} = \alpha_{\mathbf{n}} \sqrt{\frac{-iC_{\mathrm{norm}}}{\hbar M}} \sum_{\tilde{\mathbf{n}}} e^{i\mathbf{k}_{\tilde{\mathbf{n}}}\cdot\mathbf{x}_{\mathbf{n}}} \left\{ \sqrt{\widetilde{U}'_{\tilde{\mathbf{n}}}} d\zeta^{(\alpha)}_{\tilde{\mathbf{n}}} + \sqrt{\widetilde{U}''_{\tilde{\mathbf{n}}}} d\widetilde{\zeta}^{(\alpha)}_{\tilde{\mathbf{n}}} \right\} \tag{5.46a}$$

$$dX^{(\beta)}_{\mathbf{n}} = \beta_{\mathbf{n}} \sqrt{\frac{iC_{\mathrm{norm}}}{\hbar M}} \sum_{\tilde{\mathbf{n}}} e^{i\mathbf{k}_{\tilde{\mathbf{n}}}\cdot\mathbf{x}_{\mathbf{n}}} \left\{ \sqrt{\widetilde{U}'_{\tilde{\mathbf{n}}}} d\zeta^{(\beta)}_{\tilde{\mathbf{n}}} + \sqrt{\widetilde{U}''_{\tilde{\mathbf{n}}}} d\widetilde{\zeta}^{(\beta)}_{\tilde{\mathbf{n}}} \right\}. \tag{5.46b}$$

All four $\zeta^{(z)}_{\tilde{\mathbf{n}}}$ and $\widetilde{\zeta}^{(z)}_{\tilde{\mathbf{n}}}$ complex noises per (Fourier space) lattice point are independent of each other, and of the noises at all other (momentum) lattice points and times. Explicitly they have the form (5.45) in terms of the $4M$ real Wiener increments[2] $dW_{\tilde{\mathbf{n}},j}$. Storage space for $M$ complex variables $\widetilde{U}_{\tilde{\mathbf{n}}}$ is required, and calculation of these[3] takes a time $\propto M \log M$ — much more tractable than the calculations of $v_{\mathbf{nm}}$. The $dX^{(z)}_{\mathbf{n}}$ reduce to the noise terms of (5.17) under local interactions $U_{\mathbf{n}} = 2\hbar\chi\delta_{\mathbf{n},\mathbf{0}}$.

With no drift gauges, the two-particle interaction terms of the Ito stochastic equations become (the terms due to other processes are unchanged)

$$d\alpha_{\mathbf{n}} = \cdots - i \sum_{\mathbf{m}} \frac{U_{|\mathbf{n}-\mathbf{m}|}}{\hbar} \alpha_{\mathbf{n}}\alpha_{\mathbf{m}}\beta_{\mathbf{m}} + dX^{(\alpha)}_{\mathbf{n}}, \tag{5.47a}$$

$$d\beta_{\mathbf{n}} = \cdots + i \sum_{\mathbf{m}} \frac{U_{|\mathbf{n}-\mathbf{m}|}}{\hbar} \beta_{\mathbf{n}}\alpha_{\mathbf{m}}\beta_{\mathbf{m}} + dX^{(\beta)}_{\mathbf{n}}. \tag{5.47b}$$

[1] $M + 1$ if $M$ is even.
[2] Or $4(M + 1)$ if $M$ is even.
[3] Using the "fast Fourier transform" algorithm.

Drift gauges can be introduced by making the replacements

$$dW_{\mathbf{n},j} \to dW_{\mathbf{n},j} - \mathcal{G}_{\mathbf{n},j}\, dt, \tag{5.48}$$

in (5.45) (this follows straight from the standard form (4.90)) and

$$d\Omega = \cdots + \Omega \sum_{\mathbf{n}} \sum_{j} \mathcal{G}_{\mathbf{n},j} dW_{\mathbf{n},j}. \tag{5.49}$$

Simulations of such models pose no fundamental problem (see e.g. Sections 10.5 and 10.6), however the required computer time scales more steeply with $M$. There are now $2M$ complex terms to calculate in the equation for each variable rather than the 2 for a local interaction model (5.17).

## 5.6 Thermodynamics of interacting Bose gas

The grand canonical thermodynamics of a system with Hamiltonian $\widehat{H}$ in thermal and diffusive contact with a reservoir at temperature $T$ and chemical potential $\mu$ can be simulated using the master equation (2.29).

With the locally-interacting Hamiltonian (2.17), using the operator correspondences (5.7), and the methods of Sections 3.4.1, 3.4.3, one can obtain the FPE, and then directly by (4.90) (not using diffusion gauges here, so $g_{jk} = 0$) the stochastic equations. Using the same notation as in Section 5.3, these can be written

$$d\alpha_{\mathbf{n}} = -\hbar \sum_{\mathbf{m}} \omega_{\mathbf{nm}} \alpha_{\mathbf{m}}\, d\tau + (\mu_e - 2\hbar\chi\alpha_{\mathbf{n}}\beta_{\mathbf{n}})\, \alpha_{\mathbf{n}}\, d\tau + i\alpha_{\mathbf{n}} \sqrt{2\hbar\chi}\, (dW_{\mathbf{n}} - \mathcal{G}_{\mathbf{n}}) \tag{5.50a}$$

$$d\beta_{\mathbf{n}} = 0, \tag{5.50b}$$

$$d\Omega = \Omega \left[ -\hbar \sum_{\mathbf{nm}} \omega_{\mathbf{nm}} \alpha_{\mathbf{m}} \beta_{\mathbf{n}}\, d\tau + \sum_{\mathbf{n}} (\mu_e - \hbar\chi\alpha_{\mathbf{n}}\beta_{\mathbf{n}})\, \alpha_{\mathbf{n}}\beta_{\mathbf{n}}\, d\tau + \sum_{\mathbf{n}} \mathcal{G}_{\mathbf{n}} dW_{\mathbf{n}} \right] \tag{5.50c}$$

There are $M$ real Wiener increments $dW_{\mathbf{n}}$, and hence the same number of complex drift gauges $\mathcal{G}_{\mathbf{n}}$.

The asymmetric form (no $\beta_{\mathbf{n}}$ evolution) arises because the Kamiltonian acts only from the left on the density matrix in (2.27). The initial $\beta_{\mathbf{n}}$ takes on a range of random initial values (see (5.59) below), which then remain constant. A symmetric set of equations is also possible by starting from the middle (anticommutator) term

of (2.27), however this appears to serve no useful purpose but needs more noises (another set of $M$ for the $\beta_{\mathbf{n}}$ evolution).

The initial condition (2.31) is $\widehat{\rho}_u(0) = \exp\left[-\lambda_n \widehat{N}\right] = \otimes_{\mathbf{n}} \widehat{\rho}_{\mathbf{n}}(0)$, where $\lambda_n$ is given by (2.32), and with

$$\widehat{\rho}_{\mathbf{n}}(0) = \exp\left[-\lambda_n \widehat{a}_{\mathbf{n}}^\dagger \widehat{a}_{\mathbf{n}}\right]. \tag{5.51}$$

One could use (5.9) and (3.10) to obtain a gauge P distribution corresponding to this initial state, but a more compact distribution can be found as follows:

Since $\widehat{\rho}_u(0)$ is separable, let us just consider the initial conditions in a single mode $\mathbf{n}$ (all modes are in this same state initially). In a local Fock number state complete orthogonal basis $|n\rangle$, the initial state can be written

$$\begin{aligned} \widehat{\rho}_{\mathbf{n}}(0) = \exp\left[-\lambda_n \widehat{n}_{\mathbf{n}}\right] \widehat{I}_{\mathbf{n}} &= \sum_p \frac{(-\lambda_n)^p}{p!} \widehat{n}_{\mathbf{n}}^p \sum_n |n\rangle \langle n| \\ &= \sum_n e^{-\lambda_n n} |n\rangle \langle n|. \end{aligned} \tag{5.52}$$

The local kernel (5.4) , on the other hand, expanding the Bargmann states, is

$$\begin{aligned} \widehat{\Lambda}_{\mathbf{n}} &= e^{\alpha_{\mathbf{n}} \widehat{a}_{\mathbf{n}}^\dagger} |0\rangle \langle 0| e^{\beta_{\mathbf{n}} \widehat{a}_{\mathbf{n}}} e^{-\alpha_{\mathbf{n}} \beta_{\mathbf{n}}} \\ &= \sum_{n\widetilde{n}} \frac{\alpha_{\mathbf{n}}^n \beta_{\mathbf{n}}^{\widetilde{n}}}{\sqrt{n!\widetilde{n}!}} |n\rangle \langle \widetilde{n}| e^{-\alpha_{\mathbf{n}} \beta_{\mathbf{n}}}. \end{aligned} \tag{5.53}$$

Since the high temperature state should be classical let us try a gauge P distribution over just diagonal coherent states and so postulate $\boldsymbol{\alpha} = \boldsymbol{\beta}^*$. Also, at high temperature the modes should be separable, so let us try a distribution where the amplitudes at each mode are independent. From (5.51), the state of each mode should be identical, and lastly, for simplicity, let us choose the initial weight of each trajectory to be equal: $\Omega(0) = e^{z_0(0)} = 1$ Let us start, then, with the Gaussian ansatz

$$P_G^{\text{try}}(\boldsymbol{\alpha}, \boldsymbol{\beta}, z_0) = \delta^2(z_0) \delta^{2M}(\boldsymbol{\beta} - \boldsymbol{\alpha}^*) \prod_{\mathbf{n}} \frac{1}{2\pi\sigma^2} \exp\left(\frac{-|\alpha_{\mathbf{n}}|^2}{2\sigma^2}\right). \tag{5.54}$$

To see whether this is sufficient to represent the initial state, and to find the value of $\sigma$, let us substitute into (5.5) and see if (5.52) can be satisfied. Integrating over $\Omega$ and $\boldsymbol{\beta}$, and separating modes, one has (for each mode $\mathbf{n}$):

$$\widehat{\rho}_{\mathbf{n}}^{\text{try}}(0) = \int \frac{1}{2\pi\sigma^2} \exp\left(\frac{-|\alpha_{\mathbf{n}}|^2}{2\sigma^2}\right) \sum_{n\widetilde{n}} \frac{\alpha_{\mathbf{n}}^n (\alpha_{\mathbf{n}}^*)^{\widetilde{n}}}{\sqrt{n!\widetilde{n}!}} |n\rangle \langle \widetilde{n}| e^{-|\alpha_{\mathbf{n}}|^2} d^2\alpha_{\mathbf{n}}. \tag{5.55}$$

Writing $\alpha_{\mathbf{n}} = re^{i\theta}$, one has

$$\begin{aligned}\widehat{\rho}_{\mathbf{n}}^{\,\mathrm{try}}(0) &= \frac{1}{2\pi\sigma^2}\sum_{n\widetilde{n}}\frac{1}{\sqrt{n!\widetilde{n}!}}\int_{-\pi}^{\pi}d\theta\, e^{i\theta(n-\widetilde{n})}\int_0^{\infty}dr\, r^{n+\widetilde{n}+1}\exp\left(-\frac{r^2}{1+1/2\sigma^2}\right)|n\rangle\langle\widetilde{n}| \\ &= \frac{1}{\sigma^2}\sum_n\frac{1}{n!}\int_0^{\infty}dr\, r^{2n+1}\exp\left(-\frac{r^2}{1+1/2\sigma^2}\right)|n\rangle\langle n|\,, \qquad (5.56)\end{aligned}$$

and using[72] $\int_0^{\infty} r^{2n+1}e^{-fr^2}dr = n!/2f^{n+1}$,

$$\widehat{\rho}_{\mathbf{n}}^{\,\mathrm{try}}(0) = \frac{1}{1+2\sigma^2}\sum_n\left(\frac{\sigma^2}{1+2\sigma^2}\right)^n|n\rangle\langle n|\,. \qquad (5.57)$$

One wants to have $\widehat{\rho}_{\mathbf{n}}^{\,\mathrm{try}}(0) = \widehat{\rho}_{\mathbf{n}}(0)/\mathrm{Tr}\,[\,\widehat{\rho}_{\mathbf{n}}(0)]$. Since $\mathrm{Tr}\,[\widehat{\rho}_{\mathbf{n}}(0)] = 1/[1-e^{-\lambda_n}]$, this implies

$$\sigma = \frac{1}{\sqrt{2\,(e^{\lambda_n}-1)}} = \sqrt{\frac{\overline{n}_0}{2}}, \qquad (5.58)$$

($\overline{n}_0 = 1/[e^{\lambda_n}-1]$ is the mean occupation per mode). So then, it has been verified that a gauge P distribution for $\widehat{\rho}_u(0)$ is just a Gaussian in $\boldsymbol{\alpha}$.

$$P_G(\boldsymbol{\alpha},\boldsymbol{\beta},z_0) = \delta^2(z_0)\delta^{2M}(\boldsymbol{\beta}-\boldsymbol{\alpha}^*)\prod_{\mathbf{n}}\frac{1}{\pi\overline{n}_0}\exp\left(\frac{-|\alpha_{\mathbf{n}}|^2}{\overline{n}_0}\right). \qquad (5.59)$$

This is easily sampled to obtain initial values of $\alpha_{\mathbf{n}} = \beta_{\mathbf{n}}^*$, and $z_0 = 0$ for each trajectory.

For the case of extended interparticle interactions $u_{\mathbf{nm}} = U_{|\mathbf{n}-\mathbf{m}|}$, a similar procedure can be followed as was done for the dynamics in Section 5.5. The diffusion matrix in the FPE is now

$$\begin{aligned}D_{\mathbf{nm}}^{(\alpha)} &= -u_{\mathbf{nm}}\alpha_{\mathbf{n}}\alpha_{\mathbf{m}}, &(5.60a)\\ D_{\mathbf{nm}}^{(\beta)} &= 0, &(5.60b)\end{aligned}$$

rather than (5.25). With no drift gauges, the Ito stochastic equations are

$$\begin{aligned}d\alpha_{\mathbf{n}} &= -\hbar\sum_{\mathbf{m}}\omega_{\mathbf{nm}}\alpha_{\mathbf{m}}\,d\tau + \mu_e\alpha_{\mathbf{n}}\,d\tau - \sum_{\mathbf{m}}U_{|\mathbf{n}-\mathbf{m}|}\alpha_{\mathbf{n}}\alpha_{\mathbf{m}}\beta_{\mathbf{m}}\,d\tau + dX_{\mathbf{n}}^{(\alpha)} &(5.61a)\\ d\beta_{\mathbf{n}} &= 0, &(5.61b)\\ d\Omega &= \Omega\left[-\hbar\sum_{\mathbf{nm}}\omega_{\mathbf{nm}}\alpha_{\mathbf{m}}\beta_{\mathbf{n}} + \sum_{\mathbf{n}}\left(\mu_e - \sum_{\mathbf{m}}\frac{U_{|\mathbf{n}-\mathbf{m}|}}{2}\alpha_{\mathbf{m}}\beta_{\mathbf{m}}\right)\alpha_{\mathbf{n}}\beta_{\mathbf{n}}\right]d\tau &(5.61c)\end{aligned}$$

With the stochastic increments given by

$$dX_{\mathbf{n}}^{(\alpha)} = i\alpha_{\mathbf{n}}\sqrt{\frac{C_{\text{norm}}}{M}}\sum_{\widetilde{\mathbf{n}}} e^{i\mathbf{k}_{\widetilde{\mathbf{n}}}\cdot\mathbf{x}_{\mathbf{n}}}\left\{\sqrt{\widetilde{U}'_{\widetilde{\mathbf{n}}}}d\zeta_{\widetilde{\mathbf{n}}}^{(\alpha)} + \sqrt{\widetilde{U}''_{\widetilde{\mathbf{n}}}}d\widetilde{\zeta}_{\widetilde{\mathbf{n}}}^{(\alpha)}\right\}. \tag{5.62}$$

Here the noises $d\zeta_{\mathbf{n}}^{(\alpha)}$ and $d\widetilde{\zeta}_{\widetilde{\mathbf{n}}}^{(\alpha)}$ are given again by (5.45), but the $2M$ real Wiener increments $dW_{\widetilde{\mathbf{n}},j}$ now have variance $d\tau$ instead of $dt$. Drift gauges can again be introduced by making the replacements

$$dW_{\mathbf{n},j} \to dW_{\mathbf{n},j} - \mathcal{G}_{\mathbf{n},j}\, d\tau, \tag{5.63}$$

in (5.45) and

$$d\Omega = \cdots + \Omega\sum_{\mathbf{n}}\sum_{j}\mathcal{G}_{\mathbf{n},j}dW_{\mathbf{n},j}. \tag{5.64}$$

## 5.7 Comparison with historical distributions

To put the gauge P representation in perspective, let us compare to the more commonly used phase-space representations from the field of quantum optics where phase-space distributions have arguably been most used. This section is based on Section 2 of the published article by Drummond and Deuar[56]. The concepts and general layout of this section are due to P. D. Drummond.

To understand the reasons for development of the various distributions, it is useful to peruse the requirements listed in Section 3.6 that they have to satisfy to result in stochastic simulations of many-body models.

Phase-space mappings were first introduced by Wigner as the famous Wigner representation[57]. Historically, phase-space distributions have developed in three stages:

- **Stage one (classical-like phase space):** A classical-like phase space was used in which the number of real configuration variables in $C$ was the same as the number of classical degrees of freedom. Typically the kernel is of the form of a diagonal projector, and not all quantum states can be represented by positive nonsingular $P$. This usually manifests itself as either a non positive-definite propagator or 3rd order terms in the FPE in master equations involving several-body processes. Either way, a quantum-equivalent stochastic

process is not recovered. The Wigner[57], Husimi Q[73], Glauber-Sudarshan P[58, 74, 59], and the Poisson[75, 76, 62] representations, among others, all fall into this category.

- **Stage two (doubled phase space):** By the use of off-diagonal kernels, representations in a higher-dimensional phase space were developed, for which a non-singular distribution $P$ exists for all quantum states. These typically have at least two real configuration variables for each classical degree of freedom (one for the ket and one for the bra in the kernel). Examples of such representations are the Glauber R[58, 74] and the positive P[10, 11] representations. While these work very well for highly damped systems, in models with several-body processes and low damping, they typically develop unstable trajectories. This leads to large sampling uncertainties or even systematic "boundary term errors"[70, 71].

- **Stage three (global amplitude and stochastic gauges):** Addition of a global weight to the kernel allows the introduction of drift stochastic gauges as in Section 4.3, and (by appropriate gauge choice) modification of the stochastic equations to remove the instabilities. The gauge P representation introduced above is of this type, as is the stochastic wavefunction method of Carusotto *et al*[1, 65]. This work of Carusotto *et al* is in some ways complementary to that presented in this thesis, and has been developed approximately in parallel. One fundamental difference between the two representations is that the gauge P representation allows the particle number to vary, allowing open behavior such as lasing or evaporative cooling, whereas the stochastic wavefunction method is hardwired to a constant particle number $N$.

How do these various representations compare? A check of their applicability to interacting Bose gas simulations with Hamiltonians (2.17) or (2.12) is shown in Table 5.1. One can see that the early distributions were often hindered in obtaining a many-body simulation by a whole variety of problems.

For completeness, it should be mentioned that there are other distributions of the general form (3.1) that are more suited to non-stochastic calculations. For example

Table 5.1: Check list of required representation properties for the more commonly used phase-space representations, when applied to a lattice interacting Bose gas Hamiltonianof the forms (2.17) or (2.12), with no external coupling.

| distribution type | positive real | complete non-singular | FPE[a] | positive propagator | stable unbiased | UV convergent | open systems |
|---|---|---|---|---|---|---|---|
| Wigner | no | yes | no | varies[b] | – | no | yes |
| Q | yes | yes | yes | no | – | no | yes |
| P | yes | no | yes | no | – | yes | yes |
| R | no | yes | yes | no | – | yes | yes |
| positive P | yes | yes | yes | yes | no | yes | yes |
| sw.[c] Fock | yes | yes | yes | yes | yes[d] | yes | no |
| sw.[b] coherent | yes | yes | yes | yes | yes[c] | yes | no |
| gauge P | yes | yes | yes | yes | yes[c] | yes | yes |

[a] i.e. only 1st and 2nd partial derivative terms in $\partial P/\partial t$.
[b] There are no second order terms in the FPE for dynamics, while for thermodynamics the propagator may or may not be positive semi-definite, depending on occupation of modes.
[c] Stochastic wavefunction
[d] Given an appropriate choice of gauge — see Chapter 7

the symplectic tomography scheme of Mancini *et al*[77, 78], which expresses the quantum state as a probability distribution of a quadrature observable depending on a range of lab parameters. This has been used to investigate quantum entanglement and failure of local realism, but apparently has not led to many-mode quantum simulations, presumably due to the lack of a positive propagator in nonlinear evolution. The complex P representation[11] allows one to derive exact results for certain problems, but does not lead to stochastic equations, since the distribution is neither real nor positive.