

Derivation of the coordinate-momentum commutation relations from canonical invariance

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Based on (i) the spectral resolution definition of the momentum operator, (ii) the linearity of correspondence between physical observables and quantum Hermitian operators, (iii) the definition of conjugate coordinate-momentum variables in classical mechanics, and (iv) the invariance of the classical Hamiltonian to canonical transformations (transformations that change from one set of conjugate variables to another), we show that the $[\hat{x}, \hat{p}]$ coordinate-momentum commutator must have the value $i\hbar$ where \hbar is a real nonzero number (which we can identify with the experimentally determined \hbar). The results are then extended to include all generalized coordinates and their conjugate momenta as well as the Cartesian special-relativistic case.

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I. INTRODUCTION

The quest for deriving all the laws of physics from invariance requirements with respect to some basic symmetry is one of the most important and rewarding directions in physics. It is, however, the case that no such derivation exists for the very act of *quantization*, namely the imposition of commutation relations between quantum operators that correspond to certain observables. Thus the coordinate-momentum commutation relations

$$[\hat{q}, \hat{p}] = i\hbar \quad (1)$$

are usually imposed *by fiat*, their justification being given *a posteriori*. The procedure usually adopted in the formal development of quantum mechanics [1] is that after introducing the definition of the momentum operator in terms of its observed spectrum as $\hat{p} \equiv \int_{-\infty}^{\infty} dp p |p\rangle\langle p|$, the commutation relations are imposed and the identification of the wave function for the free particle in Cartesian coordinates as

$$\langle x|p\rangle = (2\pi\hbar)^{-1/2} \exp(ipx/\hbar) \quad (2)$$

is made. Using Eq. (2) and the above definition of \hat{p} one obtains the coordinate representation of \hat{p} and all other operators depending on it.

It was pointed out by Dirac [2] that it is possible to go by the reverse order: to assume Eq. (2) and *derive* from it Eq. (1). In order to motivate what follows we now briefly summarize this route. Assuming Eq. (2) and using the spectral resolution of the \hat{p} operator we have that

$$\begin{aligned} \langle x'|\hat{p}|x\rangle &= \int_{-\infty}^{\infty} dp p \langle x'|p\rangle\langle p|x\rangle \\ &= (2\pi\hbar)^{-1} \int_{-\infty}^{\infty} dp p \exp[ip(x-x')/\hbar] \\ &= \frac{-i}{2\pi} \frac{\partial}{\partial x} \int_{-\infty}^{\infty} dp \exp[ip(x-x')/\hbar] = -i\hbar \frac{\partial}{\partial x} \delta(x-x'). \end{aligned} \quad (3)$$

Using Eq. (3) we can write that

$$\begin{aligned} \langle \Psi'|\hat{p}\hat{x}|\Psi\rangle &= \int \int dx dx' \Psi'^*(x) \langle x|\hat{p}|x'\rangle x' \Psi(x') \\ &= -i\hbar \int \int dx dx' \Psi'^*(x) \frac{\partial}{\partial x} \delta(x-x') x' \Psi(x') \\ &= -i\hbar \int dx \Psi'^*(x) \frac{\partial}{\partial x} x \Psi(x). \end{aligned} \quad (4)$$

The commutation relations [Eq. (1)] follow by performing integration by parts of Eq. (4). Thus if one is able to prove Eq. (2) one would have a way of *deriving* the coordinate representation of \hat{p} and the $[\hat{x}, \hat{p}]$ commutation relations [3].

In this paper we present a *derivation* of Eq. (2) using *canonical invariance*, i.e., the invariance of the classical Hamiltonian to canonical transformations, i.e., transformations between one set of conjugate variables to another. We shall see that this invariance, plus the linear correspondence between classical observables and quantum operators and the definition of the scalar product in quantum mechanics, will suffice.

II. CANONICAL INVARIANCE IN THE NONRELATIVISTIC CASE

We begin our derivation by considering the classical kinetic energy of two freely moving noninteracting particles,

$$T = p_A^2/(2m_A) + p_B^2/(2m_B). \quad (5)$$

As a special type of canonical transformation to which T is invariant, we consider at this stage the transformation from the individual coordinates, x_A and x_B , and their conjugate momenta p_A and p_B , to the set of variables defined as X_1 , the center-of-mass coordinate, and X_2 , the relative-coordinate and their conjugate momenta P_1 and P_2 . Choosing, without loss of generality, $m_A = m_B$, we have that

$$X_1 = (x_A + x_B)/2, \quad X_2 = x_A - x_B,$$

with P_1 and P_2 , the conjugate momenta to X_1 and X_2 , being given as

$$P_1 = p_A + p_B, \quad P_2 = (p_A - p_B)/2. \quad (6)$$

The (invariant) kinetic energy is expressed in the transformed coordinates as

$$T = P_1^2/(4m_A) + P_2^2/m_A. \quad (7)$$

Due to the linear correspondence between classical observables and quantum operators, the same relation as in Eq. (5) holds between the kinetic energy operator \hat{T} and the momenta operators \hat{p}_A and \hat{p}_B . Likewise, the relation between \hat{T} and \hat{P}_1 and \hat{P}_2 is the same as that of Eq. (7).

Remembering that by the definition of a function of an operator, the kinetic energy operator \hat{T} commutes with both the \hat{p}_A and \hat{p}_B momenta and with the \hat{P}_1 and \hat{P}_2 momenta, and using the fact that in Cartesian coordinates the kinetic energy operator \hat{T} is a sum of single-momentum dependent terms in either set of variables allows us to write a given eigenfunction of the kinetic energy operator as a product of an eigenfunction of \hat{p}_A and an eigenfunction of \hat{p}_B , or as a product of an eigenfunction of \hat{P}_1 and an eigenfunction of \hat{P}_2 , as

$$\langle x_A | p_A \rangle \langle x_B | p_B \rangle = \langle X_1 | P_1 \rangle \langle X_2 | P_2 \rangle. \quad (8)$$

Choosing two particular eigenvalues, $p_A = p_B \equiv p$ we have that $P_1 = 2p$, $P_2 = 0$, with Eq. (8) now reading

$$\langle x_A | p \rangle \langle x_B | p \rangle = \langle (x_A + x_B)/2 | 2p \rangle \langle x_A - x_B | 0 \rangle. \quad (9)$$

If we now also choose the particular values $x_A = x_B \equiv x$ we have that

$$\langle x | p \rangle \langle x | p \rangle = \langle x | 2p \rangle \langle 0 | 0 \rangle. \quad (10)$$

Writing the complex amplitude explicitly as

$$\langle x | p \rangle \equiv A(p, x) \exp[i\Phi(p, x)],$$

where the absolute value $A(p, x)$ is per definition a real positive function, we obtain by taking the absolute value of Eq. (10) that

$$A'(x, 2p) = [A'(x, p)]^2, \quad (11)$$

where $A'(x, p) \equiv A(x, p)/A(0, 0)$.

Defining $\delta \equiv p/2^n$, we have from Eq. (11) that

$$A'(x, p) = A'(x, 2^n \delta) = [A'(x, \delta)]^{2^n}.$$

Hence

$$\ln A'(x, p) = 2^n \delta f'(x, \delta) = p f'(x, \delta),$$

where $f'(x, \delta) = \frac{1}{\delta} \ln[A'(x, \delta)]$. For every p value we can find an n value, such that δ is sufficiently small so that $f'(x)$ is sufficiently close to its limiting value

$$f(x) = \lim_{\delta \rightarrow 0} \frac{\ln[A'(x, \delta)]}{\delta} = \frac{dA'(x, p)/dp|_{p=0}}{A'(x, 0)}.$$

Since $A'(x, 0) > 0$ (otherwise the $\langle x | 0 \rangle$ would not be normalizable) and bounded, the $f(x)$ limit exists and is nondivergent.

Thus for sufficiently small δ we replace all $f'(x, \delta)$ functions by $f(x)$ and obtain that $A'(x, p) = \exp[pf(x)]$ or that

$$A(x, p) = a \exp[pf(x)],$$

where $a = A(0, 0)$ is a constant to be determined by normalization.

In a similar fashion we can choose in Eq. (8) $x_A = -x_B \equiv x$ and $p_A = -p_B \equiv p$. We have that $P_1 = 0$, $P_2 = p$, with Eq. (9) now reading

$$\langle x | p \rangle \langle -x | -p \rangle = \langle 0 | 0 \rangle \langle 2x | p \rangle. \quad (12)$$

We now use the vector property of p , according to which a re-definition of the coordinates $x \rightarrow -x$ entails $p \rightarrow -p$. Hence $\langle -x | -p \rangle = \langle x | p \rangle$ and Eq. (12) now reads as

$$\langle x | p \rangle \langle x | p \rangle = \langle 0 | 0 \rangle \langle 2x | p \rangle.$$

Hence

$$A'(2x, p) = [A'(x, p)]^2. \quad (13)$$

Defining $\delta = x/2^n$, we have from Eq. (13) that

$$A'(x, p) = A'(2^n \delta, p) = [A'(\delta, p)]^{2^n}.$$

Hence

$$\ln A'(x, p) = 2^n \delta g'(\delta, p) = x g'(\delta, p),$$

where $g'(\delta, p) = \frac{1}{\delta} \ln[A'(\delta, p)]$. Repeating the same arguments as for $f'(x, \delta)$ we replace $g'(\delta, p)$ by its limiting value

$$g(p) = \lim_{\delta \rightarrow 0} \frac{\ln[A'(\delta, p)]}{\delta} = \frac{dA'(x, p)/dx|_{x=0}}{A'(0, p)},$$

and obtain that

$$A(x, p) = a \exp[xg(p)]. \quad (14)$$

Since $\langle x | p \rangle = (\langle p | x \rangle)^*$, which means for the absolute values that $A(p, x) = A(x, p)$, it follows that

$$\exp[pf(x)] = \exp[xg(p)],$$

i.e.,

$$pf(x) = xg(p) \quad \text{or} \quad g(p)/p = f(x)/x = \beta,$$

where β is a real constant, independent of either p or x . Hence from Eq. (14)

$$A(p, x) = a \exp(\beta px). \quad (15)$$

This solution is unacceptable for $\beta \neq 0$ because the probability density diverges at either $x = \pm\infty$ boundary, thus violating flux conservation. Therefore the only acceptable value of β is

$$\beta = 0,$$

which renders

$$A(p, x) = A(0, 0) = a, \quad (16)$$

a constant independent of either p or x .

Given Eq. (16), we can now apply a similar set of considerations to the entire complex amplitude which we now know is given as

$$\langle x|p\rangle = a \exp[i\Phi(x,p)]$$

where Φ is a real function. Choosing $\Phi(0,0)=0$, Eq. (10) now reads

$$\{\exp[i\Phi(x,p)]\}^2 = \exp[i\Phi(x,2p)], \quad (17)$$

hence

$$\Phi(x,2p) = 2\Phi(x,p).$$

By the same line of arguments as above it follows immediately that $\Phi(x,p)=pf(x)$ and also that $\Phi(x,p)=xg(p)$, whose only solution is

$$\Phi(x,p) = \gamma px,$$

where γ is another real constant of dimension [coordinate \times momentum] $^{-1}$.

The solution we have now obtained,

$$\langle x|p\rangle = a \exp(i\gamma px), \quad (18)$$

is acceptable because its absolute value remains bounded.

The exact value of the constant γ , which depends on the (rather arbitrary) historical units of coordinates and momenta, cannot be determined theoretically and must be derived from experiment. It is interesting to note, however, that even without resorting to experiment, the above derivation definitely precludes the possibility that $\gamma=\infty$, i.e., that $[\hat{x},\hat{p}]=i/\gamma=0$, because in that case the solution presented in Eq. (18) will not be continuous. Naturally we identify γ as $1/\hbar$.

This concludes the proof of Eq. (2) and hence the derivation of the $[\hat{x},\hat{p}]$ commutation relations for Cartesian coordinates.

III. GENERALIZED COORDINATES AND THEIR CANONICAL MOMENTA

We now extend the derivation to generalized coordinates q_l and their canonical momenta p_l . Clearly if one goes the quantum route, it is possible to prove the $[\hat{q}_l,\hat{p}_l]$ commutation relation by expressing the \hat{q}_l coordinate operators and their canonical momenta operators \hat{p}_l in terms of the Cartesian coordinates and momenta. This, however, is a tedious procedure, requiring a separate derivation for each type of generalized coordinate and its canonical momentum. It is much more powerful to be able to prove the commutation relations in general using the classical definition of canonical variables and the correspondence between a classical observable and a quantum operator.

Expressed in generalized coordinates the classical kinetic energy is given as a bilinear form

$$T = \frac{1}{2} \sum_{k,l} \mathbf{t}(\mathbf{q})_{k,l} \dot{q}_l \dot{q}_k = \frac{1}{2} \sum_{k,l} [\mathbf{t}(\mathbf{q})^{-1}]_{k,l} p_l p_k, \quad (19)$$

where

$$p_l = \partial T / \partial \dot{q}_l, \quad (20)$$

and

$$\mathbf{t}(\mathbf{q})_{l,k} = \sum_i m_i (\partial \mathbf{r}_i / \partial q_l) (\partial \mathbf{r}_i / \partial q_k), \quad (21)$$

with \mathbf{q} denoting the *vector* of coordinates $\{q_1, q_1, \dots, q_N\}$.

Defining *mass-weighted* coordinates,

$$q'_l = t_{l,l}^{1/2}(\mathbf{q}_e) q_l, \quad p'_l = t_{l,l}^{-1/2}(\mathbf{q}_e) p_l, \quad (22)$$

where \mathbf{q}_e is some point in the \mathbf{q} configuration space, and their quantum analogs \hat{q}' and \hat{p}' , we form a classical invariant and its quantum analog,

$$K = \frac{1}{2} \sum_{l=1,2} p_l'^2, \quad \hat{K} = \frac{1}{2} \sum_{l=1,2} \hat{p}_l'^2. \quad (23)$$

As in the Cartesian case, K and \hat{K} are invariant to a canonical transformation of the type

$$P_1 = p'_1 + p'_2, \quad P_2 = (p'_1 - p'_2)/2,$$

provided the canonical coordinates conjugate to these momenta are obtained [4] from the F_2 generator,

$$\begin{aligned} F_2(q_1, q_2, P_1, P_2) &\equiv \int^{q'_1} p'_1 dq''_1 + \int^{q'_2} p'_2 dq''_2 \\ &= \int^{q'_1} (P_1/2 + P_2) dq''_1 + \int^{q'_2} (P_1/2 - P_2) dq''_2, \end{aligned}$$

as

$$Q_1 = \frac{\partial F_2}{\partial P_1} = (q'_1 + q'_2)/2, \quad Q_2 = \frac{\partial F_2}{\partial P_2} = q'_1 - q'_2.$$

As in the Cartesian case this transformation entails [see Eq. (21)] the doubling of the effective mass for Q_1 and the halving of the effective mass for Q_2 [see also Eq. (7)].

We see that the relations between the Q_l and q'_l and between P_l and p'_l , with $l=1,2$, are formally identical to those used in the Cartesian case. Moreover, because $[\hat{p}'_l, \hat{K}]=0$ all the conditions which form the basis for the proof presented in the Cartesian case hold. Hence the equality

$$\langle q'_l | p'_l \rangle = a \exp(i\gamma p'_l q'_l)$$

follows in exactly the same manner as in the Cartesian case. By virtue of Eq. (22)

$$\exp(i\gamma p'_l q'_l) = \exp(i\gamma p_l q_l).$$

The above two equations lead to the inescapable conclusion that

$$\langle q_l | p_l \rangle = \langle q'_l | p'_l \rangle = a \exp(i\gamma p_l q_l) \quad (\gamma = 1/\hbar). \quad (24)$$

We note that, as usual, whenever the Jacobian implicit in Eqs. (3) and (4) differs from 1, the coordinate representation of \hat{p}_l may deviate from the simple $-i\hbar \partial / \partial q_l$ form [e.g., $\hat{p}_r = (-i\hbar / r) \partial / \partial r$]. Nevertheless, the $[\hat{q}_l, \hat{p}_l]$ commutation relations remain unchanged and follow immediately from Eq. (24) and the analog of Eq. (4).

The derivation can be repeated for the most general case [e.g., a particle in the presence of an electromagnetic field $A_l(\mathbf{q})$] in which the generalized momenta are given not by

Eq. (20) but as $p_i = \partial \mathcal{L} / \partial \dot{q}_i$, where \mathcal{L} is the *Lagrangian*. One forms exactly the same invariant as in Eq. (23) and proceeds from there.

IV. THE SPECIAL-RELATIVISTIC EXTENSION IN CARTESIAN COORDINATES

In the special-relativistic case the momentum is derived from a Lagrangian that is related differently from the nonrelativistic case to the kinetic energy. For two free particles of equal mass ($m_A = m_B = m$) the relativistic Lagrangian assumes the form [6]

$$\mathcal{L} = \mathcal{L}_A + \mathcal{L}_B, \quad (25)$$

where

$$\mathcal{L}_s = -mc^2(1 - \beta_s^2)^{1/2}, \quad s = A \text{ or } B, \quad (26)$$

where $\beta_s = v_s/c$. The canonical momenta are obtained as in nonrelativistic mechanics as

$$p_s = \partial \mathcal{L} / \partial v_s = mv_s / (1 - \beta_s^2)^{1/2}.$$

We can make a canonical transformation to

$$X_1 = (x_A + x_B)/2^{1/2}, \quad X_2 = (x_A - x_B)/2^{1/2}. \quad (27)$$

The untransformed velocities are related to the transformed velocities, $V_i = \dot{X}_i$, $i = 1, 2$, as

$$v_A = (V_1 + V_2)/2^{1/2}, \quad v_B = (V_1 - V_2)/2^{1/2}. \quad (28)$$

Substituting Eq. (28) in Eq. (25) we have that

$$-\mathcal{L}/(mc) = \{c^2 - (V_1 + V_2)^2/2\}^{1/2} + \{c^2 - (V_1 - V_2)^2/2\}^{1/2}.$$

Therefore the conjugate momenta to X_1 and X_2 are given as

$$\begin{aligned} P_1 &= \partial \mathcal{L} / \partial V_1 = \frac{mc}{2} (V_1 + V_2) \{c^2 - (V_1 + V_2)^2/2\}^{-1/2} \\ &\quad + \frac{mc}{2} (V_1 - V_2) \{c^2 - (V_1 - V_2)^2/2\}^{-1/2} \\ &= (p_A + p_B)/2^{1/2}. \end{aligned}$$

Likewise, $P_2 = \partial \mathcal{L} / \partial V_2 = (p_A - p_B)/2^{1/2}$.

In relativistic dynamics an obvious invariant to the canonical transformation to the X_1 and X_2 variables is the sum of the *squares* of the kinetic energies of the two particles,

$$\mathcal{T} = T_A^2 + T_B^2 = c^2 \{2m^2 c^2 + p_A^2 + p_B^2\}. \quad (29)$$

Substituting Eq. (28) into Eq. (29) we see that \mathcal{T} is indeed invariant to this canonical transformation,

$$\begin{aligned} \mathcal{T} &= T_A^2 + T_B^2 = c^2 \{2m^2 c^2 + (P_1 + P_2)^2/2 + (P_1 - P_2)^2/2\} \\ &= c^2 \{2m^2 c^2 + P_1^2 + P_2^2\}. \end{aligned}$$

Since the invariant \mathcal{T} is a function of p_A and p_B and also of P_1 and P_2 , $\hat{\mathcal{T}}$, the quantum operator corresponding to it, commutes with all four momenta operators,

$$[\hat{\mathcal{T}}, \hat{p}_A] = [\hat{\mathcal{T}}, \hat{p}_B] = [\hat{\mathcal{T}}, \hat{P}_1] = [\hat{\mathcal{T}}, \hat{P}_2] = 0.$$

As in the nonrelativistic case, we can therefore write the eigenstates of $\hat{\mathcal{T}}$ in two different ways,

$$\langle x_A | p_A \rangle \langle x_B | p_B \rangle = \langle X_1 | P_1 \rangle \langle X_2 | P_2 \rangle. \quad (30)$$

Choosing two particular eigenvalues, $p_A = p_B \equiv p$ we have that $P_1 = 2^{1/2}p$, $P_2 = 0$, with Eq. (30) now reading

$$\langle x_A | p \rangle \langle x_B | p \rangle = \langle (x_A + x_B)/2^{1/2} | 2^{1/2}p \rangle \langle (x_A - x_B)/2^{1/2} | 0 \rangle.$$

If we now also choose the particular values $x_A = x_B \equiv x$ we have that

$$\langle x | p \rangle \langle x | p \rangle = \langle 2^{1/2}x | 2^{1/2}p \rangle \langle 0 | 0 \rangle.$$

We obtain that

$$\langle 2^{1/2}x | 2^{1/2}p \rangle' = (\langle x | p \rangle')^2, \quad (31)$$

where $\langle x | p \rangle' \equiv \langle x | p \rangle / \langle 0 | 0 \rangle$. Defining $\delta_p \equiv p/2^{n/2}$ and $\delta_x \equiv x/2^{n/2}$, we have from Eq. (31) that

$$\langle x | p \rangle' = \langle 2^{n/2} \delta_x | 2^{n/2} \delta_p \rangle' = (\langle \delta_x | \delta_p \rangle')^{2^n}.$$

Hence

$$\ln \langle x | p \rangle' = 2^{n/2} \delta_x 2^{n/2} \delta_p f'(\delta_x, \delta_p) = p x f'(\delta_x, \delta_p),$$

where $f'(\delta_x, \delta_p) = \ln \langle \delta_x | \delta_p \rangle' / (\delta_p \delta_x)$. For every p and x value we can find an n value, such that δ_x and δ_p are sufficiently small so that $f'(\delta_x, \delta_p)$ is sufficiently close to its limiting value

$$f = \lim_{\delta_p \rightarrow 0, \delta_x \rightarrow 0} \frac{\ln \langle \delta_x | \delta_p \rangle'}{\delta_x \delta_p} = \left. \frac{\partial^2 \ln \langle x | p \rangle'}{\partial x \partial p} \right|_{x,p=0}.$$

Hence

$$\ln \langle x | p \rangle / \langle 0 | 0 \rangle = p x f \text{ or } \langle x | p \rangle = \langle 0 | 0 \rangle \exp(p x f).$$

As in the nonrelativistic case, in order for $\langle x | p \rangle$ to be normalizable to $\delta(x - x')$, namely

$$\int \int dp dx' \langle x | p \rangle \langle p | x' \rangle = 1,$$

the constant f must be a purely imaginary number, $f = i\gamma$ (otherwise $\langle x | p \rangle$ would diverge, either as $x \rightarrow \infty$ or as $x \rightarrow -\infty$). By again identifying γ with $1/\hbar$, we obtain that even for the relativistic case

$$\langle x | p \rangle = \langle 0 | 0 \rangle \exp(i\gamma p x) = (2\pi\hbar)^{-1/2} \exp(ipx/\hbar)$$

and

$$\langle x' | \hat{p} | x \rangle = -i\hbar \frac{\partial}{\partial x} \delta(x - x').$$

V. SUMMARY AND CONCLUSIONS

In this paper we have derived both the Cartesian and the curvilinear $\langle q_l | p_l \rangle$ transformation matrices and the $[\hat{q}_l, \hat{p}_l]$ commutation relations. The derivation can be traced back to (i) the identification, via its spectral resolution [Eq. (3)], of

the momentum operator, (ii) the linear correspondence between classical observables and Hermitian quantum operators, and (iii) the definition of conjugate coordinate-momentum variables in classical mechanics and the invariance of the Hamiltonian to canonical transformations. We have shown that these building blocks are sufficient to enforce the $a \exp(i\gamma q_l p_l)$ form of the $\langle q_l | p_l \rangle$ transformation matrices and the ensuing momentum-coordinate commutation relations. The results are then generalized to the special-

relativistic case for Cartesian coordinates and momenta. Work on further generalizing the relativistic case to *curvilinear* coordinates is now in progress.

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 [3] The statement (cf., Ref. [5]) that \hat{p} is the generator of the shift operator $\exp(i\delta x \hat{p}/\hbar)$, and, for generalized coordinates, the appropriate Lie algebra, is not a *derivation* of the commutation relation, because this statement relies on the form of the coordinate representation of \hat{p} which we in fact wish to derive.

Likewise the correspondence between Poisson brackets and commutation relations is not a derivation of the latter, as it relies on our accepting the commutation relation between \hat{q} and \hat{p} .

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