

Coherent states

Rocco Martinazzo

E-mail: rocco.martinazzo@unimi.it

Contents

1	Introduction	1
2	Definition	2
3	Basic properties	3
3.1	Relation to harmonic oscillators	3
3.2	Creation operators for coherent states	4
3.3	Completeness relation	6
3.4	Derivatives	7
4	Time-evolution	7
4.1	Harmonic oscillator	7
4.2	Shifted harmonic oscillator	8

1 Introduction

In these notes we introduce the coherent states and show their main properties. The discussion is based on the results contained in the book of Craig and Thirunamachandran [1] and various papers by Shalashilin and Child [2, 3, 4, 5], who have developed a coherent-state based method for quantum dynamics, the so-called Coupled Coherent States method. The method has been successfully applied to a variety of problems [6, 7, 8, 9]. Relations to semiclassical propagation and real-time path-integral dynamics have also been discussed [10, 5]. More recent applications of coherent states can be found in Ref.[11, 12, 13].

2 Definition

Application of the Schwartz inequality to the basic coordinate-momentum commutator relationship

$$i\hbar = \langle \psi | [x - x_0, p - p_0] | \psi \rangle = 2i \text{Im} \langle (x - x_0)\psi | (p - p_0)\psi \rangle$$

$$\begin{aligned} \frac{\hbar}{2} &= \text{Im} \langle (x - x_0)\psi | (p - p_0)\psi \rangle \\ &\leq | \langle (x - x_0)\psi | (p - p_0)\psi \rangle | \\ &\leq \| (x - x_0)\psi \| \| (p - p_0)\psi \| \end{aligned}$$

when x_0 and p_0 are the average position and momentum, respectively, gives rise to the well-known Heisenberg uncertainty principle, since in that case $\| (x - x_0)\psi \| = \Delta x$ and analogously for Δp . The equality sign in the above equation holds, if and only if,

$$(p - p_0) | \psi \rangle = \alpha (x - x_0) | \psi \rangle$$

where α is a complex number ($\text{Re}\alpha = 0$) related to the coordinate spreading of the state $\langle (x - x_0)\psi | (p - p_0)\psi \rangle = \Delta x^2 \alpha = i\hbar/2$. The above equation may be rewritten in terms of Δx and Δp (which are to be considered as parameters satisfying the minimum uncertainty $\Delta x \Delta p = \hbar/2$)

$$\left\{ \frac{x}{2\Delta x} + i \frac{p}{2\Delta p} \right\} | \psi \rangle = \left\{ \frac{x_0}{2\Delta x} + i \frac{p_0}{2\Delta p} \right\} | \psi \rangle$$

or, introducing the *annihilation* operator

$$a = \left\{ \frac{x}{2\Delta x} + i \frac{p}{2\Delta p} \right\}$$

also in the form

$$(a - z) | \psi \rangle = 0$$

The solution vectors of this eigenvalue equation define the set of *coherent states* of coordinate width Δx . The eigenvalues z map the complex plane into the classical phase-space of the system, through the mean values of the position and momentum observables,

$$x_0 = 2\Delta x \text{Re}z \text{ and } p_0 = 2\Delta p \text{Im}z$$

Explicit expressions for the coherent states can be obtained by integrating the above equation in coordinate representation,

$$-i\hbar \frac{d\psi}{dx} = \left\{ i \frac{\hbar}{2\Delta x^2} (x - x_0) + p_0 \right\} \psi$$

to get the (normalized) function

$$\psi(x) = \left(\frac{1}{2\pi\Delta x^2} \right)^{1/4} e^{-\frac{(x-x_0)^2}{4\Delta x^2} + i \frac{p_0(x-x_0)}{\hbar}}$$

3 Basic properties

3.1 Relation to harmonic oscillators

The operator a defined above (with $\Delta x \Delta p = \hbar/2$) and its adjoint a^\dagger can be used to re-write the Harmonic Oscillator (HO) hamiltonian

$$H^{HO} = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$$

once $x = 2\Delta x \text{Re}a$ and $p = 2\Delta p \text{Im}a$ have been inserted and Δx has been related to the HO frequency using the virial theorem and the known ground-state energy

$$\epsilon_0 = \frac{\hbar\omega}{2} = 2 \langle V \rangle_0 = m\omega^2 \Delta x^2$$

The well-known result is

$$H^{HO} = \frac{\hbar\omega}{2} (aa^\dagger + a^\dagger a) = \hbar\omega (a^\dagger a + \frac{1}{2})$$

where use has been made of

$$[a, a^\dagger] = 1$$

The operators a, a^\dagger allow one to readily obtain the eigenvalues and eigenvectors of this hamiltonian. Indeed, let $|\epsilon\rangle$ be an eigenvector of H^{HO} with eigenvalue ϵ . From the above commutation relation follows

$$H^{HO} a^\dagger |\epsilon\rangle = (\epsilon + \hbar\omega) a^\dagger |\epsilon\rangle$$

that is, $a^\dagger |\epsilon\rangle$ is eigenvector of H^{HO} with the eigenvalue $(\epsilon + \hbar\omega)$. With the same token, using the adjoint of $H^{HO} a^\dagger = (\epsilon + \hbar\omega) a^\dagger$, it follows that $a |\epsilon\rangle$ is eigenvector of H^{HO} with eigenvalue $(\epsilon - \hbar\omega)$. Now, since the energy spectrum is bound from below,

$$\langle H^{HO} \rangle \geq \frac{\hbar\omega}{2}$$

the eigenvalues must have the form

$$\epsilon_n = \hbar\omega(n + \frac{1}{2}) \text{ with } n \in \mathbb{N}$$

and

$$a |0\rangle = 0$$

where $|0\rangle$ is the eigenvector with $n = 0$ (i.e. eigenvalue $\hbar\omega/2$). The last equation determines the ground-state eigenvector of the HO hamiltonian and identifies it as a coherent state with $x_0 = 0$ and $p_0 = 0$. Excited-state eigenvectors can be obtained by repeated application of a^\dagger ,

$$|n\rangle \propto (a^\dagger)^n |0\rangle$$

The proportionality constant follows from the normalization condition applied to

$$|n+1\rangle = \lambda a^\dagger |n\rangle$$

when the phase has been fixed such that

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

holds. Analogously,

$$a |n\rangle = \sqrt{n} |n-1\rangle$$

Thus,

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle \quad (1)$$

The above expression for the complete set of eigenvectors of H^{HO} can be used to expand the coherent states in terms of HO eigenstates,

$$\begin{aligned} |z\rangle &= \sum_{n=0}^{\infty} |n\rangle \langle n|z\rangle = \sum_{n=0}^{\infty} |n\rangle \langle 0| \frac{a^n}{\sqrt{n!}} |z\rangle \\ &= \langle 0|z\rangle \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle \end{aligned}$$

where the coefficient $\langle 0|z\rangle$ may be fixed, apart from an irrelevant phase factor, by the normalization condition

$$|\langle z|z\rangle|^2 = |\langle 0|z\rangle|^2 \sum_{n=0}^{\infty} \frac{z^{2n}}{n!} = |\langle 0|z\rangle|^2 e^{-|z|^2} = 1$$

i.e.

$$|z\rangle = e^{-\frac{|z|^2}{2}} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle \quad (2)$$

This is the equation we were looking for. It expresses the generic coherent state in terms of harmonic oscillators eigenstates and fixes its phase factor.

3.2 Creation operators for coherent states

Equation 2 may be rewritten by explicitly showing the creation of the n -th state from the ground-state $n=0$ (the ‘vacuum’ state), eq. 1. The result is

$$|z\rangle = e^{-\frac{|z|^2}{2}} e^{za^\dagger} |0\rangle \quad (3)$$

where the operator on the r.h.s. is a *coherent-state creation operator* from the vacuum. This formula may also be written in another form upon noticing

that $e^{\alpha a} |0\rangle = |0\rangle$, and choosing α in such a way to eliminate the normalization factor. The following property

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]} \quad (4)$$

which holds whenever $[A, [A, B]] = [B, [A, B]] = 0$, is of interest.

Its proof is as follows. First let us show that when $[A, [A, B]] = 0$

$$e^{-\lambda A} B e^{\lambda A} = B + \lambda[A, B]$$

holds. Let be $F(\lambda) = e^{-\lambda A} B e^{\lambda A}$; then $F'(\lambda) = e^{-\lambda A} [A, B] e^{\lambda A} \equiv [A, B]$ and thus

$$F(\lambda) \equiv F(0) + F'(\lambda)\lambda = B + \lambda[A, B]$$

With this formula at hand let us now consider $F(\lambda) = e^{\lambda A} e^{\lambda B}$ and its derivative,

$$\begin{aligned} F'(\lambda) &= AF(\lambda) + e^{\lambda A} B e^{-\lambda A} F(\lambda) \\ &= (A + e^{\lambda A} B e^{-\lambda A}) F(\lambda) = \\ &= (A + B + \lambda[A, B]) F(\lambda) \end{aligned}$$

Since the λ integral of the first operator on the left of the r.h.s. commutes with the operator itself, this equation may be integrated to give

$$F(\lambda) = e^{\lambda(A+B) + \frac{\lambda^2}{2}[A,B]}$$

The above property follows by using again the commutation relation between A , B and their commutator.

Now, noting that $[a, a^\dagger] = 1$, we have

$$e^{z a^\dagger} e^{\alpha a} = e^{z a^\dagger + \alpha a} e^{-\frac{z\alpha}{2}}$$

and, thus, the choice $\alpha = -z^*$ allows to write

$$|z\rangle = e^{z a^\dagger - z^* a} |0\rangle \quad (5)$$

where the operator on the r.h.s is a (further) creation operator for coherent states from the vacuum.

The above equations may be generalized for creation operators out from arbitrary coherent states. Indeed, application of Eq. 3 allows us to write

$$e^{\lambda a^\dagger} |z\rangle = e^{-\frac{|z|^2}{2}} e^{(\lambda+z)a^\dagger} |0\rangle = e^{\frac{|\lambda+z|^2 - |z|^2}{2}} |\lambda+z\rangle$$

or

$$e^{-\frac{|\lambda|^2}{2}} e^{\lambda a^\dagger} |z\rangle = e^{\text{Re}(\lambda^* z)} |\lambda+z\rangle \quad (6)$$

This equation tells us that coherent states may be generated starting with arbitrary coherent states upon application of an appropriate creation operator. Changing the notation, it is not hard to show that

$$|z\rangle = e^{i\text{Im}(\alpha^*z)} e^{-\frac{|z-\alpha|^2}{2}} e^{(z-\alpha)(a-\alpha)^\dagger} |\alpha\rangle \quad (7)$$

which generalizes eq. 3 to arbitrary starting vectors. The interpretation of this formula is simple: it arises from an α translation in the complex plane, and $|\alpha\rangle$ is the vacuum state of the operator $(a - \alpha)$.

3.3 Completeness relation

The set of coherent states of a given width is *non*-orthogonal. The generic overlap matrix element follows directly from eq. 2

$$\langle z|z'\rangle = e^{-\frac{|z|^2}{2}} e^{-\frac{|z'|^2}{2}} \sum_{n=0}^{\infty} \frac{z'^n (z^*)^n}{n!} = e^{z^*z' - \frac{|z|^2}{2} - \frac{|z'|^2}{2}} \quad (8)$$

and satisfies

$$|\langle z|z'\rangle|^2 = e^{-|z-z'|^2} \quad (9)$$

However, the set is *complete* and forms what it is called a *tight* frame.

The proof is as follows. Let us consider the following integral (operator)

$$\frac{1}{\pi} \int d^2z |z\rangle \langle z| = \frac{1}{\pi} \sum_{n,m} \frac{|n\rangle \langle m|}{\sqrt{n!m!}} \int e^{-|z|^2} z^n (z^*)^m d^2z$$

where eq. 2 has been used. The integrals on the r.h.s. are standard

$$\int_0^{2\pi} e^{i(n-m)\theta} d\theta = 2\pi\delta_{nm} \quad \text{and} \quad \int_0^\infty e^{-r^2} r^{2n+1} dr = \frac{n!}{2}$$

once the polar coordinates have been introduced, and therefore we get

$$\frac{1}{\pi} \int d^2z |z\rangle \langle z| = 1 \quad (10)$$

where the completeness property of the HO eigenstates has been used.

Note that in the above derivation we haven't used any specific property of the HO states other than orthogonality and completeness; it follows that the same relation holds for any set defined by eq. 2 in terms of a complete¹, orthonormal set $\{|n\rangle\}$. The above equation 2, therefore, maps hilbert spaces into classical phase-spaces.

¹More generally, if the original set is not complete "1" has to be replaced with the appropriate projection operator.

3.4 Derivatives

The creation operator for coherent state used in eq. 3 may be employed to get explicit expressions for the derivatives of an arbitrary coherent state with respect to a parameter λ upon which z may depend. Let then be $z = z(\lambda)$,

$$\begin{aligned} \frac{d}{d\lambda} |z\rangle &= \left(-\frac{1}{2} \frac{d|z|^2}{d\lambda} + \frac{dz}{d\lambda} a^\dagger \right) e^{-\frac{|z|^2}{2} + za^\dagger} |0\rangle \\ &= \left(-\frac{1}{2} \frac{d|z|^2}{d\lambda} + \frac{dz}{d\lambda} a^\dagger \right) |z\rangle \end{aligned} \quad (11)$$

It follows

$$\langle z' | \frac{dz}{d\lambda} \rangle = \left(-\frac{1}{2} \frac{d|z|^2}{d\lambda} + \frac{dz}{d\lambda} z'^* \right) \langle z' | z \rangle \quad (12)$$

where $|\frac{dz}{d\lambda}\rangle$ has *not* to be confused with the coherent state corresponding to the complex number $dz/d\lambda$ (actually, $d|z\rangle/d\lambda$ is *not* a coherent state). In particular, for $z' = z$, eq. 12 becomes

$$\langle z | \frac{dz}{d\lambda} \rangle = i\text{Im} \left(\frac{dz}{d\lambda} z^* \right)$$

Analogously, one may obtain explicit expressions for higher derivatives and overlap matrix elements between derivatives and coherent states. For example,

$$\langle z | \frac{d^2 z}{d\lambda^2} \rangle = i\text{Im} \left(\frac{d^2 z}{d\lambda^2} z^* \right) - \text{Im}^2 \left(\frac{dz}{d\lambda} z^* \right) - \frac{dz}{d\lambda} \frac{dz^*}{d\lambda}$$

Note that in the above manipulation it is not straightforward to employ the creation operator for coherent states used in eq. 5. The reason is that the derivative of $A(z) = za^\dagger - z^*a$, i.e. $A'(z) = z'a^\dagger - z'^*a$, does *not* commute with A itself ($[A, A'] = 2i\text{Im}(zz'^*)$) and thus the theorem of the derivative of a compound function cannot be applied to $f(A) = \exp(A)$. Indeed, from the definition of $f'(A)$

$$\begin{aligned} f'(A) &= \lim_{h \rightarrow 0} \frac{e^{A+A'h} - e^A}{h} \\ &= \lim_{h \rightarrow 0} \frac{e^A e^{A'h} e^{-\frac{h}{2}[A, A']} - e^A}{h} \\ &= e^A (A' - [A, A']/2) \end{aligned}$$

where use has been made of eq. 4.

4 Time-evolution

4.1 Harmonic oscillator

The discussion of section 3.1 suggests that coherent states of width Δx have a simple time-evolution under the action of the harmonic oscillator

hamiltonian with frequency $\omega = \hbar/2m\Delta x^2$. Indeed, using eq. 2,

$$\begin{aligned} e^{-\frac{H^{HO}}{\hbar}t} |z_0\rangle &= e^{-\frac{H^{HO}}{\hbar}t} e^{-\frac{|z_0|^2}{2}} \sum_{n=0}^{\infty} \frac{z_0^n}{\sqrt{n!}} |n\rangle \\ &= e^{-\frac{|z_0|^2}{2}} \sum_{n=0}^{\infty} \frac{z_0^n}{\sqrt{n!}} e^{-i(n+\frac{1}{2})\omega t} |n\rangle \end{aligned}$$

i.e. with $z_t = z_0 e^{-i\omega t}$,

$$e^{-\frac{H^{HO}}{\hbar}t} |z_0\rangle = e^{-\frac{i}{2}\omega t} |z_t\rangle$$

Thus, under the action of the HO hamiltonian a coherent state remains coherent and its representative point z moves in the complex plane just like the classical coordinates and momenta move classically in phase-space ($\dot{z} = -i\omega z$ means $\dot{x} = p/m$ and $\dot{p} = -m\omega^2 x$). Note that the average energy of the system in a coherent state $|z\rangle$ is given by

$$\langle H^{HO} \rangle = \hbar\omega(|z|^2 + \frac{1}{2}) = \frac{p_0^2}{2m} + \frac{m\omega^2 x_0^2}{2} + \frac{\hbar\omega}{2}$$

that is, it is function of the modulus of the complex number z .

4.2 Shifted harmonic oscillator

Let us now consider the hamiltonian with a general ‘coupling’ linear in a and a^\dagger ,

$$H = \hbar\omega(a^\dagger a + \frac{1}{2}) - (\beta^* a + \beta a^\dagger)$$

Putting $\beta = \hbar\omega\lambda$, we get

$$H = \hbar\omega(b^\dagger b + \frac{1}{2}) - |\beta|^2$$

where the operator $b = a - \lambda$ has been introduced. Addition of a general linear term to an HO hamiltonian gives rise to another HO hamiltonian (as it should be) with *shifted* creation/annihilation operators, b^\dagger and b . The ‘vacuum’ state of the operator b is the coherent state vector $|\lambda\rangle$. It may be used to obtain the eigenvectors of H ,

$$|n_\lambda\rangle = \frac{(b^\dagger)^n}{\sqrt{n!}} |\lambda\rangle$$

$$H |n_\lambda\rangle = \hbar\omega(n_\lambda + \frac{1}{2}) - |\beta|^2$$

where the subscript λ remember us that they refer to the ‘shifted’ HO hamiltonian, $H_\lambda = \hbar\omega(b^\dagger b + \frac{1}{2})$. The time-evolution of a coherent state $|z_0\rangle$ under

the action of the above hamiltonian may thus be obtained by using the general creation operator defined in eq. 7 to write

$$|z_0\rangle = e^{i\text{Im}(\lambda^* z_0)} e^{-\frac{|z_0-\lambda|^2}{2}} e^{(z_0-\lambda)b^\dagger} |\lambda\rangle$$

and the spectral representation of the hamiltonian. After some manipulations, the result can be put in the form

$$e^{-i\frac{H}{\hbar}t} = e^{-i(\frac{\omega}{2} + \frac{|\beta|^2}{\hbar})t} e^{-i\text{Im}(\lambda^*(z_t-z_0))} |z_t\rangle$$

where $z_t = \lambda + (z_0 - \lambda)e^{-i\omega t}$ or, equivalently,

$$\dot{z}_t = -i\omega(z_t - \lambda)$$

Therefore, the coherent state remains coherent and its representative point moves ‘classically’ in the complex plane.

References

- [1] D. P. Craig and T. Thirunamachandran, *Molecular quantum electrodynamics*, Dover Publications Inc., Mineda, New York, 1998.
- [2] D. V. Shalashilin and M. S. Child, *J. Chem. Phys.* **113**, 10028 (2000).
- [3] D. V. Shalashilin and M. S. Child, *J. Chem. Phys.* **114**, 9296 (2001).
- [4] D. V. Shalashilin and M. S. Child, *J. Chem. Phys.* **115**, 5367 (2001).
- [5] D. V. Shalashilin and M. S. Child, *J. Chem. Phys.* **118**, 2061 (2003).
- [6] D. V. Shalashilin and M. S. Child, *J. Chem. Phys.* **119**, 1961 (2003).
- [7] D. V. Shalashilin and M. S. Child, *J. Chem. Phys.* **121**, 2563 (2004).
- [8] D. V. Shalashilin and M. S. Child, *J. Chem. Phys.* **122**, 224108 (2005).
- [9] D. V. Shalashilin and M. S. Child, *J. Chem. Phys.* **122**, 224109 (2005).
- [10] J. C. Burant and V. S. Batista, *J. Chem. Phys.* **116**, 2748 (2002).
- [11] R. Martinazzo, M. Nest, P. Saalfrank, and G. F. Tantardini, *The Journal of Chemical Physics* **125**, 194102 (2006).
- [12] S. Lopez-Lopez, M. Nest, and R. Martinazzo, *The Journal of Chemical Physics* **134**, 014102 (2011).
- [13] S. Lopez-Lopez, R. Martinazzo, and M. Nest, *The Journal of Chemical Physics* **134**, 094102 (2011).