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Properties of a discretized coherent state representation and the relation to Gabor analysis

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Abstract
Properties of a discretized coherent state representation (DCSR) and its connection to Gabor frame analysis are discussed. The DCSR approach was recently shown (Andersson L M 2001 *J. Chem. Phys.* **115** 1158) to yield a practical computational scheme for quantum dynamics, and an iterative scheme for finding the identity operator was proposed. In the present work, we suggest a proof of fast convergence of the iterative scheme for computing the canonical dual to any given countable frame in a Hilbert space. The method of frames is concerned with the use of a non-orthogonal, over-complete set of functions for expansion of an arbitrary function. We also introduce the concept of 'representations of the identity operator' and show how to expand arbitrary vectors using the frame elements, without explicit diagonalization to an orthonormal basis. Numerical examples that illustrate the method are shown.

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1. Introduction

The aim of this paper is to use a discrete set of Gaussian coherent states as an adaptable and economic way of representing wavefunctions. In a previous work [1], an iterative refinement for computing expansion coefficients was proposed and shown numerically to give a stable way of representing functions using coherent states. Here, we extend to present a proof of convergence of the iterative scheme and generalize to any countable frame. As will be shown, the convergence is very rapid requiring only a few iterations. We give a mathematical foundation to the coherent state representation and present an efficient and practical way to use this set and more general non-orthogonal sets of functions for representing arbitrary functions.

The general question of using non-orthogonal and overcomplete sets to represent vectors is studied using the concept of frames [2]. In the present paper, we connect the discrete coherent state representation to the method of Gabor analysis [3], which builds on frames. Gabor analysis has mostly been applied to signal analysis, but could potentially be of great interest also to the physics community. It is perhaps not unexpected that the question of economic representation of wavefunctions is related to optimal representations of time signals.

In signal analysis the aim is to find suitable expansion coefficients and then reconstruct the signal in a robust way. For Gabor analysis this can be achieved by using a Gaussian windowed Fourier transform to compute Gabor frame coefficients. To reconstruct the signal an inverse Fourier transform with a different window is performed. This window is called a dual window to the Gaussian window, and may in general not be easy to find. To be of use in quantum dynamics it must also be possible to perform various operations *within* the representation, such as scalar products, application of operators, etc. This is where *matrix representations of the identity*, as defined in this paper, become of use. We also show how to economize the computation in the case of coherent states by using phase-space translation properties to construct the entire matrix from a single column. By the use of this, the iterative scheme becomes very efficient computationally.

Coherent states have been of great use in quantum mechanics and especially for quantum optics [4, 5]. Many different types of coherent states exist, but here we consider the Gaussian coherent states. These have, for example, been useful for deriving semi-classical approximations of the propagator due to the 'classical' properties of these space and momentum localized states [6]. One of the motivations for this study is the possibility of using the coherent state representation for solving the time-dependent Schrödinger equation [1, 7, 8].

Previous attempts to use coherent states as a basis set for wavefunctions have solved the problem of non-orthogonality by traditional methods, e.g. singular-value decomposition (SVD) to construct a (pseudo) inverse to the overlap matrix [7]. The problem is the unfavourable scaling of the SVD with respect to the number of coherent states. Also the SVD procedure gives a full matrix whereas the present scheme can give a sparse matrix. Another possibility is to take a dense enough sampling of coherent states [8] in order for the frame operator to be close to the identity operator. This requires about a factor of ten oversampling to reach double precision accuracy, as will be shown.

This paper is organized as follows. In section 2 we review general properties of frames. Section 3 defines frames of coherent states and makes the connection to Gabor frames. Section 4 introduces the iterative method for computing matrix representations of the identity. Phase-space translation properties are studied in section 5 and are shown to reduce the effort needed for performing the iterations. Examples on how to compute operator matrix elements by normal ordering are shown in section 6. Finally, in section 7 we show a few illustrations.

2. Frames

In the following $\mathcal{H}$ denotes a complex separable Hilbert space. The inner product of the Hilbert space is denoted by $\langle\cdot|\cdot\rangle$ and $\|\cdot\| = \sqrt{\langle\cdot|\cdot\rangle}$ denotes the norm. $\mathcal{H}$ can in general be any separable complex Hilbert space, finite-dimensional or infinite-dimensional. In the concrete examples, $\mathcal{H}$ will be the space $L^2(\mathbb{R})$ of square integrable complex-valued functions over the real numbers. A *frame* (see, e.g., [2, 3], and references therein) is a set of vectors $\{|\psi_x\rangle\}_{x\in X}$ with $|\psi_x\rangle \in \mathcal{H}$ and where X is an index set (possibly overcountable), such that

$$A\|\psi\|^2 \leqslant \langle\psi|\hat{Q}|\psi\rangle \leqslant B\|\psi\|^2 \qquad \forall\psi \in \mathcal{H} \tag{1}$$

$$0 < A \leqslant B < \infty \tag{2}$$

where the *frame operator* is defined as $\hat{Q} = \int |\psi_x\rangle\langle\psi_x|\,\mathrm{d}x$. In the following, we will assume that A, B are the optimal frame bounds, i.e. with A the largest and B the smallest numbers fulfilling (1). Here, we will be concerned with *countable frames* for which the index set X is countable. Then the frame operator is defined as

$$\hat{Q} = \sum_k |\psi_k\rangle\langle\psi_k| \tag{3}$$

with each $|\psi_k\rangle \in \mathcal{H}$. (In the case of an infinite number of elements the summation should be interpreted in the sense of strong operator convergence [9].)

Frames admit representation of vectors by superposition,

$$|\chi\rangle = \sum_k |\psi_k\rangle d_k. \tag{4}$$

Note that the vectors that constitute a frame do not need to be orthogonal or normalized. However, the connection between the overlaps, $c_k = \langle\psi_k|\chi\rangle$, and the expansion coefficients, d_k, in the above equation is not straightforward (cf for an orthonormal set where $d_k = c_k$). One complication is that in general the coefficients d_k in (4) are not uniquely determined by $|\chi\rangle$. We seek a simple method of computation of the expansion coefficients.

An especially simple case is if the constants A and B in (2) can be chosen equal,

$$\hat{Q} = A\hat{1} \tag{5}$$

for some $A > 0$, where $\hat{1}$ is the identity operator. Then the frame is a *tight frame*. The special case of tight frames can be seen as a generalization of the concept of bases, in that they can be used for expansion of a state similar to the way bases can. If $\{|\psi_k\rangle\}_k$ is a tight frame (with A given by equation (5)) then

$$|\chi\rangle = \frac{1}{A}\sum_k |\psi_k\rangle\langle\psi_k|\chi\rangle \qquad \forall|\chi\rangle \in \mathcal{H} \tag{6}$$

which follows directly from equation (5). Note that also for tight frames the coefficients d_k in (4) are not uniquely determined by $|\chi\rangle$, and (6) is just one possible choice.

To compute the expansion coefficients for a general frame, the dual frame is introduced. A frame $\{|\widetilde{\psi}_k\rangle\}_k$ is a *dual frame* to $\{|\psi_k\rangle\}_k$ if

$$\sum_k |\widetilde{\psi}_k\rangle\langle\psi_k| = \sum_k |\psi_k\rangle\langle\widetilde{\psi}_k| = \hat{1}. \tag{7}$$

In general there are many dual frames to a given frame. The *canonical dual frame* (or just canonical dual) is defined as

$$|\widetilde{\psi}_k^{\circ}\rangle = \hat{Q}^{-1}|\psi_k\rangle \tag{8}$$

with $\hat{Q}$ being the frame operator. That the frame operator $\hat{Q}$ is invertible was shown in [2]. In essence, the invertibility of $\hat{Q}$ follows from the fact that $\hat{Q}$ is a bounded positive operator with $\hat{Q} \geqslant A\hat{1}$ with $A > 0$. This condition guarantees that the spectrum of $\hat{Q}$ is 'kept away' from zero, which is the problematic point of the inverse. Another important consequence is that the inverse $\hat{Q}^{-1}$ is a bounded operator with $\hat{Q}^{-1} \leqslant A^{-1}\hat{1}$. As seen from equation (7), duals give us a possibility of calculating expansion coefficients in (4) as $d_k = \langle\widetilde{\psi}_k|\chi\rangle$. We will discuss how to practically compute the dual and the expansion coefficients in section 4.

The canonical dual has the special property that if $\{|\psi_k\rangle\}_k$ is a frame, $|\chi\rangle$ is an arbitrary element in $\mathcal{H}$ and $(c_k)_k$ is a sequence of complex numbers such that

$$|\chi\rangle = \sum_k c_k|\psi_k\rangle \tag{9}$$

then

$$\sum_k |c_k|^2 \geqslant \sum_k |\langle \widetilde{\psi}_k^{\circ} | \chi \rangle|^2. \tag{10}$$

For a proof see [2]. Hence, the canonical dual gives us, in this respect, the minimal size of the expansion coefficient vector.

Although definitions (1), (2) give a precise description of what a frame is, it may perhaps be useful to give a short description of the flexibility of the frame concept. The elements of a frame need not be orthogonal to each other, nor do they have to be normalized. They need not be linearly independent. In the case of a frame on a finite-dimensional Hilbert space, the number of frame elements may exceed the dimension of the space (the number of elements may even be infinite). A frame is always a complete set, but every complete set is not a frame. A frame may be overcomplete, which means that an element can be taken away and the set is still complete. In other words, frames are much more flexible objects than complete orthonormal bases. For a review of completeness and of some of the many different versions of definitions of linear independence in infinite-dimensional Hilbert spaces, see [10, 11].

3. Gabor frames and coherent states

In this section, we discuss two types of frames, regular *Gabor frames* and the closely related frames of coherent states. For a recent review on Gabor analysis, see [3].

Given a function $g \in L^2(\mathbb{R})$ we can construct a set of translated and momentum shifted functions

$$g_{m,n}(x) = g(x - na)\,\mathrm{e}^{2\pi \mathrm{i} mbx} \tag{11}$$

where (m, n) are integers and $a, b > 0$ are lattice parameters. The function $g \in L^2(\mathbb{R})$ is called the *Gabor atom*. The set $\{g_{m,n}\}_{m,n}$ forms a regular Gabor set. The word 'regular' refers to the regularity with which we distribute translation and momentum shifts. If the Gabor set is a frame it is called a Gabor frame. A common choice of Gabor atom is a Gaussian function,

$$g(x) = \pi^{-1/4} \exp[-x^2/2] \tag{12}$$

with the width being equal to unity. For a Gabor set to form a frame it is a necessary (but not sufficient) condition that the lattice is sufficiently dense in the phase plane. In the case of regular Gabor frames it has been shown that it is a necessary condition that $ab < 1$ [12, 13] (see [3] for an explanation). In the specific case of regular frames of Gaussian functions it has been shown that $ab < 1$ is both a sufficient and necessary condition for the formation of a frame [14–16].

As for any frame we can define the dual frames and specifically the canonical dual $\widetilde{g}^{\circ}_{m,n} = \hat{Q}^{-1} g_{m,n}$ as given by (8), where $\hat{Q}$ is the frame operator of $\{g_{m,n}\}_{m,n}$. From the properties of Gabor frames one can show [3, 17] that the dual frame $\{\widetilde{g}^{\circ}_{m,n}\}_{m,n}$ can be constructed with translations and momentum shifts as in (11) with the (canonical) dual Gabor atom $\widetilde{g}^{\circ} = \hat{Q}^{-1} g$,

$$\widetilde{g}^{\circ}_{mn}(x) = \widetilde{g}^{\circ}(x - na)\,\mathrm{e}^{2\pi \mathrm{i} mbx}. \tag{13}$$

Now we turn to a frame of coherent states which is very closely related to the Gabor frame with a Gaussian Gabor atom, equation (12). Coherent states for a harmonic oscillator are generated by a displacement of the ground state (see, for example, [18])

$$|\alpha\rangle = \hat{D}(\alpha)|0\rangle = \mathrm{e}^{\alpha \hat{a}^{\dagger} - \alpha^{*} \hat{a}} |0\rangle \tag{14}$$

where $\hat{a}$ and $\hat{a}^\dagger$ are the annihilation and creation operators of the harmonic oscillator. These states constitute a two-parameter (real) family which defines a phase-space (q, p) according to $\alpha = \frac{1}{\sqrt{2}}(q + \mathrm{i}p)$. The scalar product of two such states is given by

$$\begin{aligned}\langle\alpha|\alpha'\rangle &= \exp[-(|\alpha|^2 + |\alpha'|^2)/2 + \alpha^*\alpha'] \\ &= \exp[-(q-q')^2/4 - (p-p')^2/4 + \mathrm{i}(qp' - pq')/2].\end{aligned} \tag{15}$$

The position representation of the coherent state is given by

$$\langle x|\alpha\rangle = \pi^{-1/4}\exp[-(x-q)^2/2 + \mathrm{i}p(x - q/2)]. \tag{16}$$

A discrete set of coherent states can be defined on a phase-space lattice as

$$\{|\alpha_{m,n}\rangle\}_{mn} \qquad \alpha_{m,n} = \frac{1}{\sqrt{2}}(q_n + \mathrm{i}p_m) = \frac{1}{\sqrt{2}}(na + \mathrm{i}2\pi mb) \tag{17}$$

where $a, b > 0$ are lattice parameters and where

$$q_n = an \qquad p_m = 2\pi bm. \tag{18}$$

The Gabor frame (11) with Gaussian atom (12) and the set of coherent states defined by equations (16) and (17), differ only in the choice of phase

$$g_{m,n}(x) = \langle x|\alpha_{m,n}\rangle \exp[\mathrm{i}p_m q_n/2]. \tag{19}$$

Since these two sets differ only in phases it follows that the frame operators for the two sets are the same, and hence the set of coherent states forms a frame if and only if the corresponding Gaussian Gabor frame does. The frame condition can be formulated in terms of the phase-space sampling density

$$D = \frac{1}{ab} = \frac{2\pi}{\Delta q\,\Delta p} \tag{20}$$

where Δq, Δp are the lattice grid separations in position and momentum. Hence the coherent state set (17) is a frame if and only if $D > 1$.

4. Iterative method for calculation of the canonical dual

In the previous paper [1], an iterative method for calculating expansion coefficients of arbitrary vectors in a given frame was introduced for coherent state frames. Here we generalize this method to general countable frames. We will give a sketch of the proof and include some important aspects to understand the properties of the algorithm. For a proof with more technical details considered we refer to [19].

Consider a general countable frame $\{|\psi_j\rangle\}_j$. Similar to the case of complete orthonormal basis we can use frames to represent operators on $\mathcal{H}$ with matrices,

$$\sum_{i,j} |\psi_i\rangle W_{ij}\langle\psi_j| = \hat{W}. \tag{21}$$

As in the case of expansion of vectors in the frame, we have that the matrix W_{ij} is not unique. The matrix element W_{ij} can be computed with

$$W_{ij} = \langle\widetilde{\psi}_i|\hat{W}|\widetilde{\psi}_j\rangle \tag{22}$$

where $\{|\widetilde{\psi}_j\rangle\}_j$ is any dual frame to $\{|\psi_j\rangle\}_j$. Now consider matrix representations of the identity operator. Given a frame $\{|\psi_k\rangle\}_k$ there always exists a matrix with elements F_{ij} such that

$$\sum_{i,j} |\psi_i\rangle F_{ij}\langle\psi_j| = \hat{1}. \tag{23}$$

(For example, $F_{ij} = \langle\tilde{\psi}_i|\tilde{\psi}_j\rangle$.) Hence, the matrix F_{ij} is a representation of the identity operator in the frame. (It is important to note that F_{ij} in general is different from the identity matrix δ_{ij}, and that the identity matrix δ_{ij} is a representation of the identity operator *only* in the cases where the frame operator is the identity operator, i.e. only for a tight frame with $A = 1$.) Such an identity representation matrix F_{ij} can be used to expand an arbitrary vector

$$|\chi\rangle = \sum_{ij} |\psi_i\rangle F_{ij} \langle\psi_j|\chi\rangle. \tag{24}$$

This suggests a very close relation between these representations of the identity operator and dual frames. Indeed, given two dual frames $\{|\widetilde{\psi_k^a}\rangle\}_k$ and $\{|\widetilde{\psi_k^b}\rangle\}_k$ we can construct a representation of the identity operator such as $F_{ij} = \langle\widetilde{\psi_i^a}|\widetilde{\psi_j^b}\rangle$, by the use of equation (7) for each dual frame. This illustrates a point crucial for the understanding of the following derivations, namely that the representation of the identity operator with respect to a frame is, in general, not unique. Among all the representations there is, however, one special representation, which we will call the *canonical identity representation* (or just *canonical representation*) which we define as

$$F_{ij}^{\circ} = \langle\widetilde{\psi}_i^{\circ}|\widetilde{\psi}_j^{\circ}\rangle. \tag{25}$$

Hence, the canonical representation of the identity operator is nothing but the overlap matrix of the canonical dual. As will be seen, the canonical representation is closely related to the iterative scheme discussed below.

The following iterative method to compute a representation of the identity operator was proposed in [1]. It was formulated in terms of the special case of a coherent state frame. Here we will formulate it in terms of general countable frames. Define the sequence of matrices $F_{ij}^{(n)}$ according to

$$\begin{cases} F_{ij}^{(0)} = \delta_{ij} \\ F_{ij}^{(n+1)} = 2F_{ij}^{(n)} - \sum_{k,l} F_{ik}^{(n)} \langle\psi_k|\psi_l\rangle F_{lj}^{(n)}. \end{cases} \tag{26}$$

We will show that this iterative scheme gives a sequence of matrices $F_{ij}^{(n)}$ that yield better and better approximations of a representation of the identity operator. Suppose that we have a matrix F_{ij}^{appr} that gives an approximation to a representation of the identity operator. This approximate representation can be used, as in (24), to give an approximate expansion of an arbitrary vector of the Hilbert space. A reasonable choice of error measure would be the norm of the difference between the approximately expanded vector and the original vector and find the vector that gives the maximum error (among the normalized vectors). The maximal error is then

$$\begin{aligned} \mathrm{err}(F^{\mathrm{appr}}) &= \sup_{\|\chi\|=1} \left\| |\chi\rangle - \sum_{ij} |\psi_i\rangle F_{ij}^{\mathrm{appr}} \langle\psi_j|\chi\rangle \right\| \\ &= \left\| \hat{1} - \sum_{ij} |\psi_i\rangle F_{ij}^{\mathrm{appr}} \langle\psi_j| \right\| \end{aligned} \tag{27}$$

where $\|\cdot\|$ in the second line denotes the standard operator norm

$$\|\hat{W}\| = \sup_{\|\chi\|=1} \|\hat{W}|\chi\rangle\|. \tag{28}$$

As seen, the same symbol $\|\cdot\|$ will be used both for the norm of vectors in a Hilbert space and for the operator norm of operators on a Hilbert space. Which one is intended is determined by the object it acts on. Since the sequence of approximations produced by (26) is to be used for expansions of arbitrary vectors, a suitable criterion of convergence of (26) is whether or not $\mathrm{err}(F^{(n)})$ goes to zero. Hence, it is not really important whether these matrices themselves converge to a *specific* representation of the identity operator, but whether or not the error measure goes to zero. In a sense we could say that we are satisfied that the sequence $F_{ij}^{(n)}$ converges to the *set* of representations of the identity operator.

With the convergence criterion established we may now proceed to prove that (26) indeed gives better and better expansions. We define the operators

$$\hat{Q}_n = \sum_{i,j} |\psi_i\rangle F_{ij}^{(n)} \langle\psi_j|. \tag{29}$$

Note that $\hat{Q}_0$ is the frame operator $\hat{Q}$ in (3). By combining (29) with (26) we obtain

$$\hat{Q}_{n+1} = 2\hat{Q}_n - \hat{Q}_n^2. \tag{30}$$

With our error measure (27) in mind we define the nth error operator as

$$\hat{R}_n = \hat{1} - \hat{Q}_n \tag{31}$$

and obtain from (30)

$$\hat{R}_{n+1} = \hat{R}_n^2 = \hat{R}_0^{2^{n+1}}. \tag{32}$$

Hence

$$\mathrm{err}(F^{(n)}) = \|\hat{R}_n\| = \left\|\hat{R}_0^{2^n}\right\| = \|\hat{R}_0\|^{2^n}. \tag{33}$$

It should be noted that in the last equality we have used the fact that $\hat{R}_0$ is a bounded self-adjoint operator. For a general bounded operator $\hat{T}$ holds $\|\hat{T}^n\| \leqslant \|\hat{T}\|^n$, but for bounded self-adjoint operators the equality always holds [19]. Hence the *logarithm* of the error decreases in an *exponential* fashion, if $\|\hat{R}_0\| < 1$. It is not difficult to realize that this is true if and only if the upper frame bound is strictly less than 2. (The requirement that the lower frame bound should be strictly larger than zero is already met, since we have a frame.)

To summarize we have shown that the iterative scheme given by (26) gives a good approximation of a representation of the identity operator very quickly. In the following, we will show stronger results, namely that with the aid of this algorithm we are able to generate approximations to the *canonical* dual and the *canonical* representation of the identity operator.

Define the sequence of vectors

$$\left|\psi_j^{(n)}\right\rangle = \sum_i |\psi_i\rangle F_{ij}^{(n)}. \tag{34}$$

We will now show that if $F_{ij}^{(n)}$ is calculated as described in (26), then $\left|\psi_j^{(n)}\right\rangle$ converge to $|\widetilde{\psi}_j^{\circ}\rangle$ for each j. Hence, the iterative scheme in (26), together with (34), will generate successive approximations to the canonical dual. With $\hat{Q}_n$ defined as in (29), by (34) we have

$$\hat{Q}_n = \sum_j \left|\psi_j^{(n)}\right\rangle\langle\psi_j| \tag{35}$$

and $\left|\psi_j^{(0)}\right\rangle = |\psi_j\rangle$. When combining (34) and (26) we obtain

$$\left|\psi_j^{(n+1)}\right\rangle = 2\left|\psi_j^{(n)}\right\rangle - \sum_k \left|\psi_k^{(n)}\right\rangle\left\langle\psi_k\middle|\psi_j^{(n)}\right\rangle. \tag{36}$$

Using (35) we can rewrite this as

$$\left|\psi_j^{(n+1)}\right\rangle = (2\hat{1} - \hat{Q}_n)\left|\psi_j^{(n)}\right\rangle = \left(\hat{1} + \hat{R}_0^{2^n}\right)\left|\psi_j^{(n)}\right\rangle \tag{37}$$

where we, in the last equality, have made use of (32). Hence

$$\left|\psi_j^{(n)}\right\rangle = \prod_{m=0}^{n-1}\left(\hat{1} + \hat{R}_0^{2^m}\right)|\psi_j\rangle. \tag{38}$$

This operator product is possible to write in a closed form using the product limit for complex numbers [20],

$$\lim_{n\to\infty}\prod_{m=0}^{n-1}\left(1 + z^{2^m}\right) = \frac{1}{1-z} \qquad |z| < 1 \quad z \in \mathbb{C}. \tag{39}$$

Then follows for the operator product (for a proof, see [19])

$$\lim_{n\to\infty}\prod_{m=0}^{n-1}\left(\hat{1} + \hat{R}_0^{2^m}\right) = (\hat{1} - \hat{R}_0)^{-1} = \hat{Q}_0^{-1}. \tag{40}$$

For the above convergence to hold it is necessary that the spectrum of $\hat{R}_0$ is within an interval $[c, d]$ with $-1 < c \leqslant d < 1$. This is translated to the requirement that the upper frame bound of $\{|\psi_k\rangle\}_k$ should be strictly less than 2. By combining (38) and (40) we have

$$\lim_{n\to\infty}\left|\psi_j^{(n)}\right\rangle = \hat{Q}_0^{-1}|\psi_j\rangle = |\widetilde{\psi}_j^{\circ}\rangle. \tag{41}$$

Hence, the iterative scheme (26) together with (34) gives a scheme that converges to the canonical dual of $\{|\psi_k\rangle\}_k$.

Now we turn to the sequence of matrices $F_{ij}^{(n)}$ themselves. As we have argued, the question of whether this sequence converges element-wise or not, is not really important for the use of these matrices. At the present stage of investigation, we do not know whether this sequence does converge or not, although there are numerical indications that it does not. However, we will now show that from the sequence $F_{ij}^{(n)}$ created by (26), we may construct another sequence of matrices $G_{ij}^{(n)}$ that converge to the canonical representation of the identity operator F_{ij}°. We define

$$G_{ij}^{(n)} = \left\langle\psi_i^{(n)}\middle|\psi_j^{(n)}\right\rangle = \sum_{kl} F_{ik}^{(n)}\langle\psi_k|\psi_l\rangle F_{lj}^{(n)}. \tag{42}$$

By the just established fact that $\left|\psi_j^{(n)}\right\rangle$ converge to the canonical dual element $|\widetilde{\psi}_j^{\circ}\rangle$ it follows that $G_{ij}^{(n)}$ converge element-wise to the canonical representation F_{ij}° as n goes to infinity.

4.1. Prescaling of the frame

As the previous demonstrations have shown, the iterative scheme converges if the upper frame bound is strictly less than 2. This is a quite trivial restriction because of the following reason: if $\{|\psi_k\rangle\}_k$ is a frame with frame bounds A, B and if $r > 0$ then $\{\sqrt{r}|\psi_k\rangle\}_k$ is a frame with frame bounds rA, rB. Hence, if we have a frame with upper frame bound larger than or equal to 2 we can trivially construct a new frame with upper frame bound less than 2 simply by multiplying all the frame elements with a sufficiently small number. If we accept the error measure $\mathrm{err}(F^{(n)})$, we realize from (33) that the speed of convergence is determined by the size of $\|\hat{R}_0\|$. The smaller this norm gets the faster the error bounds shrink. This tells us that we can gain in convergence speed of the iterative scheme by first multiplying the elements of the given frame with a positive number $\sqrt{r}$. We call this procedure *prescaling* of the frame. Among all these scaled frames we may find an optimal r that makes $\|\hat{1} - r\hat{Q}\|$ as small as possible. We wish to solve the minimization problem

$$w_{\min} = \min_{r>0}\|\hat{1} - r\hat{Q}\| \tag{43}$$

where $\hat{Q}$ is the frame operator of the given frame. For a bounded, self-adjoint operator $\hat{W}$ holds [9]

$$\|\hat{W}\| = \max(|m|, |M|) \tag{44}$$

where

$$m = \inf_{\|\chi\|=1} \langle\chi|\hat{W}|\chi\rangle \qquad M = \sup_{\|\chi\|=1} \langle\chi|\hat{W}|\chi\rangle. \tag{45}$$

Here m and M are the optimal lower and upper bounds of $\hat{W}$. The frame operator is a bounded self-adjoint operator and it is not difficult to realize that $m = A$ and $M = B$, by comparing with (1) and (2). Hence $\|\hat{Q}\| = B$. Moreover, one realizes that

$$\|\hat{1} - r\hat{Q}\| = \max(|1 - rA|, |1 - rB|). \tag{46}$$

With (46) and (43) we can write

$$\min_{r>0} \|\hat{1} - r\hat{Q}\| = \min_{r>0} \max(|1 - rA|, |1 - rB|). \tag{47}$$

Using $0 < A \leqslant B$ we have

$$\max(|1 - rA|, |1 - rB|) = \begin{cases} 1 - rA & r \leqslant \frac{2}{A+B} \\ rB - 1 & r \geqslant \frac{2}{A+B} \end{cases}. \tag{48}$$

By this

$$w_{\min} = \min_{r>0} \|\hat{1} - r\hat{Q}\| = \frac{B - A}{B + A} \tag{49}$$

and this minimum is obtained at

$$r = r_{\min} = \frac{2}{A + B}. \tag{50}$$

We call the minimal value (49) the *essential tightness* of the frame. Hence given a frame with frame bounds A, B we precondition the frame by multiplying the frame elements with $\sqrt{r_{\min}}$ (which is the same as dividing the frame operator with the average of the upper and lower frame bounds). We say that the frame is *optimally prescaled* if the norm of the operator R_0 is equal to the essential tightness. We note that due to $A > 0$ we have that $1 > w_{\min}$ and $B \geqslant A$ leads to $w_{\min} \geqslant 0$ with equality if and only if the frame is tight.

In summary, the algorithm (26) works if the frame is sufficiently tight, i.e. if the upper frame bound is strictly less than 2. By multiplying the frame with a sufficiently small positive number we can always get the iterative scheme to work. Among all these trivially different frames the optimally prescaled frame is the one that gives the fastest convergence. To make a frame optimally prescaled requires knowledge of the frame bounds. In many cases it can be a very difficult task to get the frame bounds and one must be satisfied with estimates. But to get the iterative scheme to converge (but perhaps not in the fastest way) it is sufficient to multiply the frame elements with $\sqrt{2/B_{\mathrm{est}}}$, where B_{est} is a (strict) *upper* estimate of the upper frame bound.

5. Phase-space translations

We have seen that the canonical representation, F°_{ij}, of the identity operator can be used to expand arbitrary vectors in the frame. If this is to be used as a numerical method in practice we must have an efficient method for computing and using F°_{ij}. In this section, we study translation properties of Gabor frames and coherent state frames, which are especially appealing from the computational point of view.

Let $\{|g_{m,n}\rangle\}_{m,n}$ be a regular Gabor frame with lattice constants a, b as in (11). Using equation (11) gives for the overlap matrix

$$\langle g_{m+k,n+l}|g_{m'+k,n'+l}\rangle = \langle g_{m,n}|g_{m',n'}\rangle\, \mathrm{e}^{2\pi \mathrm{i}ab(m'-m)l}. \tag{51}$$

This is, as a special case, true for the Gabor frame with a Gaussian Gabor atom (12). This should be compared with the corresponding expression for the coherent states, as defined in equations (16) and (17),

$$\langle \alpha_{m+k,n+l}|\alpha_{m'+k,n'+l}\rangle = \langle \alpha_{m,n}|\alpha_{m',n'}\rangle\, \mathrm{e}^{\mathrm{i}\pi ab((m'-m)l-(n'-n)k)} \tag{52}$$

which can be derived either directly from the definition of this frame, (16) and (17), or from (51) and the expression for the phase difference (19). From (13) it follows that the overlap matrix of the canonical duals of the Gabor frame $\langle \widetilde{g}^{\circ}_{m,n}|\widetilde{g}^{\circ}_{m',n'}\rangle$ has the same translation properties (51) as the overlap matrix $\langle g_{m,n}|g_{m',n'}\rangle$. As discussed in section 3, both the Gaussian Gabor frame and the corresponding frame of coherent states have the same frame operator. By the definition of the canonical dual (8) the same phase relation as in (19) follows

$$|\widetilde{g}^{\circ}_{m,n}\rangle = |\widetilde{\alpha}^{\circ}_{m,n}\rangle\, \mathrm{e}^{\mathrm{i}p_m q_n/2}. \tag{53}$$

Hence it follows that the coherent state canonical dual frame has the phase-space translation property

$$\langle \widetilde{\alpha}^{\circ}_{m+k,n+l}|\widetilde{\alpha}^{\circ}_{m'+k,n'+l}\rangle = \langle \widetilde{\alpha}^{\circ}_{m,n}|\widetilde{\alpha}^{\circ}_{m',n'}\rangle\, \mathrm{e}^{\mathrm{i}\pi ab((m'-m)l-(n'-n)k)}. \tag{54}$$

In the rest of this section we will concentrate on the frame of coherent states $\{|\alpha_{m,n}\rangle\}_{m,n}$. For the sake of notational simplicity we introduce a collective index $i = (m, n)$ and denote the set of coherent states as $\{|\alpha_i\rangle\}_i$, with $q_i = q_n$ and $p_i = p_m$. Using this collective index, we rewrite equation (54) by inserting $k = -m'$, $l = -n'$ and letting $j = (m', n')$ to finally get

$$F^{\circ}_{i,j} = F^{\circ}_{i-j,0}\, \mathrm{e}^{\mathrm{i}(p_j q_i - p_i q_j)/2}. \tag{55}$$

Hence, given a row (or a column) of the canonical representation we can reconstruct the whole matrix. (Note that we say 'row' in spite of the fact that this 'row' due to the collective index actually is a matrix. The whole 'matrix' F° is a four-dimensional array.)

Now we use these translation properties of the coherent states to simplify the calculations in the iterative procedure described in section 4. What we want to show is that in the case of a frame of coherent states, the iterative procedure described by (26) can be simplified in that we never need the whole matrix $F^{(n)}_{ij}$, but only one row of it. The overlap matrix $S_{i,j} = \langle \alpha_i|\alpha_j\rangle$ have the same translation property as in (55); moreover, the identity matrix δ_{ij} (to be interpreted as $\delta_{n,n'}\delta_{m,m'}$) trivially possesses the same translation property. It is, moreover, possible to show (by direct calculation) that if two matrices possess this translation property, then both their sum and their product possess the same translation property (with the same phase factors). By induction we can now show that each matrix $F^{(n)}$ in the sequence defined by (26) has the translation property. This makes the following reformulation of (26) possible in the case of a frame of coherent states

$$\begin{cases} F^{(0)}_{i,0} = \delta_{i0} r \\ F^{(n+1)}_{i,0} = 2F^{(n)}_{i,0} - \sum_{j,k} F^{(n)}_{i-j,0} F^{(n)}_{k,0}\, \mathrm{e}^{\frac{\mathrm{i}}{2}\phi_{i,j,k} - \frac{1}{4}((q_j-q_k)^2+(p_j-p_k)^2)} \end{cases}$$
$$\phi_{i,j,k} = p_j q_i - p_i q_j + q_j p_k - p_j q_k \tag{56}$$

where r is the prescaling factor. To derive this we made use of the expression for the coherent state overlap matrix (15). The fact that we in this way can restrict the computation to a single column of the $F^{(n)}$ matrix means a very large saving in both memory needed and the number of operations needed in the computation.

6. Useful expressions

In this section, we list a series of useful expressions in order to facilitate the practical use of the representation. For the sake of simplicity, we will assume throughout this section that the frames used are the frames of coherent states and that the representation of identity used is the canonical representation, although some of the rules to a varying degree can be generalized to more general frames and more general representations of the identity. The canonical representation of the identity F°_{ij} gives a method to compute the canonical expansion coefficients f_i in $|\chi\rangle = \sum_i |\alpha_i\rangle f_i$, given the overlap coefficients $c_j = \langle\alpha_j|\chi\rangle$, via the equation

$$f_i = \sum_j F^{\circ}_{ij} c_j. \tag{57}$$

If one wishes to perform computations within the representation that the frame provides, it is important to express standard manipulations as scalar products and application of operators. Consider c_i and c'_j to be the overlap coefficients of $|\chi\rangle$ and $|\psi\rangle$ respectively, then the scalar product is computed as

$$\langle\chi|\psi\rangle = \sum_{ij} c^*_i F^{\circ}_{ij} c'_j. \tag{58}$$

Suppose now that the vectors are related via application of an operator $\hat{A}$ as $|\psi\rangle = \hat{A}|\chi\rangle$, and that $\hat{A}$ has the matrix elements $A_{ij} = \langle\alpha_i|\hat{A}|\alpha_j\rangle$ then the relation between the overlap coefficients becomes

$$c'_j = \sum_k A_{jk} F^{\circ}_{ki} c_i. \tag{59}$$

In general, the matrix elements A_{ij} must be computed by numerical quadrature. However, in the cases when the operator $\hat{A}$ can be written as $\hat{A} = A(\hat{a}^\dagger, \hat{a})$, where A is a function possible to express in series expansion, we can find analytic expressions for the matrix elements $\langle\alpha_i|A(\hat{a}^\dagger, \hat{a})|\alpha_j\rangle$, cf [8]. For such operators

$$\langle\alpha_i|A(\hat{a}^\dagger, \hat{a})|\alpha_j\rangle = \langle\alpha_i|\alpha_j\rangle A_{\mathrm{ord}}(\alpha^*_i, \alpha_j) \tag{60}$$

where $A_{\mathrm{ord}}(\hat{a}^\dagger, \hat{a})$ is $A(\hat{a}^\dagger, \hat{a})$ written in a normal ordered form. That is, we rewrite $A(\hat{a}^\dagger, \hat{a})$ using commutation relations, such that it only contains summands where in each summand all annihilation operators stand to the left of the creation operators. As an example consider

$$\hat{A} = \hat{a} + \hat{a}^2\hat{a}^\dagger. \tag{61}$$

Using the commutation relation $[\hat{a}, \hat{a}^\dagger] = \hat{1}$ this can be written in the normal order

$$\hat{A} = 3\hat{a} + \hat{a}^\dagger\hat{a}^2 \tag{62}$$

and hence

$$\langle\alpha_i|\hat{A}|\alpha_j\rangle = \langle\alpha_i|\alpha_j\rangle\left(3\alpha_j + \alpha^*_i\alpha^2_j\right). \tag{63}$$

Using the normal ordering we can derive the following expressions for the matrix elements of powers of the position and of the momentum operator. The higher powers are expressed in terms of recursion relations. Define

$$X^{(n)}_{ij} = \langle\alpha_i|\hat{x}^n|\alpha_j\rangle \qquad P^{(n)}_{ij} = \langle\alpha_i|\hat{p}^n|\alpha_j\rangle. \tag{64}$$

By using $\hat{x} = \frac{1}{\sqrt{2}}(\hat{a}^\dagger + \hat{a})$ and $\hat{p} = \frac{\mathrm{i}}{\sqrt{2}}(\hat{a}^\dagger - \hat{a})$ follows

$$\begin{cases} X^{(1)}_{ij} = \frac{1}{\sqrt{2}}(\alpha^*_i + \alpha_j)S_{ij} \\ X^{(2)}_{ij} = \frac{1}{2}(1 + (\alpha^*_i + \alpha_j)^2)S_{ij} \\ X^{(n)}_{ij} = \frac{1}{\sqrt{2}}(\alpha^*_i + \alpha_j)X^{(n-1)}_{ij} + \frac{n-1}{2}X^{(n-2)}_{ij} \end{cases} \tag{65}$$

$$\begin{cases} P_{ij}^{(1)} = \frac{\mathrm{i}}{\sqrt{2}}(\alpha_i^* - \alpha_j)S_{ij} \\ P_{ij}^{(2)} = \frac{1}{2}(1 - (\alpha_i^* - \alpha_j)^2)S_{ij} \\ P_{ij}^{(n)} = \frac{\mathrm{i}}{\sqrt{2}}(\alpha_i^* - \alpha_j)P_{ij}^{(n-1)} + \frac{n-1}{2}P_{ij}^{(n-2)} \end{cases} \tag{66}$$

where

$$S_{ij} = \langle \alpha_i | \alpha_j \rangle \qquad \alpha_i = \frac{1}{\sqrt{2}}(q_i + \mathrm{i}p_i). \tag{67}$$

Potentials that can be expressed as a sum of exponentials can also be put in a normal form in a straightforward way. One such example which has relevance for molecular physics is the Morse potential [21]

$$V(x) = 1 + \mathrm{e}^{-2\beta(x-x_0)} - 2\mathrm{e}^{-\beta(x-x_0)} \tag{68}$$

where x_0 and β are parameters. The operator $V(\hat{x})$ can be put in normal order by the use of the Campbell–Baker–Hausdorff theorem, see e.g. [5], which states that if $[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0$ then

$$\mathrm{e}^{s(\hat{A}+\hat{B})} = \mathrm{e}^{s\hat{B}}\,\mathrm{e}^{s\hat{A}}\,\mathrm{e}^{\frac{1}{2}s^2[\hat{A},\hat{B}]} \tag{69}$$

for any real number s. By this

$$\begin{aligned} V(\hat{x}) &= \hat{1} + \mathrm{e}^{2\beta x_0}\,\mathrm{e}^{-\sqrt{2}\beta(\hat{a}+\hat{a}^\dagger)} - 2\,\mathrm{e}^{\beta x_0}\,\mathrm{e}^{-\frac{1}{\sqrt{2}}\beta(\hat{a}+\hat{a}^\dagger)} \\ &= \hat{1} + \mathrm{e}^{2\beta x_0+\beta^2}\,\mathrm{e}^{-\sqrt{2}\beta\hat{a}^\dagger}\mathrm{e}^{-\sqrt{2}\beta\hat{a}} - 2\,\mathrm{e}^{\beta x_0+\frac{1}{4}\beta^2}\,\mathrm{e}^{-\frac{1}{\sqrt{2}}\beta\hat{a}^\dagger}\,\mathrm{e}^{-\frac{1}{\sqrt{2}}\beta\hat{a}} \end{aligned} \tag{70}$$

where the last line is normal ordered. Hence

$$V_{ij} = \langle \alpha_i | V(\hat{x}) | \alpha_j \rangle = S_{ij}\left[1 + \mathrm{e}^{2\beta x_0+\beta^2-\sqrt{2}\beta(\alpha_i^*+\alpha_j)} - 2\mathrm{e}^{\beta x_0+\frac{1}{4}\beta^2-\frac{1}{\sqrt{2}}\beta(\alpha_i^*+\alpha_j)}\right]. \tag{71}$$

7. Some illustrations

Here, we give some examples of the use of frames of coherent states, i.e. the discretized coherent state representation. For all the examples presented we have used a symmetric phase-space sampling with $\Delta q = \Delta p$, which have turned out to be the most efficient in terms of convergence. The convergence of the iterative scheme for computing the expansion coefficients is shown in figure 1, and confirms the very rapid decay of the representation error. The test vector used was a squeezed Gaussian centred on an arbitrary position in phase-space, but identical results are obtained for all functions that are sufficiently supported on the selected phase-space grid points. Also a similar convergence of the canonical dual defined from (34) was found. In order to have a frame and to get convergence of the iterative scheme the density D has to be larger than one. However, only a slight oversampling is necessary, e.g. $D = 1.2$ gives convergence to double precision in five iterations. In practice, it is found that using $r = 1/D$ as a prescaling in equation (56) gives good convergence speeds. As can be inferred from the figure, the frame operator becomes the identity operator for sufficiently dense sampling, e.g. for $D = 10$ the error is down to 10^{-13}. But this large oversampling means a tenfold increase in the number of expansion coefficients necessary for representing a given function.

The canonical matrix representation of the identity, F_{ij}°, is localized around the diagonal, and the magnitude decreases away from the diagonal, i.e. with increasing phase-space distance. In figure 2, we show the row $F_{i,0}^{\circ}$, which is real valued, as a function of the phase-space position (q_i, p_i). In practical computations we truncate the row at a specified distance from the origin, i.e. far off-diagonal elements are put to zero.

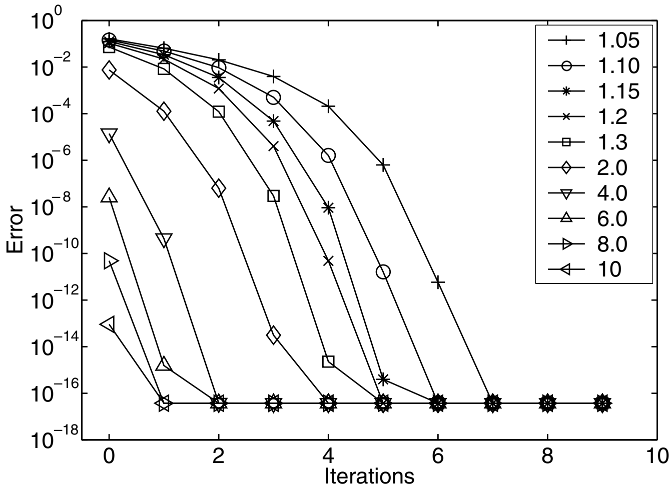

Figure 1. Convergence of iterative scheme for different sampling densities D. The representation error $\||\psi_{\text{expanded}}\rangle - |\psi_{\text{exact}}\rangle\|$ of a test vector is shown. Note the fast convergence even for only minor oversampling. The zero iteration error represents the error in the frame operator as compared to identity.

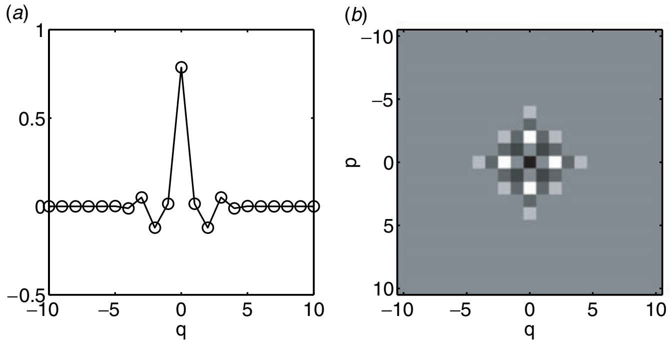

Figure 2. One row F°_{i0} of the canonical matrix representation of the identity for a density of $D = 1.2$. In (*b*) the elements are shown as a function of phase-space position (q_i, p_i), in units of Δq and Δp resp. Black is positive and white is negative. In (*a*) the values are given for the line $p_i = 0$. Note the symmetry which is due to the symmetric sampling of the phase-space.

Two examples of functions that may arise in molecular context are eigenstates in the Morse [21] and the Rosen–Morse [22] potentials. In figure 3, the wavefunctions for the $n = 40$ eigenstate, close to the dissociation limit, are shown together with the magnitude of the overlap coefficients as a function of the phase-space position.

8. Summary

In an earlier investigation a numerical method for calculating representations of arbitrary quantum states in frames of coherent states was presented. This was motivated by the goal of developing a compact and fast technique for state propagation in realistic models of molecular systems. In this investigation, we have formalized this method in terms of frames and specifically in terms of frames of coherent states and the closely related Gabor frames, which

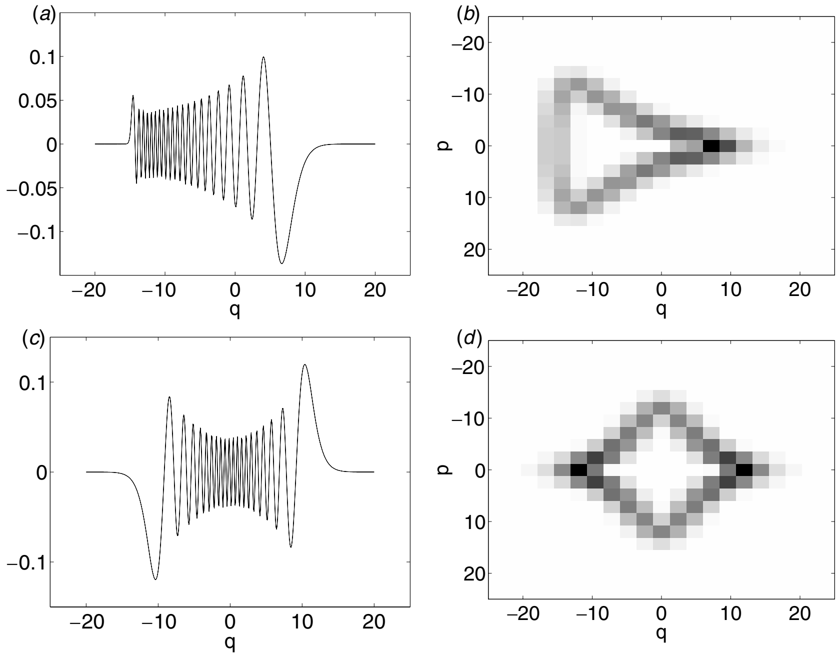

Figure 3. (*a*) and (*b*) The $n = 40$ eigenstate in a Morse potential ($D = 1.2$). (*c*) and (*d*) The $n = 40$ eigenstate in a symmetric Morse potential ($D = 1.2$). In (*a*) and (*c*) the position representations are shown and in (*b*) and (*c*) the discretized coherent state representations are shown. The magnitudes of the complex overlap coefficients are shown with white being zero and increasing values as darker shades.

have been used in the context of signal analysis. In this setting, we have presented an overview of a proof of the iterative method and have confirmed the high convergence rate that the earlier numerical experiments indicated. We have shown that the iterative method is not limited to frames of coherent states and Gabor frames, but can be applied to any countable frame on a complex separable Hilbert space, after a prescaling of the frame. Moreover, we have shown that in the special case of regular frames of coherent states, certain phase-space translation properties can reduce the computational and memory needs. The iterative scheme might also be of use in Gabor analysis as a tool for computing dual windows.

For future use and to facilitate applications of this method we have also demonstrated some simple but important rules how to make calculations within the coherent state representation. We have shown with examples and explicit formulae that many operators which can be written as combinations of creation and annihilation operators (e.g. position and momentum operators) have matrix elements, in the coherent state representation, that can be calculated analytically by the use of normal ordering and hence are straightforward to implement in numerical calculations. Finally, we have presented some examples to give a feeling for the 'phase-space picture' of quantum mechanics that the coherent state frames provide and how this can be used for efficient and flexible representations of wavefunctions.

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