

Comment on phase-space representation of quantum state vectors

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A simple approach to phase-space representation of quantum state vectors using the displacement-operator formalism is presented. Although the resulting expressions for the fundamental operators (position and momentum) are equivalent to those obtained by other methods, this approach provides both alternative mathematical foundation as well as physical interpretation of phase-space representation of quantum state vectors. © 1999 American Institute of Physics.

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I. INTRODUCTION

Over the past few years there has been a renewed interest in phase-space descriptions of quantum systems. In a recent paper by Ban¹ a novel approach to phase-space representation of quantum state vectors is obtained within the relative-state formulation, and in this Comment we make a few remarks on the physical contents of this construction. Also, we relate it to another approach to phase-space representation of quantum state vectors, the so-called displacement-operator approach.

The idea of phase-space representation of quantum state vectors, i.e., representation of a quantum state as a probability amplitude depending on *two real* variables related to the position and momentum coordinates goes back to the works of Fock² and Bargmann.³ In their formulation, a quantum state is represented as a complex function depending on *one complex* coordinate whose real and imaginary part is proportional to the position and momentum coordinate, respectively. This is a result of regarding the bosonic creation and annihilation operators as the fundamental operators.

The relative-state formulation, on the other hand, treats the position and momentum operators themselves as the fundamental operators and is therefore more closely related to the works of Torres-Vega and Frederick⁴ and Harriman.⁵ Both of these works rely to a certain extent on Dirac's representation theory of quantum mechanics,⁶ either as a Hilbert-space-vector approach postulating the existence of a complete set of states depending on two real parameters that can be used as a basis in phase space or a linear transformation onto phase space from position or momentum space.

In fact, the relative-state representation of Ban¹ becomes, under certain conditions, equivalent to those of Torres-Vega and Frederick⁴ and Harriman.⁵ The relative-state formulation may therefore serve as a mathematical and physical foundation for the representations presented by these authors since it is derived from first principles without assumptions or transformations from other representations.

However, the relative-state formulation is not the only way to construct a phase-space representation of quantum state vectors from first principles that becomes equivalent to those of Torres-Vega and Frederick⁴ and Harriman.⁵ Below, we present an alternative construction, using the displacement operators, and discuss the mathematical and physical differences between this method the relative-state approach.

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The displacement-operator approach is essentially equivalent to the coherent-state formalism as put forward by, for instance, Klauder and Skagerstam⁷ and studied in some detail by the present author.⁸ Hence, the presentation given here is extracted from these earlier works and put in a form relevant for the present discussion. For a thorough review and analysis of the use of displacement operators, the reader is referred to Refs. 7 and 8 and the references therein.

II. RELATIVE-STATE FORMULATION

The relative-state formulation is presented in great detail by Ban¹ and here we only include a few results relevant for the further discussion. The key of this approach is to enlarge the Hilbert space \mathcal{H} of a quantum system by introducing an auxiliary (reference) quantum system and treat quantum state vectors in the extended Hilbert space $\tilde{\mathcal{H}} = \mathcal{H} \otimes \mathcal{H}_r$, where \mathcal{H}_r is the Hilbert space of the reference system. A state vector in the extended Hilbert space $\tilde{\mathcal{H}}$ then becomes $|\Psi\rangle \equiv |\psi\rangle \otimes |\phi\rangle_r$ where $|\phi\rangle_r$ is the reference state.

A set of state vectors $\{|\omega(r, k; s)\rangle | r, k \in \mathbf{R}\}$ may be introduced¹ that becomes a complete orthonormal system in $\tilde{\mathcal{H}}$. These state vectors, which can be written on the following form:

$$|\omega(r, k; s)\rangle \equiv \frac{1}{\sqrt{2\pi}} e^{-i(1+s)kr/2} \int_{-\infty}^{\infty} dx e^{ikx} |x\rangle \otimes |x-r\rangle_r \tag{1}$$

(as in Ref. 1, we set $\hbar=1$ throughout this Comment) are simultaneous eigenstates of the operators $\hat{x} - \hat{x}_r$, and $\hat{p} + \hat{p}_r$,

$$(\hat{x} - \hat{x}_r)|\omega(r, k; s)\rangle = r|\omega(r, k; s)\rangle, \tag{2}$$

$$(\hat{p} + \hat{p}_r)|\omega(r, k; s)\rangle = k|\omega(r, k; s)\rangle. \tag{3}$$

However, when we investigate the properties of the relevant quantum system, we only need a description of this system in the Hilbert space \mathcal{H} . Thus, the extended Hilbert space is reduced again by fixing the state vector of the reference system. For any fixed state vector $|\phi\rangle_r$ of the reference system, the set $\{|\omega(r, k; s)\rangle | r, k \in \mathbf{R}\}$, where

$$|\omega(r, k; s)\rangle \equiv_r \langle \phi | \omega(r, k; s) \rangle = \frac{1}{\sqrt{2\pi}} e^{-i(1+s)kr/2} \int_{-\infty}^{\infty} dx e^{ikx} \phi^*(x-r) |x\rangle, \tag{4}$$

becomes an overcomplete system in the Hilbert space \mathcal{H} .¹ Therefore, the relevant quantum system can be represented by an $\mathcal{L}^2(2)$ normalized wave function $\psi_\omega(r, k; s) \equiv \langle \omega(r, k; s) | \psi \rangle$ depending of the two real parameters k and r . In this representation, the fundamental operators \hat{x} and \hat{p} take the form

$$\langle \omega(r, k; s) | \hat{x} | \psi \rangle = \left[\frac{1}{2} (1+s)r + i \frac{\partial}{\partial k} \right] \psi_\omega(r, k; s), \tag{5}$$

$$\langle \omega(r, k; s) | \hat{p} | \psi \rangle = \left[\frac{1}{2} (1-s)k - i \frac{\partial}{\partial r} \right] \psi_\omega(r, k; s). \tag{6}$$

Apart from some notational differences these are essentially the expressions given by Torres-Vega and Frederick⁴ and Harriman⁵ in their representations. Thus, the construction by Ban¹ may serve as a mathematical foundation for the work of Torres-Vega and Frederick⁴ and Harriman.⁵ Furthermore, the relative-state formulation provides a physical interpretation of the wave function $\psi_\omega(r, k; s)$ and the parameters k and r as phase-space coordinates. In light of Eqs. (2) and (3), the function $|\psi_\omega(r, k; s)|^2$ represents the probability distributions of the eigenvalues of the operators $\hat{x} - \hat{x}_r$ and $\hat{p} + \hat{p}_r$ in the extended Hilbert space $\tilde{\mathcal{H}}$.

Alternatively, one may utilize $|\psi_\omega(r, k; s)|^2$ as a combined probability distribution directly in the r, k -parametrized space as follows:

$$\bar{r} \equiv \int_{-\infty}^{\infty} dr \int_{-\infty}^{\infty} dk r |\psi_\omega(r, k; s)|^2 = x_\psi - x_\phi, \tag{7}$$

$$\bar{k} \equiv \int_{-\infty}^{\infty} dr \int_{-\infty}^{\infty} dk k |\psi_\omega(r, k; s)|^2 = p_\psi + p_\phi. \tag{8}$$

Here, $x_\psi = \langle \psi | \hat{x} | \psi \rangle$ and so on. Thus, r and k may be interpreted as phase-space coordinates in the sense that the average value of r equals the relative position between the relevant and the reference system, and the average value of k equals the sum of the momenta of the relevant and the reference system. Hence, the physical interpretation of the wave function depends on the reference state, although the operator expressions, Eqs. (5) and (6), do not, and from this point of view the most satisfactory representation is obtained using a reference state with $\langle \phi | \hat{x} | \phi \rangle = 0$ and $\langle \phi | \hat{p} | \phi \rangle = 0$. In general, also the physical interpretation of higher momenta of r and k depend on the reference system.¹

III. DISPLACEMENT-OPERATOR APPROACH

Here we present an alternative derivation from first principles of the phase-space representation of quantum state vectors that also becomes equivalent to the ones of Torres-Vega and Frederick⁴ and Harriman⁵ and therefore to the result of Ban,¹ as well. However, the derivation presented here differs from the one obtained in the relative-state formulation in both the mathematical foundation and in the physical interpretation of the phase-space wave functions. In fact, it resembles closely Dirac's construction of the usual position and momentum representations.⁶

Two things are important for the definitions of these representations. First, the basis states, denoted by $|r\rangle_x$ and $|k\rangle_p$, are eigenstates of the position and momentum operator, respectively,

$$\hat{x}|r\rangle_x = r|r\rangle_x \quad \text{and} \quad \hat{p}|k\rangle_p = k|k\rangle_p. \tag{9}$$

Second, the position (momentum) eigenstate with eigenvalue $r(k)$ can be generated from the eigenstate with eigenvalue $r=0$ ($k=0$) by a displacement operator,

$$|r\rangle_x = \hat{D}_x(r)|0\rangle_x \quad \text{and} \quad |k\rangle_p = \hat{D}_p(k)|0\rangle_p, \tag{10}$$

where the displacement operators are given as $\hat{D}_x(r) = \exp(-ir\hat{p})$ and $\hat{D}_p(k) = \exp(ik\hat{x})$.⁶ The wave function in position (momentum) space is then obtained by projection onto a position (momentum) eigenstate, $\psi(r) \equiv \langle r | \psi \rangle$ ($\psi(k) \equiv \langle k | \psi \rangle$). This implies that the displacement operators when acting on a state displace the expectation value of the position or momentum by r and k , respectively.

An identical approach to a phase-space representation of quantum state vectors would require the existence of an Hermitian operator representing a point in phase space. Torres-Vega and Frederick⁴ claim that such an operator exist but without proof and, in fact, the existence of such an operator would violate the Heisenberg uncertainty relation. In the relative-state formulation, a close resemblance is obtained for the basis states $|\omega(r, k; s)\rangle$ in the extended Hilbert space; cf. Eqs. (2) and (3).

Nevertheless, an r, k -parametrized basis *can* be constructed utilizing displacement operators. In general, a displacement operator that displaces the expectation values of the position and momentum for any state by r and k simultaneously, can be defined as^{7,8}

$$\hat{D}_s(r, k) = \exp[i(k\hat{x} - r\hat{p} - skr/2)], \tag{11}$$

where s is real number determining the phase such that $\hat{D}_1(r,k) = \hat{D}_q(r)\hat{D}_p(k)$, $\hat{D}_{-1}(r,k) = \hat{D}_p(k)\hat{D}_q(r)$, and $\hat{D}_0(r,k)$ is a symmetric combination. An r,k -parametrized state vector may then be defined as $|\Omega(r,k;s)\rangle \equiv (2\pi)^{-1/2}\hat{D}_s(r,k)|\chi\rangle$, where $|\chi\rangle$ is an arbitrary normalized state, and the set $\{|\Omega(r,k;s)\rangle | r,k \in \mathbf{R}\}$ becomes an overcomplete set of normalized vectors.⁷ The set $\{|\Omega(r,k;s)\rangle | r,k \in \mathbf{R}\}$ can therefore be used as a basis and the relevant quantum system represented by the $\mathcal{L}^2(2)$ normalized wave function $\psi_\Omega(r,k;s) \equiv \langle \Omega(r,k;s) | \psi \rangle$, depending on the two real parameters k and r . These basis vectors obviously satisfy the displacement relation

$$|\Omega(r,k;s)\rangle = \hat{D}_s(r,k)|\Omega(0,0;s)\rangle. \tag{12}$$

Using that

$$i \frac{\partial}{\partial k} \hat{D}(r,k;s) = \left[\frac{1}{2}(1+s)r - \hat{x} \right] \hat{D}(r,k;s), \tag{13}$$

$$i \frac{\partial}{\partial r} \hat{D}(r,k;s) = - \left[\frac{1}{2}(1-s)k - \hat{p} \right] \hat{D}(r,k;s), \tag{14}$$

it is seen that in this representation, the fundamental operators \hat{x} and \hat{p} take the same form as in the relative-state formulation, given by Eqs. (5) and (6).

Therefore, the displacement-operator approach provides an alternative derivation from first principles to the results obtained within the relative-state formalism. Here, the state of the relevant system is projected onto an auxiliary (reference) state $|\chi\rangle$, displaced by r and k , whereas the auxiliary state $|\phi\rangle$ in the relative-state formulation is utilized to project the orthonormal basis in the extended Hilbert space onto a reduced Hilbert space. Thus, the auxiliary states play different physical roles, as can also be seen from the relations

$$\bar{r} \equiv \int_{-\infty}^{\infty} dr \int_{-\infty}^{\infty} dk r |\psi_\Omega(r,k;s)|^2 = x_\psi - x_\chi, \tag{15}$$

$$\bar{k} \equiv \int_{-\infty}^{\infty} dr \int_{-\infty}^{\infty} dk k |\psi_\Omega(r,k;s)|^2 = p_\psi - p_\chi. \tag{16}$$

Hence, r and k may here be interpreted as phase space coordinates, in the sense that the average values obtained using $|\psi_\Omega(r,k;s)|^2$ as a combined probability distribution equal the relative position and momentum, respectively, between the relevant and the auxiliary system. Hence, the displacement-operator approach provides a more symmetrical interpretation of the r,k -parametrized representation of the quantum state vector.

Since

$$\hat{D}_s(r,k)|\chi\rangle = e^{-i(1+s)kr/2} \int_{-\infty}^{\infty} dx e^{ikx} \chi(x-r)|x\rangle, \tag{17}$$

we see that the displacement-operator approach and the phase-space representation obtained within the relative-state formulation become formally identical if $\chi(x) = \phi^*(x)$; cf. Eq. (4), which implies that $p_\phi = -p_\chi$, as expected [compare Eqs. (8) and (16)].

In conclusion, we have shown that the two different mathematical approaches to a phase-space representation of quantum state vectors lead to identical expressions for the fundamental operators. However, usage of the well-known technique of displacement operators is in spirit closer to the construction of the usual position and momentum representations and, also, it provides a more transparent physical interpretation of the auxiliary state as a ‘‘probe’’ state in phase

space.⁸ With this interpretation, phase-space representation of quantum state vectors becomes a powerful tool and has been applied recently in the study of quantum dynamics directly in phase space⁹ or as a route to semiclassical approximations.¹⁰

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¹M. Ban, J. Math. Phys. **39**, 1744 (1998).

²V. Fock, Z. Phys. **49**, 339 (1928).

³V. Bargmann, Commun. Pure Appl. Math. **14**, 187 (1961).

⁴Go. Torres-Vega and J. H. Frederick, J. Chem. Phys. **98**, 3103 (1993).

⁵J. E. Harriman, J. Chem. Phys. **100**, 3651 (1994).

⁶P. A. M. Dirac, *The Principles of Quantum Mechanics*, 4th ed. (Oxford University Press, Oxford, 1958); W. H. Louisell, *Quantum Statistical Properties of Radiation* (Wiley, New York, 1973), Chap. 1.

⁷J. R. Klauder and B.-S. Skagerstam, *Coherent States* (World Scientific, Singapore, 1985).

⁸K. B. Møller, T. G. Jørgensen, and Go. Torres-Vega, J. Chem. Phys. **106**, 7228 (1997).

⁹Go. Torres-Vega, K. B. Møller, and A. Zúñiga-Segundo, Phys. Rev. A **57**, 771 (1998).

¹⁰S. Jang, M. Zhao, and S. A. Rice, Chem. Phys. **230**, 237 (1998).