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Hermiticity of Quantum Observables Versus Commutation Relations

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In order to obtain sum rules and spectral representations the Hermiticity property $\langle\Psi, A\Phi\rangle = \langle A\Psi, \Phi\rangle$ of observables is used. It is shown that for certain Ψ and Φ the property turns out to be inconsistent with the commutation relations that contain A. The known Schwinger paradox is explained by this inconsistency.

KEY WORDS: quantum mechanics; quantum field theory; commutation relations; hermitian operators; schwinger paradox; sum rules.

1. INTRODUCTION

Quantum observable A must satisfy the equation

$$\langle\Psi, A\Phi\rangle = \langle A\Psi, \Phi\rangle. \tag{1}$$

Note that this Hermiticity property (HP) is necessary but not sufficient for A to be an observable possessing a complete set of eigenvectors with real eigenvalues, see Richtmyer (1978). Equation (1) must hold for vectors Ψ, Φ belonging to Hilbert space $\mathcal{H}$ (more exactly belonging to A domain (Richtmyer, 1978)). In fact Eq. (1) is also valid when Ψ, Φ are A eigenvectors that may not belong to $\mathcal{H}$. In practice physicists use Eq. (1) for any Ψ and Φ they come across. For example, let us mention the derivations of spectral representations (Schweber, 1961) and sum rules (Lipkin, 1973). In other words, Eq. (1) is assumed (usually tacitly) to be a working tool that allows one to perform calculations.

Therefore, it seems urgent to give examples of Ψ and Φ for which Eq. (1) turns out to be invalid. This is done in Section 2.

In Section 3, the known Schwinger paradox is considered in detail in order to show that its derivation assumes the validity of a particular HP. This makes it possible to suggest the resolution of the paradox: this assumption must be rejected.

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The so-called Schwinger term and sum rules are dicussed in Sections 4 and 5. For conclusion see Section 6.

2. COMMUTATION RELATIONS VERSUS HERMITICITY

Let us show that for some Ψ and Φ, Eq. (1) turns out to be invalid.

Along with A consider an operator B such that $[A, B] = C \neq 0$ (note that A is multiple of the unit operator if $[A, B] = 0$ for all B). Let φ_a be A eigenvectors

$$A\varphi_a = a\varphi_a, \quad a \ \text{ are real.} \tag{2}$$

Consider the averages of $[A, B] - C$ in the state φ_a. We have

$$\begin{aligned}\langle\varphi_a, AB\varphi_a\rangle &= \langle\varphi_a, BA\varphi_a\rangle + C_{aa}\\ &= \langle a\varphi_a, B\varphi_a\rangle + C_{aa} = \langle A\varphi_a, B\varphi_a\rangle + C_{aa}.\end{aligned} \tag{3}$$

Equation (2) was used; C_{aa} denotes $\langle\varphi_a, C\varphi_a\rangle$. The consequence of Eq. (3) is that Eq. (1) is invalid for $\Psi = \varphi_a$, $\Phi = B\varphi_a$ when $C_{aa} \neq 0$ and must be replaced by

$$\langle\varphi_a, A\Phi\rangle - \langle A\varphi_a, \Phi\rangle = C_{aa}, \quad \Phi \equiv B\varphi_a. \tag{4}$$

Conversely, if Eq. (1) is postulated to be valid unconditionally, then $\langle\varphi_a, [A, B]\varphi_a\rangle$ must vanish in contradiction to $[A, B] \neq 0$ (C_{aa} being nonzero). Assuming that both Eq. (1) and commutation relations (CR) are valid we get paradoxes that mean that Eq. (1) and CR are inconsistent.

Example. Let A be a momentum operator $P = -id/dx$ and B be a function $g(x)$ of the position operator x, so that $[P, g(x)] = -ig'(x)$. Then Eq. (3) turns into

$$\begin{aligned}\langle\varphi_p, Pg\varphi_p\rangle - \langle P\varphi_p, g\varphi_p\rangle &= \langle\varphi_p, (-i)g'\varphi_p\rangle\\ &= (-i)[g(\infty) - g(-\infty)].\end{aligned} \tag{5}$$

Here $\varphi_p = \exp(ipx)$. The r.h.s. of Eq. (5), does not depend on p, is not zero and is finite if, e.g., $g(x) = \tanh x$. So Eq. (1) in the case $A = P$, $\Psi = \varphi_p$, and $\Phi = g\varphi_p$ is not consistent with $[P, x] = -i$.

It will be shown in the next section that analogous inconsistency of HP and CR explains (resolves) Schwinger's paradox.

3. SCHWINGER'S PARADOX

Let us consider a spinor field ψ that is free or interacts with other fields. Usual canonical CR are assumed for Schrödinger operators $\psi_\mu(\vec{x})$ and $\psi_\mu^+(\vec{x})$ (see, e.g., Bjorken and Drell, 1965)

$$\{\psi_\mu(\vec{x}), \psi_\nu^+(\vec{y})\}_+ = \delta_{\mu\nu}\delta(\vec{x}-\vec{y}). \tag{6}$$

Here $\mu, \nu = 1, 2, 3, 4$; ψ_ν^+ denotes Hermitian conjugated to ψ_ν. Zero anticommutators are not written out.

3.1. Let us calculate the double commutator $[j^0(\vec{x}), [H, j^0(\vec{y})]]$ where H is the total Hamiltonian and

$$j^0(\vec{x}) = \sum_\mu \psi_\mu^+(\vec{x})\psi_\mu(\vec{x}) \equiv \psi^\dagger(\vec{x})\psi(\vec{x})$$

(the column of ψ_ν is denoted by ψ and the row of ψ_ν^+ by $\psi^\dagger$). Zero commutators follow from Eq. (6) for Dirac charge and current densities

$$[j^0(\vec{x}), j^0(\vec{y})] = 0 \tag{7}$$

$$[j^0(\vec{x}), j^k(\vec{y})] = 0, \quad j^k(\vec{x}) \equiv \psi^\dagger(\vec{x})\alpha^k\psi(\vec{x}). \tag{8}$$

Suppose that the interaction terms in H depend only on bilinear combinations of the spinor fields, namely such as j^0, j^k, $\psi^\dagger\beta\psi$, $\psi^\dagger\beta\gamma_5\psi$ (without derivatives of ψ). Then it follows from Eq. (6) (in particular from Eqs. (7) and (8)) that $[j^0(\vec{x}), H]$ is equal to $[j^0(\vec{x}), H_{0s}]$, H_{0s} being the free spinor Hamiltonian

$$H_{0s} = \int d^3x\,\psi^\dagger(\vec{x})(-i\alpha^k\nabla_k + \beta m)\psi(\vec{x}), \tag{9}$$

see Bjorken and Drell (1965, chap. 13, Eq. (13.46)). Using Eq. (6) one gets

$$[j^0(\vec{x}), H] = -i\sum_k \nabla_k j^k(\vec{x}). \tag{10}$$

Equation (10) also follows from $\partial_t j^0 + div\vec{j} = 0$ and $[j^0, H] = i\partial_t j^0$. Because of Eq. (8) the double commutator $[j^0(\vec{x}), [H, j^0(\vec{y})]]$ equals zero. In particular, we have

$$[F, [H, F]] = 0, \quad F = \int d^3x f(\vec{x}) j^0(\vec{x}). \tag{11}$$

Stating the Schwinger paradox Itzykson and Zuber (1980, Vol. 2, chap. 11.3) assumed $f(\vec{x}) = \delta(\vec{x})$ so that $F = j^0(0)$.

In particular Eq. (11) leads to

$$D \equiv \langle\Omega, [F, [H, F]]\Omega\rangle = 0, \tag{12}$$

where Ω is the physical vacuum state. Let us assume that $H\Omega = 0$.

3.2. Schwinger (1959) calculated D in a different way, which results in a nonzero value for D in paradoxical contradiction to Eq. (12). The way begins as follows:

$$D = \langle \Omega, [F, [H, F]]\Omega \rangle = \langle \Omega, (FHF - FFH - HFF + FHF)\Omega \rangle$$
$$= -\langle \Omega, HF^2\Omega \rangle + 2\langle \Omega, FHF\Omega \rangle. \tag{13}$$

Only the equation $H\Omega = 0$ has been used. The positiveness of the second term in the r.h.s. of Eq. (13) will be argued in the next subsection. Schwinger (1959) as well as Itzykson and Zuber (1980, Vol. 2, chap. 11.3) tacitly assumed that the first term in the r.h.s. of Eq. (13) vanishes because of Eq. (1) for $A = H$, $\Psi = \Omega$, $\Phi = F^2\Omega$ and $H\Omega = 0$. So in this way one obtains $D > 0$ instead of $D = 0$.

To resolve the paradox the Eqs. (7) and (8) are usually stated to be false (the term "naive" is used). I suggest another resolution. Equation (6) is postulated, so Eqs. (7) and (8) are valid and the r.h.s. of Eq. (13) must vanish. This means that $\langle \Omega, HF^2\Omega \rangle$ must be equal to $2\langle \Omega, FHF\Omega \rangle > 0$ (and not to zero). In other words, the paradox shows that Eq. (1) is false for $A = H$, $\Psi = \Omega$, $\Phi = F^2\Omega$.

3.3. Now turn to the derivation of the inequality $\langle \Omega, FHF\Omega \rangle > 0$. This needs some assumptions. At first, the validity of the spectral resolution $H = \sum_n |n\rangle E_n \langle n|$ is assumed, $|n\rangle$ being H eigenvectors, $E_n \geq 0$. Further Eq. (1) in the form

$$\langle \Omega, Fn \rangle = \langle F\Omega, n \rangle = \langle n, F\Omega \rangle^* \tag{14}$$

is used. The result is strictly positive

$$\langle \Omega, FHF\Omega \rangle = \sum_n E_n |\langle n|F|\Omega \rangle|^2 \tag{15}$$

if $\langle n, F\Omega \rangle \neq 0$ for some $|n\rangle \neq \Omega$.

In the case of the free spinor field one may prove the inequality $2\langle \Omega, FHF \rangle > 0$ using canonical anticommutators for fermion creation–destruction operators (the anticommutators being tantamount to Eq. (6)). One obtains that $\langle \Omega, FHF\Omega \rangle$ diverges, i.e., in this case the paradox assumes the extreme form "0 equals ∞."

4. REGULARIZATION AND SCHWINGER TERMS

To regularize $\langle \Omega, FHF\Omega \rangle$ Schwinger (1959) proposed to replace $j^0(\vec{x}) = \psi^\dagger(\vec{x})\psi(\vec{x})$ by

$$j_r^0(\vec{x}) = \psi^\dagger(\vec{x} - \vec{\varepsilon})\psi(\vec{x} + \vec{\varepsilon})$$

(the subsequent symmetrical averaging over all $\vec{\varepsilon}$ directions being implied). It follows from Eq. (6) that the commutators $[j_r^0(\vec{x}), j_r^0(\vec{y})$ and $[j_r^0(\vec{x}, j_r^k(\vec{y}))]$ are nonzero and, therefore, $[F_r, [H, F_r]] \neq 0$. Schwinger did not verify the equality

$$\langle \Omega, [F_r, [H, F_r]]\Omega \rangle = 2\langle \Omega, F_r H F_r \Omega \rangle.$$

Meanwhile if the equality does not hold, the paradox still exists though it does not have a simple form "zero equals nonzero." Schwinger's purpose was to demonstrate that $\langle\Omega, [j_r^0(\vec{x}), j_r^k(\vec{y})]\Omega$ contains a nonvanishing contribution proportional to $\nabla_k\delta(\vec{x}-\vec{y})$. It is called Schwinger's term and has been discussed in Itzykson and Zuber (1980, Vol. 2, chap. 11.3) and Weinberg (2000). Weinberg noted that dimensional regularization does not lead to the Schwinger term. Then Schwinger's paradox survives under regularization.

Let us mention a modification of Schwinger's paradox. There exists a way of calculating the average $\langle\Omega, [j^0(\vec{x}), j^k(\vec{y})]\Omega\rangle$ that gives to it a nonzero value (proportional to $\nabla_k\delta(\vec{x}-\vec{y})$ in contradiction to Eq. (8). See, e.g., Brown (1966, Appendix A) and Itzykson and Zuber (1980, Vol. 1, chap. 5.1.7) (in the latter reference see Eq. (5.98) that follows from Eqs. (5.91) and (5.89), or from Eq. (5.81)). The modification looks simpler than Schwinger's version. However, its derivation uses among others the assumptions of the kind represented by Eq. (14) needed to obtain absolute squares of matrix elements, cf. Eq. (15).

5. "SUM RULES" AND SCHWINGER PARADOX

To illustrate the relation between "sum rules" and Schwinger's paradox I consider a simple case of nonrelativistic quantum mechanics when the Hamiltonian is equal to $p^2/2m + V(x)$. Similarly to Section 3 an average of the double commutator $[F, [H, F]]$ is calculated in two ways, F being now some function of x. The first way uses only the canonical CR $[p, x] = -i$ and gives

$$\langle\Omega, [F, [H, F]]\Omega\rangle = \langle\Omega, (F'(x))^2\Omega\rangle/m.$$

The second way is carried out analogously to Subsection 3.2 and assumes the validity of Eq. (1) in the form

$$\langle\Omega, HF^2\Omega\rangle = \langle H\Omega, F^2\Omega\rangle. \tag{16}$$

Here and below Ω denotes H eigenvector with eigenvalue E_0.

"Sum rules" are obtained when we equate the results of these ways of calculation, e.g., see Lipkin (1973),

$$\left\langle\Omega, \frac{1}{m}\left(\frac{dF}{dx}\right)^2\Omega\right\rangle = 2\sum_2(E_n - E_0)|\langle n|F|\Omega\rangle|^2. \tag{17}$$

For possible physical applications of "sum rules" see Lipkin (1973). However, it should be stressed that their theoretical validity depends on the validity of Eq. (16). We may use "sum rules" for verification of Eq. (16). For this purpose one must calculate directly the sum in the r.h.s. of Eq. (17) and compare the r.h.s. with the l.h.s. Their inequality will mean that we have a paradox that shows that Eq. (16) is inconsistent with $[p, x] = -i$. Schwinger's paradox may be considered as an example of "sum rules" that is obviously violated.

6. CONCLUSION

It was shown that the HP, see Eq. (1), for some A, Ψ, Φ may turn out to be inconsistent with CR.

The usual way of the Schwinger paradox resolution is to doubt canonical CR, HP being tacitly assumed. I suggest another resolution: CR must be considered as fundamental fixed postulates that are necessary for quantum calculations. To resolve the paradox, one must accept that HP is invalid for some A, Ψ, Φ.

It was stressed in Section 5 that “sum rules” derivation uses HP as in the case of Schwinger’s paradox. Therefore, the rules may be invalid as theoretical statements. Their derivation should be complemented by the proof of the corresponding HP.

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