

Quantum nonlinear lattices and coherent state vectors

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Abstract

Quantized nonlinear lattice models are considered for two different classes, boson and fermionic ones. The quantum discrete nonlinear Schrödinger model (DNLS) is our main objective, but its so called modified discrete nonlinear (MDNLS) version is also included, together with the fermionic polaron (FP) model.

Based on the respective dynamical symmetries of the models, a method is put forward which by use of the associated boson and spin coherent state vectors (CSV) and a factorization ansatz for the solution of the Schrödinger equation, leads to quasiclassical Hamiltonian equations of motion for the CSV parameters. The so obtained evolution equations are intimately related to the respective evolution equations for the classical lattices, provided we account for the ordering rules (normal, symmetric) adopted for their quantization.

Analysing the geometrical content of the factorization ansatz made for the state vectors invokes the study of the Riemannian and symplectic geometry of the CSV manifolds as generalized phase spaces. Next, we investigate analytically and numerically the behavior of mean values and uncertainties of some physically interesting observables as well as the modifications in the quantum regime of processes such as the discrete self trapping (DST), in terms of the Q-function and the distribution of excitation quanta of the lattice sites. Quantum DST in the symmetric ordering of lattice operators is found to be relatively enhanced with respect to the classical DST. Finally, the meaning of the factorization ansatz for the lattice wave function is explained in terms of disregarded quantum correlations, and as a quantitative figure of merit for that ansatz a correlation index is introduced. This index is given in terms of the norm of the difference between the true and factorized state vectors, and accounts for the quantum correlations of the lattice sites that develop during the time evolution of the systems.

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1 Introduction

Nonlinear lattice equations are abundant in physical applications and their study constitutes a well developed field of research. In many cases where models are described by classical lattice differential equations this is done as a first approximation to what is essentially a quantum mechanical lattice system. Quantized nonlinear lattice equations are the main target of the most successful method of the quantum inverse scattering method (QISM) [25]. Recent attempts to treat quantum lattice equations with arbitrary number of lattice sites have led to such schemes as the so called number state method (NSM) [34, 14], and the Hartree approximation [38] (see also [4] for a discussion about QISM and NSM). On the other hand it seems highly desirable when treating quantum versions of classical lattices to be able to utilize in some sense the available classical solutions of the nonlinear evolution equations and to keep a conceptual framework *viz.* phase spaces, Poisson brackets, coordinate transformations etc. akin to that of the classical models. It is in that direction that this work focuses and provides an alternative to the above mentioned methods.

Specifically we deal with lattices related to the nonintegrable generalized discrete nonlinear Schrödinger equation (DNLS) [7] (also known as the generalized discrete self-trapping (GDST) equation) [35] and with a modified version of it (MDNLS) [21]. We also discuss a fermionic lattice associated to the fermionic polaron (FP) model [15]. The DNLS models quantized by the canonical quantization method lead to a configuration of f sites, described by tensoring the Weyl-Heisenberg (WH) algebra attached to each lattice site. The ordering rule adopted when the classical wave amplitude variables are substituted by boson operators [6, 37] is essential for the form of the obtained Hamiltonian operator. Our method of solving the resulting Schrödinger equation is based on the assumption that the lattice state vector can be factorized to a tensor product of coherent state vectors ([33, 17, 2, 28, 39]) each one living in the Hilbert space associated to each lattice site. This leads to a set of Hamiltonian equations for the CSV coordinates, which provide an approximate quasiclassical solution for the exact quantum dynamics. As the CS are the most classical state vectors [33, 17] for boson systems the resulting equations are quasiclassical in nature and govern the motion of CS wavepackets. To elucidate the meaning of the ansatz we recall that the boson CS labels are coordinates of the canonical phase plane and therefore the quasiclassical dynamics occurs in the f -fold cartesian product of harmonic oscillator phase space. That dynamics is the classical dynamics if the normal ordering of the bosons is used and diverges from that for symmetric ordering. Therefore the CS mean values for normally ordered observables coincide with their classical values in the former case while their quantum mechanical fluctuations are constant and minimum in the course of time evolution. To try the method to more general quantum systems we have also studied the FP model, which is first mapped by means of the Jordan-Wigner transformation to its equivalent XXZ model [3]. The resulting spin Hamiltonian is expressed by tensoring the $su(2)$ algebra generators attached to each site of the model. By the same token as in the boson case the quantum dynamics is studied by assuming factorization of the state vector of the system to a product of spin CS. However the geometrical framework for the dynamics of the spin CSV's is different in this case. The $su(2)$ CS space is a spherical surface with a noncanonical symplectic structure defined on it, as it results by looking at the so called ray metric of the CSV [23, 30]; the classical Hamiltonian equations generate a flow in the f -fold cartesian product of spherical (or rather complex projective) coordinates.

The plan of the paper is as follows: in section two the general framework for the construction of CSV is outlined and the needed formulas for the special cases of the canonical and the spin CSV are provided. In the next section the DNLS model is quantized and the associated quasiclassical equations are derived and studied. Attention is paid to the problem of discrete self trapping (DST) phenomenon in the quantum regime, by illustrating the situation with plots of the Poisson distribution and the Q-function of the quantized modes of the system. Next section explains the physical meaning of the factoring of the lattice state vector as adopted for all models, and gives a validity measure for that approximation. In the following two appendices we illustrate the same idea by taking up first the MDNLS quantum lattice and then the FP model. The final section contains a number of conclusions and offers some prospects.

Throughout the text we consider $\hbar = 1$ and we denote CS expectation values of any generator with brackets around it.

2 Coherent state manifolds

The notion of coherent state vector was essentially introduced in the early days of quantum mechanics by Schrödinger [33], in his successful attempt to construct a nonspreading Gaussian wavepacket for a quantum harmonic potential. The wavepacket center was evolving following the classical path while the dispersion was kept to a minimum compatible with the minimum uncertainty principle. The regeneration of the theory took place in the sixties and seventies when to a wealth of physical applications of CS a mathematical group theoretical foundation was also provided [24, 16, 28, 39].

For our needs here a brief introduction of the CS concept goes as follows: consider a Lie group \mathcal{G} , with a unitary irreducible representation $T(g)$, $g \in \mathcal{G}$, in a Hilbert space \mathcal{H} . We select a reference vector $|\Psi_0\rangle \in \mathcal{H}$, to be called the "vacuum" state vector, and let $\mathcal{G}_0 \subset \mathcal{G}$ be its isotropy subgroup, *i.e.* for $h \in \mathcal{G}_0$, $T(h)|\Psi_0\rangle = e^{i\varphi(h)}|\Psi_0\rangle$. The map from the factor group $\mathcal{M} = \mathcal{G}/\mathcal{G}_0$ to the Hilbert space \mathcal{H} , introduced in the form of an orbit of the vacuum state under a factor group element, defines a CSV $|x\rangle = T(\mathcal{G}/\mathcal{G}_0)|\Psi_0\rangle$ labelled by points $x \in \mathcal{M}$ of the coherent state manifold. Coherent states form an (over)complete set of states, since by means of the Haar invariant measure of the group \mathcal{G} *viz.* $d\mu(x)$, $x \in \mathcal{M}$, they provide a resolution of unity, $\mathbf{1} = \int_{\mathcal{M}} d\mu(x) |x\rangle\langle x|$. As a consequence, any vector $|\Psi\rangle \in \mathcal{H}$ is analyzed in the CS basis, $|\Psi\rangle = \int_{\mathcal{M}} d\mu(x) \Psi(x) |x\rangle$, with coefficients $\Psi(x) = \langle x|\Psi\rangle$.

What concerns us here mostly is the geometry of the CS manifold \mathcal{M} . Indeed by its very construction \mathcal{M} inherits the structure of a Riemann manifold with in general non-constant curvature, which is also endowed with a complex structure of a Kähler manifold [19], namely it can be considered as a generalized phase space [2]. In the sequel we restrict ourselves to the case of a two dimensional surface \mathcal{M} for definiteness, although higher dimensional extensions of our statements are also possible [28]. Also we shall assume a generator G_+ creating from the vacuum state the CS vector, *i.e.*,

$$|\zeta\rangle = \mathcal{N}|\zeta\rangle = \mathcal{N}\exp(\zeta G_+)|\emptyset\rangle, \quad (1)$$

where $\zeta \in C$ and $\mathcal{N} = (\zeta|\zeta)^{-\frac{1}{2}}$ is the normalization factor. Occasionally we shall write G_- for the Hermitean conjugate of G_+ ; they should both belong to the Lie algebra of the

group for which the CS is defined. Below we shall specialize to the cases of $su(2)$ and the Weyl-Heisenberg groups but for the moment we proceed with the present general framework. The symplectic structure possessed by the state space \mathcal{M} is based on the existence of a canonical kinematical 1-form $\theta = \langle \zeta | d | \zeta \rangle = \frac{1}{2}(\langle G_+ \rangle d\zeta - \langle G_- \rangle d\bar{\zeta})$. The derivation $d = \partial_\zeta d\zeta + \partial_{\bar{\zeta}} d\bar{\zeta}$ acts on the state vectors, *e.g.*, $d|\zeta\rangle = (G_+ - \frac{1}{2}\langle G_+ \rangle)|\zeta\rangle d\zeta + (-\frac{1}{2}\langle G_- \rangle)|\zeta\rangle d\bar{\zeta}$. The symplectic 2-form ω of \mathcal{M} is derived from the canonical θ by derivation $\omega = d\theta$, and can be expressed in the form $\omega = (\langle G_- G_+ \rangle - \langle G_- \rangle \langle G_+ \rangle) d\zeta \wedge d\bar{\zeta}$.

Concerning the geometric features of our $2D$ phase space considered as a Riemannian surface with a distance function operating on it, we shall employ a meaningful metric tensor starting from the distance on the projective Hilbert space of rays $\overline{|\zeta\rangle}$, $\zeta \in C$ [23, 30]. By $\overline{|\zeta\rangle}$ we simply mean the set of CS $e^{i\phi}|\zeta\rangle$, multiplied by an arbitrary phase factor. The choice of space of rays rather than the Hilbert space is in accordance with the quantum mechanical arbitrariness of phase of the state vectors. The finite distance $\mathcal{D}(\overline{|\zeta_1\rangle}, \overline{|\zeta_2\rangle})$ between any two rays $\overline{|\zeta_1\rangle}$ and $\overline{|\zeta_2\rangle}$, which are associated with the normalized coherent states $e^{i\varphi_1}|\zeta_1\rangle$ and $e^{i\varphi_2}|\zeta_2\rangle$, is defined by

$$\mathcal{D}^2(\overline{|\zeta_1\rangle}, \overline{|\zeta_2\rangle}) = \inf_{\varphi_1, \varphi_2} \|e^{i\varphi_1}|\zeta_1\rangle - e^{i\varphi_2}|\zeta_2\rangle\|^2 = 2 - 2|\langle \zeta_1 | \zeta_2 \rangle|. \quad (2)$$

This is a proper distance function as it is positive definite and non-degenerate, it satisfies the triangular property and it is also gauge invariant. In addition its infinitesimal form gives the distance of two nearby coherent state vectors and provides the metric tensor on the CS-manifold [9], *i.e.*

$$\begin{aligned} (ds)^2 &= \frac{1}{2}\mathcal{D}^2(\overline{|\zeta + d\zeta\rangle}, \overline{|\zeta\rangle}) = 1 - |\langle \zeta + d\zeta | \zeta \rangle| \\ &= \left[\frac{\partial_\zeta \partial_{\bar{\zeta}} (\zeta || \zeta)}{(\zeta || \zeta)} - \frac{\partial_{\bar{\zeta}} (\zeta || \zeta)}{(\zeta || \zeta)} \cdot \frac{\partial_\zeta (\zeta || \zeta)}{(\zeta || \zeta)} \right] d\zeta d\bar{\zeta} \\ &= \frac{\partial}{\partial |\zeta|^2} \left[\frac{|\zeta|^2}{(\zeta || \zeta)} \frac{\partial (\zeta || \zeta)}{\partial |\zeta|^2} \right] d\zeta d\bar{\zeta} \equiv g_{\zeta\bar{\zeta}} d\zeta d\bar{\zeta}, \end{aligned} \quad (3)$$

or alternatively

$$(ds)^2 = \left[\frac{(\zeta || G_- G_+ || \zeta)}{(\zeta || \zeta)} - \frac{(\zeta || G_- || \zeta)}{(\zeta || \zeta)} \cdot \frac{(\zeta || G_+ || \zeta)}{(\zeta || \zeta)} \right] d\zeta d\bar{\zeta}. \quad (4)$$

The curvature scalar [19],

$$R = -g_{\zeta\bar{\zeta}}^{-1} \partial_\zeta \partial_{\bar{\zeta}} (\ln g_{\zeta\bar{\zeta}}), \quad (5)$$

following from the metric g involves higher correlations of the G_\pm generators and is in general not constant. It is worth noticing that the basic geometric objects of both the symplectic and Riemannian structure endowed in \mathcal{M} are given in terms of the so called symbols of the operators or their products [2], *i.e.* the coherent state mean value $\langle \zeta | G | \zeta \rangle \equiv \langle G \rangle$ of the corresponding operator G . Also the noncommutativity of the involved operators and their non-zero uncertainties in the coherent state basis is essential for the non-trivial geometric characteristics of the \mathcal{M} manifold. In effect, the CS-manifold \mathcal{M} captures some genuine quantum mechanical features despite its classical character; this property of \mathcal{M} is further manifested in the quantum mechanical evolution to be studied shortly.

As the models to be studied in the next sections are of boson and fermionic/spin type with dynamical symmetries related to the WH and the $su(2)$ algebras [16], we now exemplify the

above construction for the CS of these algebras. For the boson algebra,

$$[a, a^\dagger] = \mathbf{1} \quad [N, a^\dagger] = a^\dagger \quad [N, a] = -a, \quad (6)$$

with $N = a^\dagger a$ the number operator, the vacuum state is the zero-photon state vector $|\odot\rangle = |0\rangle$, and $G_+ = a^\dagger$ the creation operator. This defines the boson CS

$$|\alpha\rangle = e^{\alpha a^\dagger - \bar{\alpha} a} |0\rangle = \mathcal{N} e^{\alpha a^\dagger} |0\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \quad (7)$$

It is an (over)complete set of states with respect to the measure $d\mu(\alpha) = \frac{1}{\pi} e^{-|\alpha|^2} d^2\alpha$ for the non-normalized CS, and $\alpha \in \mathcal{M} = WH/U(1) \approx C$ is the CS manifold. Since $a|\alpha\rangle = \alpha|\alpha\rangle$, which implies the symbols $\langle a \rangle = \alpha$, $\langle a^\dagger \rangle = \bar{\alpha}$, $\langle N \rangle = |\alpha|^2$, \mathcal{M} is the flat canonical phase plane with the standard line element $ds^2 = d\alpha d\bar{\alpha}$. Also the symplectic 2-form $\omega = id\alpha \wedge d\bar{\alpha}$ is associated to the canonical Poisson bracket $\{f, g\} = i(\partial_\alpha f \partial_{\bar{\alpha}} g - \partial_{\bar{\alpha}} f \partial_\alpha g)$.

Next we come to the case of the $su(2)$ algebra with commutation relations,

$$[J_0, J_\pm] = \pm J_\pm \quad [J_+, J_-] = 2J_0. \quad (8)$$

The vacuum state $|\odot\rangle \equiv |j - j\rangle$ is the extremal vector in the representation module of the algebra, with $\{|j \ m\rangle\}_{m=-j}^j$, $j = 1/2, 1, 3/2, \dots$, and $-j \leq m \leq j$. The CS vector is obtained by displacing the vacuum with a $SU(2)/U(1)$ coset element:

$$|z\rangle = e^{\nu J_+ - \bar{\nu} J_-} |j - j\rangle = \mathcal{N} e^{z J_+} |j - j\rangle = \mathcal{N} \sum_{m=-j}^j \binom{2j}{j+m}^{\frac{1}{2}} z^{j+m} |j \ m\rangle, \quad (9)$$

with $z = (\nu/|\nu|)\tan|\nu|$ and normalization coefficient $\mathcal{N} = (1 + z\bar{z})^{-j}$. The CS manifold $\mathcal{M} = SU(2)/U(1) \approx S^2 \approx CP^1$ is isomorphic to the 2-sphere S^2 , with $0 \leq \theta \leq \pi$, $0 \leq \varphi \leq 2\pi$ polar and azimuthal angles respectively. It is also parametrized as the complex projection plane CP^1 with coordinate $\mathcal{M} \ni z = \tan(\frac{1}{2}\theta)e^{-i\varphi}$.

The symbols of the generators are

$$\begin{aligned} \langle J_+ \rangle &= 2j \frac{\bar{z}}{1 + z\bar{z}}, & \langle J_- \rangle &= 2j \frac{z}{1 + z\bar{z}} \\ \langle J_0 \rangle &= -j \frac{1 - z\bar{z}}{1 + z\bar{z}}, & \langle J_- J_+ \rangle &= \frac{4j^2 z\bar{z} + 2j}{(1 + z\bar{z})^2}. \end{aligned} \quad (10)$$

Based on the general scheme the above generator symbols give rise to the line element $ds^2 = (1 + z\bar{z})^{-2} dz d\bar{z}$ for the complex tangent plane \mathcal{M} . The (over)completeness of the non-normalized CS invokes the Haar invariant measure on \mathcal{M} , $d\mu(z) = \frac{2j+1}{\pi} (1 + z\bar{z})^{-2} d^2z$. The CS vector space is now the constant curvature ($R = 1$) sphere equipped with the canonical 1-form $\theta = ij \frac{\bar{z}}{1+z\bar{z}} dz + cc$, which furnishes a canonical symplectic 2-form $\omega = ij \frac{dz \wedge d\bar{z}}{(1+z\bar{z})^2}$, and the associated Poisson bracket becomes $\{f, g\} = \frac{i(1+z\bar{z})^2}{2j} (\partial_z f \partial_{\bar{z}} g - \partial_{\bar{z}} f \partial_z g)$.

3 Generalized discrete self-trapping equation

The classical Hamiltonian of the generalized discrete self-trapping (GDST) model reads [7, 35]

$$H_{\text{CL}} = \sum_{j=1}^f (\omega_0 |A_j|^2 - \frac{\gamma}{m} |A_j|^{2m}) - \sum_{j \neq k}^f \lambda_{jk} \bar{A}_j A_k, \quad (11)$$

where $j = 1, 2, \dots, f$ counts the number of complex mode amplitudes $A_j(t)$ and its complex conjugate $\bar{A}_j(t)$. The equation of motion

$$i\dot{A}_j = \omega_0 A_j - \sum_{(j \neq k)k=1}^f \lambda_{jk} A_k - \gamma |A_j|^{2(m-1)} A_j \quad (12)$$

is derived from the canonical Poisson brackets

$$\{A_j, \bar{A}_k\} = i\delta_{jk}, \quad \{A_j, A_k\} = \{\bar{A}_j, \bar{A}_k\} = 0 \quad (13)$$

using the equation of motion $\dot{A}_j = \{H, A_j\}$.

The quantization of this canonical Lie-Poisson algebra proceeds with the correspondance rule [6, 37] $A \rightarrow b, A^* \rightarrow b^\dagger$, where b^\dagger and b are the canonical creation and annihilation operators respectively. To account for problems of ordering, well known in the naive quantization rule, we shall here confine ourselves to two ordering rules, namely the normal ordering (NO) and the symmetric ordering (SO). SO is a classically motivated symmetrization of non-commuting operators and should be expected to give the right classical limit when $\hbar \rightarrow 0$. However here we study the quasiclassical limit of the quantum equations of motion by means of the CS symbol of operators and in this case the NO is the appropriate ordering. (For further discussion on the difference between semi- and quasiclassical ordering see refs. 89 and 142 in [24], ff p.64-65).

For the SO quantization rule the correspondance [18, 5]

$$|A|^{2m} \rightarrow \frac{m!}{2^m} L_m(-2x), \quad (14)$$

is valid for quantization of arbitrary positive powers of the modulus of the complex amplitude; here $x^k = : (b^\dagger b)^k : \equiv b^{\dagger k} b^k$ and $L_m(\cdot)$ is the Laguerre polynomial of zero order. Then, using the symmetric ordering quantization rule and after a constant shifting by $\frac{1}{2}\omega_0 - \gamma \frac{(m-1)!}{2^m}$, the Hamiltonian of the GDST model takes the form

$$H_{\text{SO}} = H_{\text{NO}} - \gamma \sum_{j=1}^f \sum_{n=1}^{m-1} \mu_n^{(m)} b_j^{\dagger n} b_j^n, \quad (15)$$

where $\mu_n^{(m)} = \frac{(m-1)!}{2^m} \binom{m}{m-n} \frac{2^n}{n!}$, and

$$H_{\text{NO}} = \sum_{j=1}^f (\omega_0 b_j^\dagger b_j - \frac{\gamma}{m} b_j^{\dagger m} b_j^m) - \sum_{j \neq k}^f \lambda_{jk} b_j^\dagger b_k, \quad (16)$$

is the Hamiltonian obtained by the normal ordering quantization rule. We observe that the symmetric ordering rule adds $m - 1$ additional terms in the Hamiltonian with respect to its

NO quantization. However since for $m = 2$ it is reduced to the number operator which can be absorbed in the H_{NO} by simply redefining the coefficient of the corresponding number operator term, we see that in effect the symmetric ordering modifies the Hamiltonian only for $m > 2$, *i.e.* only for higher order nonlinearity.

Next we obtain the Heisenberg equations of motion for the boson operators by using the Hamiltonian of eq. (15)

$$i\dot{b}_j = \omega_0 b_j - \gamma b_j^{\dagger m-1} b_j^m - \sum_{k=1}^f \lambda_{jk} b_k - \gamma \left(\sum_{n=1}^{m-1} \mu_n^{(m)} n b_j^{\dagger n-1} b_j^n \right). \quad (17)$$

Making use of the factorized state vector $|\beta\rangle \equiv \otimes_{j=1}^f |\beta_j\rangle$, where $b_j |\beta_j\rangle = \beta_j |\beta_j\rangle$, $j = 1, \dots, f$, we evaluate the CS mean value of the last equation to obtain

$$i\dot{\beta}_j = \omega_0 \beta_j - \gamma |\beta_j|^{2m-2} \beta_j - \sum_{(j \neq k)k=1}^f \lambda_{jk} \beta_k - \gamma \sum_{n=1}^{m-1} \mu_n^{(m)} n |\beta_j|^{2n-2} \beta_j. \quad (18)$$

By means of the canonical Poisson brackets this set of equations can be derived from the Hamiltonian

$$\mathcal{H} = \langle \beta | H | \beta \rangle = \sum_{k=1}^f (\omega_0 |\beta_k|^2 - \frac{\gamma}{m} |\beta_k|^{2m}) - \sum_{k \neq l}^f \lambda_{kl} \beta_k \bar{\beta}_l - \gamma \sum_{k=1}^f \sum_{n=1}^{m-1} \mu_n^{(m)} |\beta_k|^{2n}. \quad (19)$$

The above Hamiltonian and the norm $N = \sum_{j=1}^f |\beta_j|^2$ are the constants of motion for the dynamics issued by eq. (18). We observe that the first two sums in eq. (19) combine to give the coherent state symbol of the H_{NO} of eq. (16), while the remaining part corresponds to the symbol of the terms appearing in eq. (15) due to the SO. This implies that NO quantization induces in the CS manifold \mathcal{M} an essentially classical time evolution while the quantization by SO, due to the additional terms, induces a dynamical evolution on \mathcal{M} which departs from classical dynamics. This of course makes a difference in the dynamics of the observables of the system as well as in the wavefunction distributions. At this point we should remark that the assumption of factorization of the state vector into CSVs implies that any normal ordered function of boson operators from each mode has CS mean value expressed by the same function, *i.e.*

$$\langle \alpha | : f(a_j^\dagger, a_j) : | \alpha \rangle = f(\bar{\alpha}_j, \alpha_j). \quad (20)$$

Also for each oscillator mode the Hermitian combinations $x = \frac{1}{\sqrt{2}}(a^\dagger + a)$ and $p = \frac{i}{\sqrt{2}}(a^\dagger - a)$, *i.e.* the position and momentum operators, we obtain the minimum uncertainty property of the boson CSV,

$$\Delta x \Delta p = \frac{1}{2}, \quad (21)$$

for the uncertainties $(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle$ and $(\Delta p)^2 = \langle (p - \langle p \rangle)^2 \rangle$. We shall recall this property shortly for the Q-function.

To illustrate these differences in dynamics due to ordering we shall employ the quantum mechanical Q-distribution function [20] and the Poissonian distribution of the boson excitations of a CSV in the number state basis [17]. For the Q-distribution of a ρ density matrix we define

$$Q_j = \frac{1}{\pi} \langle \beta_r | \rho_j | \beta_r \rangle = \frac{1}{\pi} |\langle \beta_r | \beta_j \rangle|^2, \quad (22)$$

with $j = 1, \dots, f$. Here we have assumed a pure state for each mode *i.e.* $\rho_j = |\beta_j\rangle\langle\beta_j|$, and the reference CS $|\beta_r\rangle$ is labelled by the complex coordinate $\beta_r = x_r + iy_r$. The Q-function then takes the form of a displaced Gaussian function *viz.*

$$Q_j(x_r, y_r) = \frac{1}{\pi} e^{-(x_r - \text{Re}\beta_j)^2 - (y_r - \text{Im}\beta_j)^2}. \quad (23)$$

The center of the Gaussian $(\text{Re}\beta_j, \text{Im}\beta_j)$ is the expectation value of the position and momentum operators in the CS basis, *i.e.* $(\text{Re}\beta_j, \text{Im}\beta_j) = (\langle\beta|x_j|\beta\rangle, \langle\beta|p_j|\beta\rangle)$, for $j = 1, \dots, f$. However there is a nonzero quantum mechanical uncertainty around this point since $\Delta x_j = \Delta p_j = \frac{1}{\sqrt{2}}$, albeit it is the minimum acceptable one (*c.f.* eq.(21)).

In Figs. 1(a,b) the Gaussian bells of the Q-functions for the quintic ($m = 3$) GDST trimer ($f = 3$) system are plotted at a certain instant of time for SO and NO respectively. Here and in the following we use periodic boundary conditions and choose $\lambda_{jk} = 1$ for nearest neighbouring sites, and zero otherwise. The centers of the Gaussian functions of Fig. 1 are plotted in Fig. 2 for the SO (Fig. 2a,b) and the NO (Fig. 2 c,d) cases, respectively. We note that in the SO case the trajectory of the bell corresponding to the initially excited site will always be confined in a region far from the origin, while the bells corresponding to the other two sites will stay close to the origin. In our framework, this corresponds to the well known self-trapping of the classical system. It is obvious that the appearance of the extra terms in the SO-equation enhances the self-trapping compared to the NO-case.

Next we consider the Poissonian distribution of each boson mode in the coherent state,

$$P_n^j = |\langle\beta_j|n\rangle|^2 = e^{-|\beta_j|^2} \frac{|\beta_j|^{2n}}{n!}, \quad (24)$$

where $n = 0, 1, \dots$ enumerates the number states and $|\beta_j|^2 = \langle\beta_j|b_j^\dagger b_j|\beta_j\rangle$ is the expectation value of the number operator which gives the average number of quanta in the CS basis. An illustration of how the self-trapping reflects itself in the Poissonian distribution and how it gets enhanced in SO quantization, is shown in Fig. 3a and 3b for the SO and NO cases respectively. The system is here a rather large ($f = 21$) quintic ($m = 3$) GDST-system, and initially one single site ($j = 21$) is excited with the total excitation number $N = 10$. As can be seen, for the particular parameter values chosen here the main part of the excitation stays at the initially excited site in the SO-case, while it spreads more or less equally among the modes in the NO case.

To end this section, we note that in the simple case of the GDST dimer ($f = 2$) with cubic ($m = 2$) or quintic ($m = 3$) nonlinearity, it is possible to derive an analytic expression for the critical value, γ_{cr} , of the nonlinear coupling coefficient for the appearance of self-trapping in eq. (18). This is done in the standard way by considering the variable $r = |\beta_1|^2 - |\beta_2|^2$. For the ordinary GDST equation (12), it was found in ref. [22] for the cubic case and in ref. [35] for the quintic case, that \ddot{r} could be expressed as a cubic polynomial in r , and solutions in terms of Jacobi elliptic functions were obtained. In the case of eq. (18), containing both cubic and quintic nonlinearity, we find the same equation for \ddot{r} as in ref. [22], provided that we replace γ with $\gamma^{(2)} + N\gamma^{(3)}$, where $\gamma^{(2)}$ and $\gamma^{(3)}$ are the coefficients of the cubic and quintic nonlinear terms, respectively. Thus, defining γ_{cr} in the usual way as the smallest value of γ for which $|\beta_{j_0}|^2$ is always larger than $N/2$, given that the excitation initially was localized on site j_0 , we find the self-trapping condition $\frac{\gamma^{(2)} + N\gamma^{(3)}}{\lambda_{jk}} > \frac{4}{N}$ from the explicit solution for

$r(t)$ just as in ref. [22]. Using the explicit expressions for $\gamma^{(2)}$ and $\gamma^{(3)}$ in (18) and $\lambda_{jk} = 1$, the following expressions for γ_{cr} are obtained in the NO and SO cases, respectively:

$$\gamma_{\text{cr}}^{\text{NO}} = \frac{4}{N^2} \quad , \quad \gamma_{\text{cr}}^{\text{SO}} = \frac{4}{N(N+3)} . \quad (25)$$

These expressions are plotted in Fig. 4 as a function of the total number of lattice quanta N . In the limit of large number of excitations (phonons) the quantum lattice model, according to Bohr's correspondance principle, will behave classically. In particular the critical value of γ for the onset of self-trapping, which as we have also seen from previous plots is different for SO and NO, is expected to become equal in the classical limit of the quantum lattice models. In this limit the ordering of the operators, a genuine quantum characteristic, should not be of importance. Indeed the analytic expressions (25) for the critical γ 's of the GDST dimer show, that when the number of quanta becomes large, the phenomenon of DST occurs asymptotically for the same values *i.e.* $\gamma_{\text{cr}}^{\text{NO}} \approx \gamma_{\text{cr}}^{\text{SO}}$, independently of the ordering rule.

4 Validity of the factorization ansatz and quantum correlations

Let a composite quantum system be described by a general pure state $|\psi\rangle$ living in $\mathcal{H} = \otimes_{i=1}^f \mathcal{H}_i$, the tensor product of Hilbert spaces of its f subsystems. In general the form of such a generic vector $|\psi\rangle$ can be of three different types, each one signifying a specific kind of correlation among the subsystems. For vectors of the product form, $|\psi\rangle = |\phi\rangle^1 \otimes |\phi\rangle^2 \otimes \dots \otimes |\phi\rangle^f$, the subsystems are decorrelated. If $|\psi\rangle$ is a convex combination of product states *i.e.* $|\psi\rangle = \sum_i^n \lambda_i |\phi\rangle_i^1 \otimes |\phi\rangle_i^2 \otimes \dots \otimes |\phi\rangle_i^f$, with $\sum_i^n \lambda_i = 1$, the subsystems are said to be classically correlated [29]. For inseparable or entangled systems, the third case, the state vector $|\psi\rangle$ is a general superposition of states from its subsystems with no additional properties, that are further characterized by *e.g.* violation of Bell inequalities [1]; this is the case when genuine quantum correlations are developed among the subsystems.

Although the existence and the oddities of quantum nonlocal correlations and of entanglement have been pointed out since the early days of Quantum Mechanics [8], and have remained an active subject of research since then [1], it is only recently (due mainly to some striking applications of entanglement such as quantum computation, cryptography, teleportation etc; see [10, 12] and refs. therein), that measures that quantify the amount of correlations of a given state of a composite quantum system have been studied. In the above framework of quantum correlations it is clear that our factorization ansatz is equivalent to the assumption that no quantum correlations will be developed in the course of time evolution. Still, as we have seen, due to the nonlinear form of the quantum Hamiltonian the equations of motions derived from that approximate ansatz differ from the entirely classical ones. This difference captures some of the quantum features of the system, so we would like to have a figure of merit of our approximation. To this end we introduce a single index, the correlation index, that measures the distance of the true state of the model from the factorized one that is assumed, and so gauges the validity of our approximation.

Recall that the CS-vectors form a basis for the Hilbert space of a single site, so for the f

sites of the boson chain model a general state vector can be expanded as

$$|\psi\rangle = \int P(\{\alpha_i\}, \{\bar{\alpha}_i\}) \otimes_{i=1}^f |\alpha_i\rangle d\mu(\{\alpha_i\}) \quad (26)$$

with $d\mu(\{\alpha_i\}) = \prod_{i=1}^f d^2\alpha_i$. By means of the relations ([26]),

$$\begin{aligned} f(\bar{\beta}) &= \int f(\bar{\alpha}) \exp[-\frac{1}{2}(|\alpha|^2 + |\beta|^2) + \bar{\beta}\alpha] d^2\alpha, \\ f(\bar{\beta}) &= \int f(\bar{\alpha}) \langle\beta|\alpha\rangle d^2\alpha, \end{aligned} \quad (27)$$

which imply that the overlap $\langle\beta|\alpha\rangle$ of CS behaves as a delta function for the integrable functions of the Bargmann-Hilbert space, we can compute that $|\psi\rangle$ is normalized provided that $\int |P(\{\alpha_i\}, \{\bar{\alpha}_i\})|^2 d\mu(\{\alpha_i\}) = 1$. This shows that if $P(\{\alpha_i\}, \{\bar{\alpha}_i\}) = \delta(\alpha_1 - \alpha_1^r) \dots \delta(\alpha_f - \alpha_f^r)$, then the general vector $|\psi\rangle$ is reduced to the factorized state $|\psi_{ref}\rangle = \otimes_{i=1}^f |\alpha_i^r\rangle$.

We now introduce the correlation index ϵ (*c.f* eq. (2)),

$$\begin{aligned} \epsilon &= \mathcal{D}^2(\overline{|\psi\rangle}, \overline{|\psi_{ref}\rangle}) = 2 - 2 |\langle\psi|\psi_{ref}\rangle| \\ &= 2 - 2 \left| \int d\mu(\{\alpha_i\}) P(\{\alpha_i\}, \{\bar{\alpha}_i\}) \prod_{i=1}^f \exp[-\frac{1}{2}(|\alpha_i^r|^2 + |\alpha_i|^2) + \bar{\alpha}_i^r \alpha_i] \right|. \end{aligned} \quad (28)$$

Initially $\epsilon(t=0) = 0$, since we set $|\psi(t=0)\rangle = |\psi_{ref}\rangle$. In any subsequent time interval $a \leq t \leq b$, for which $\epsilon(t=0) \approx 0$, our ansatz is justified. To determine $\epsilon(t)$, we need to know the kernel $P(\{\alpha_i\}, \{\bar{\alpha}_i\})$. Substituting the expansion (26) in the Schrödinger equation we find that the kernel P satisfies the Fokker-Planck equation,

$$i\hbar\partial_t P(\{\alpha_i\}, \{\bar{\alpha}_i\}) = \mathcal{H}(\alpha_i, -\partial_{\alpha_i} + \frac{1}{2}\bar{\alpha}_i) P(\{\alpha_i\}, \{\bar{\alpha}_i\}), \quad (29)$$

where \mathcal{H} is the analytic image of the Hamiltonian operator under the substitutions $a_i \rightarrow \alpha_i$, $a_i^\dagger \rightarrow -\bar{\alpha}_i$. There are a number of approximate and analytic solution techniques available for such equations [32], most accessible *e.g.* is the technique of continued fractions. However the problem of quantum correlations in nonlinear lattice models is interesting even in the dimer case, and as far as we know it has not been addressed. In such a case the conservation of the total number of excitation quanta in the lattice sites will make the number of terms in a continued fraction method of solving the ensuing Fokker-Planck equation finite, since the dimensionality of the available Hilbert space and of the ρ -density matrix is determined by the number of quanta available. This makes possible an explicit calculation of the correlation index and allows to set a number of interesting questions concerning the relation of correlation/decorrelation versus selftrapping/non-selftrapping in the case of the quantum dimer (see *e.g.* [13] for a full quantum treatment of the quantum dimer); however more work should be anticipated along these lines [11]. Finally, we note that for non-boson lattices, as the ones of the last appendix, the introduction of the correlation index can be done again based on the distance function defined for the respective CSV, *c.f* eq.(2).

5 Conclusions

This work was inspired by the fact that for a linear quantum mechanical oscillator there is a coherent state vector defined in its Hilbert space, predicting that the motion will be

centered around the classical path with the minimum uncertainty. Here, this simple idea has been extended to some quantum nonlinear chain models. For quantum chain models with an oscillator attached at each site, the obvious assumption which has been followed here is that each site is in a CS ; the same idea however can be applied for multispin-like models with some advantages as we have shown. The essential geometric nature of our assumption has also been stated in terms of the symplectic and Riemannian geometry of the CSV spaces. Other types of special states, such as *e.g.* even/odd CSV (symmetric/antisymmetric combination of boson CS) which are associated with different geometries of their CS spaces, could have been considered; the final choice depends on the dynamical symmetry of the given Hamiltonian and on the specific form of the nonlinear interaction terms.

Also, the treatment of the DST in the quantum regime as has been presented here shows that this is a phenomenon which continues to exist after quantization of the classical DST equations. However, as has been demonstrated by means of the CS method, its exact parameter dependence is crucially affected by the quantization scheme. Contrary to the NO case where the situation is essentially classical, in the SO rule DST gets even more pronounced from its classical form. We note that a similar statement can be made also concerning the Hartree approximation treated in [38, 18, 36], since this ansatz results into similar approximate dynamics as obtained here. This can be seen by comparing our eq. (18) with eqs. (4.3) and (4.4) of ref. [18]. However, the Hartree ansatz is basically different from the factorization ansatz used here. Namely, geometrically it can be said that the two ansätze confine the dynamics in different subspaces of the total Hilbert space of the GDST model, moreover the Hartree wavefunction is not fully factorized.

Finally, we should note that although the factorization hypothesis for the state vector has been effective in treating the dynamical evolution in the model-cases studied here, its validity should be questioned. This is a crucial point, since factoring the state vector of a compound quantum system implies a loss of the quantum correlations which may be developed during the course of the time evolution. The failure of a factorized state to account for such entanglement of quantum subsystems can however be quantified by means of a correlation index, as we have shown. In future work we plan to present a study of the entanglement phenomenon versus DST in a quantum dimer model.

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Appendix 1: Modified discrete nonlinear Schrödinger equation

The ability of the CS-method to extract the quantum mechanical characteristics of the time evolution for a given lattice Hamiltonian model is very much depending on the special form of the Hamiltonian itself. Occasionally the derived equations of motion will be reducible to the classical ones indifferently of the quantization ordering rule (at least for the common rules); let us take up the following case. The so called modified discrete nonlinear Schrödinger equation (MDNLS) [21] has been recently introduced as a model describing in the adiabatic limit polaron dynamics when the excitation is coupled to an acoustic chain of oscillators. Compared to ordinary DNLS dynamics of an excitation coupled to optical oscillators, the MDNLS contains some new formal features such as off-diagonal nonlinearity, and for a ring with f -sites reads

$$i\dot{A}_j = V(A_{j+1} + A_{j-1}) - X(|A_{j+1}|^2 + |A_{j-1}|^2 + 2|A_j|^2)A_j. \quad (30)$$

Using canonical Poisson brackets, these equations can be derived from the Hamiltonian

$$H_{\text{CL}} = V \sum_{j=1}^f (A_j \bar{A}_{j+1} + \bar{A}_j A_{j+1}) - X \sum_{j=1}^f (|A_{j+1}|^2 |A_{j+2}|^2 + |A_j|^4). \quad (31)$$

The quantization of the classical Hamiltonian for the MDNLS equation leads (after a constant shifting of the Hamiltonian) to the following expression

$$H_{\text{SO}} = H_{\text{NO}} - \frac{1}{2}X \sum_{j=1}^f (b_{j+2}^\dagger b_{j+2} + b_{j+1}^\dagger b_{j+1} + b_j^\dagger b_j), \quad (32)$$

where

$$H_{\text{NO}} = V \sum_{j=1}^f (b_j b_{j+1}^\dagger + b_j^\dagger b_{j+1}) - X \sum_{j=1}^f (b_{j+1}^\dagger b_{j+1} b_{j+2}^\dagger b_{j+2} + b_j^\dagger b_j^2). \quad (33)$$

The first term in eq. (32) refers to the NO and the second one is obtained as before from the SO rule. Since the total Hamiltonian is written in terms of WH algebra elements defined at each site and by their products, we can follow exactly the same procedure as in the quantum DNLS case. Namely we assume the factorization of the state vector in terms of canonical CSVs. By the method of the previous section, and for the Hamiltonian H_{SO} , this leads to derivation of a set of quasiclassical equations of motion satisfied by the CSV parameters A_j ,

$$i\dot{A}_j = V(A_{j+1} + A_{j-1}) - X(|A_{j+1}|^2 + |A_{j-1}|^2 + 2|A_j|^2)A_j + \frac{3}{2}XA_j. \quad (34)$$

The above expression shows that the quasiclassical equation differs by a constant shift of the coefficients of the onsite variables from the corresponding classical equation. With the transformation $A_j \rightarrow e^{-\frac{3}{2}iXt}A_j$ they become the classical equations. The formal similarity of classical and quasiclassical equations allows to conclude the following: the particular form of the MDNLS Hamiltonian after quantization by NO and SO generates, (on the geometrical space singled out by the factorization of the model's quantum state in terms of boson CSV), an (almost) classical dynamics. This however as the previous sections show, should not be expected to be true in general.

Appendix 2: Fermionic polaron model (FP)

To demonstrate the ability of the proposed method to study quantum dynamics for models others than quantized boson chains, we shall take up in this appendix the fermionic polaron (FP) model. It has been recently proposed to describe the interaction of electrons with optical phonons in one spatial dimension [15]. This same model has been studied from the point of view of QISM [31, 14] and the NSM [14, 36]. Under the assumptions made in [15] the Hamiltonian of the interacting electron-phonon system with periodic boundary conditions reads

$$H = \epsilon \sum_{j=1}^N a_j^\dagger a_j - g \sum_{j=1}^N (a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) + V \sum_{j=1}^N n_j n_{j+1} , \quad (35)$$

where the fermion annihilation operator of a polaron at lattice site j , a_j and its corresponding Hermitian conjugate a_j^\dagger (the creation operator) generate the Grassmann algebra

$$[a_j, a_k]_+ = [a_j^\dagger, a_k^\dagger]_+ = 0 \quad , \quad [a_j, a_k^\dagger]_+ = \delta_{jk} . \quad (36)$$

The occupation number operator is defined by $n_j = a_j^\dagger a_j$, while g is a parameter proportional to the overlapping integral and V stands for the electron-phonon coupling constant (see [15] for details). Using the equivalence of the FP model to the XXZ model provided in [31] by means of a Jordan-Wigner transformation, we shall proceed to write the spin analogue of the fermionic model. The Grassmann algebra in eq. (36) is realized in terms of a tensor product of generators of the (spin 1/2 Pauli) algebra by means of the following Jordan-Wigner transformation

$$\begin{aligned} a_j &= \sigma_j^- \exp \left(i\pi \sum_{k=1}^{j-1} (\sigma_k^z + \frac{1}{2} \mathbf{1}_j) \right) \\ a_j^\dagger &= \sigma_j^+ \exp \left(-i\pi \sum_{k=1}^{j-1} (\sigma_k^z + \frac{1}{2} \mathbf{1}_j) \right) \\ n_j &= \sigma_j^+ \sigma_j^- = (\frac{1}{2} \mathbf{1}_j + \sigma_j^z) , \end{aligned} \quad (37)$$

and its inverse

$$\sigma_j^- = a_j \exp(-i\pi \sum_{k=1}^{j-1} n_k) \quad , \quad \sigma_j^+ = a_j^\dagger \exp(i\pi \sum_{k=1}^{j-1} n_k) \quad (38)$$

$$\sigma_j^z = n_j - \frac{1}{2} \mathbf{1}_j , \quad (39)$$

where $\sigma_j^\pm = \sigma_j^x \pm i\sigma_j^y$, and $\sigma_j^x, \sigma_j^y, \sigma_j^z$ are the Pauli matrices and $\mathbf{1}_j$ is the unit matrix at site j .

Using eq. (37) the transformed Hamiltonian of eq. (35) reads,

$$H = \frac{N}{2} \left(\epsilon + \frac{V}{2} \right) + (\epsilon + V) \sum_{j=1}^N \sigma_j^z + H_{\text{XXZ}} , \quad (40)$$

where

$$H_{\text{XXZ}} = V \sum_{j=1}^N \sigma_j^z \sigma_{j+1}^z - 2g \sum_{j=1}^N (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) , \quad (41)$$

or

$$H_{\text{XXZ}} = V \sum_{j=1}^N \sigma_j^z \sigma_{j+1}^z - g \sum_{j=1}^N (\sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+). \quad (42)$$

We now proceed with the H_{XXZ} part of the Hamiltonian as the other terms are constants of motion. Following same tactics as for the boson models we acknowledge the fact that the H_{XXZ} Hamiltonian is embedded in the $\otimes_{j=1}^N su_j(2)$ algebra and make an appropriate ansatz about the form of the wavefunction. Namely, we assume it is written in the form $|z\rangle = \otimes_{j=1}^N |z_j\rangle$, where $|z_j\rangle$ is the $su(2)$ coherent state corresponding to the j -site of the chain. To determine the dynamics of the complex amplitudes z 's we use the relation $z \langle j - J_0 \rangle = \langle J_- \rangle$, which is obtained from eq. (10). Then the time derivative of this relation for $j = 1/2$, gives the evolution equation of the complex amplitude at each site by means of the CS symbol of the Heisenberg equations, *viz.*

$$\begin{aligned} \dot{z}_j &= \frac{d/dt \langle \sigma_j^- \rangle \langle 1/2 - \sigma_j^z \rangle - \langle \sigma_j^- \rangle d/dt \langle 1/2 - \sigma_j^z \rangle}{\langle 1/2 - \sigma_j^z \rangle^2} \\ &= \frac{-i(\langle [\sigma_j^-, H] \rangle \langle 1/2 - \sigma_j^z \rangle + \langle \sigma_j^- \rangle \langle [\sigma_j^z, H] \rangle)}{\langle 1/2 - \sigma_j^z \rangle^2}. \end{aligned} \quad (43)$$

Straightforward evaluation of the CS symbols of the involved operators gives the evolution equation,

$$\begin{aligned} i\dot{z}_j &= \frac{1}{(1 + |z_{j-1}|^2)(1 + |z_{j+1}|^2)} \\ &\quad \left[-V z_j (1 - 2|z_{j-1}|^2 |z_{j+1}|^2) + (2g - 3g|z_j|^2) [z_{j-1}(1 + |z_{j+1}|^2) + z_{j+1}(1 + |z_{j-1}|^2)] \right. \\ &\quad \left. + g z_j^2 [\bar{z}_{j-1}(1 + |z_{j+1}|^2) + \bar{z}_{j+1}(1 + |z_{j-1}|^2)] \right] \end{aligned} \quad (44)$$

Returning to the original model we compute the CS mean value of the fermion operators by use of eqs. (10) and (37). This yields

$$\langle z(t) | a_j^\dagger | z(t) \rangle = \prod_{k=1}^{j-1} (-2) \langle z_k(t) | \sigma_k^z | z_k(t) \rangle \langle z_j(t) | \sigma_j^+ | z_j(t) \rangle = C_j(t) e^{-i\theta_j(t)}, \quad (45)$$

where

$$C_j(t) = \frac{|z_j(t)|}{1 + |z_j(t)|^2} \prod_{k=1}^{j-1} \frac{1 - |z_k(t)|^2}{1 + |z_k(t)|^2}, \quad (46)$$

with $z_j(t) = |z_j(t)| e^{i\theta_j(t)}$.

Also, $\langle z(t) | a_k^\dagger | z(t) \rangle = \overline{\langle z(t) | a_k^\dagger | z(t) \rangle}$, $k = 1, \dots, N$, while the average value of the fermion number operator is given by

$$\langle z(t) | n_j | z(t) \rangle = \langle z(t) | \sigma_j^z | z(t) \rangle + \frac{1}{2} = \frac{|z_j(t)|^2}{1 + |z_j(t)|^2}. \quad (47)$$

A final remark concerns the applicability of the CS method to the XXZ model; it has recently come to our attention that this method also can treat [27] the XXZ model of higher spins.

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Figure captions

Fig. 1. The Q-functions (22) for the quintic ($m = 3$) GDST-trimer ($f = 3$) plotted at the time-instant $t = 76.4$ for the cases of symmetric (a) resp. normal (b) ordering of the boson operators. Dashed line corresponds to the initially excited site $j = 2$, while solid line corresponds to the sites $j = 1$ and $j = 3$. (They are equal for all times due to the symmetric initial condition.) In both cases, the total excitation number $N = 10$, the nonlinear parameter $\gamma = 0.055$, and the linear coupling coefficient λ_{jk} is unity.

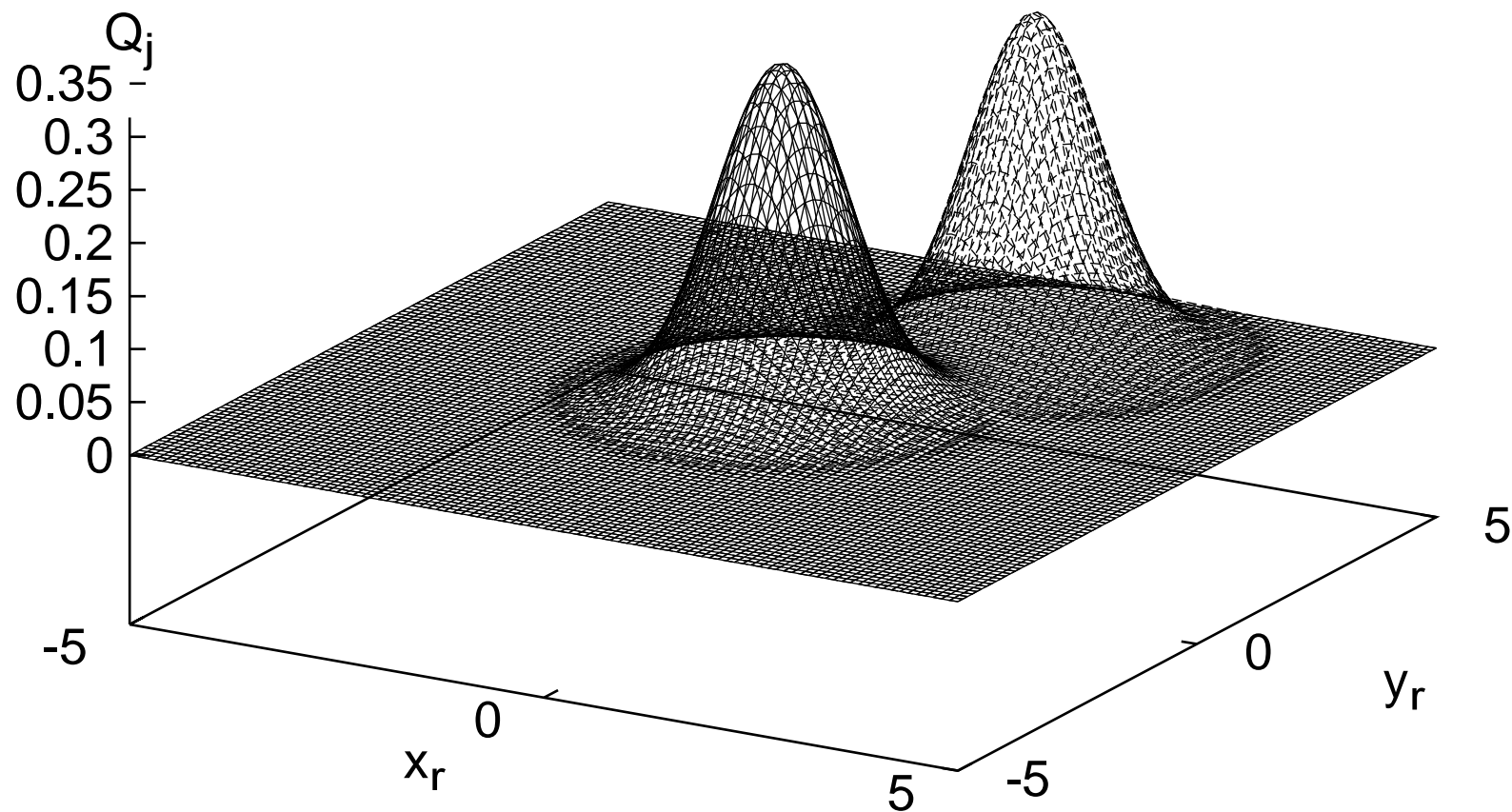
Fig. 2. The trajectories of the centers of the Gaussian bells in Fig. 1 for times $t < 260$. The parameter-values are the same as in Fig. 1. Fig. 2(a,b) (Fig. 2(c,d)) corresponds to sites 1 resp. 2 for the SO (NO) case.

Fig. 3. The Poissonian probability distribution P_n^j from eq. (24) plotted as a function of excitation number n and site index j for the quintic GDST ($m = 3$) with $f = 21$ at the time-instant $t = 50$. Fig. 3(a) shows the case of SO, while (b) corresponds to NO. In both cases, the site $j = 21$ is initially excited, and the total excitation number is $N = 10$. The value of the nonlinear parameter is $\gamma = 0.05$, which gives self-trapping in the SO-equation, but not in the NO-equation.

Fig. 4. The analytic expressions of γ_{cr} eq. (25) for a GDST quantum dimer with quintic nonlinearity (*i.e.* $f = 2, m = 3$) plotted as a function of the total excitation number N for normal (NO) and symmetric (SO) ordering. The value of the linear coupling coefficients is set equal to 1 or to $1/2$ if we consider periodic boundary conditions. We notice that the two γ 's become asymptotically equal for the moderate value of $N = 10$.

(1a)

$j=1,3$ —
 $j=2$ - - -



(1b)

$j=1,3$ ———
 $j=2$ - - - - -

