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Time in quantum mechanics and quantum field theory

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Abstract

W Pauli pointed out that the existence of a self-adjoint time operator is incompatible with the semi-bounded character of the Hamiltonian spectrum. As a result, there has been much argument about the time–energy uncertainty relation and other related issues. In this paper, we show a way to overcome Pauli's argument. In order to define a time operator, by treating time and space on an equal footing and extending the usual Hamiltonian $\hat{H}$ to the generalized Hamiltonian $\hat{H}_\mu$ (with $\hat{H}_0 = \hat{H}$), we reconstruct the analytical mechanics and the corresponding quantum (field) theories, which are equivalent to the traditional ones. The generalized Schrödinger equation $\mathrm{i}\partial_\mu\psi = \hat{H}_\mu\psi$ and Heisenberg equation $\mathrm{d}\hat{F}/\mathrm{d}x^\mu = \partial_\mu\hat{F} + \mathrm{i}[\hat{H}_\mu, \hat{F}]$ are obtained, from which we have: (1) t is to $\hat{H}_0$ as x_j is to $\hat{H}_j$ ($j = 1, 2, 3$); likewise, t is to $\mathrm{i}\partial_0$ as x_j is to $\mathrm{i}\partial_j$; (2) the proposed time operator is canonically conjugate to $\mathrm{i}\partial_0$ rather than to $\hat{H}_0$, therefore Pauli's theorem no longer applies; (3) two types of uncertainty relations, the usual $\Delta x_\mu \Delta p_\mu \geqslant 1/2$ and the Mandelstam–Tamm treatment $\Delta x_\mu \Delta H_\mu \geqslant 1/2$, have been formulated.

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1. Introduction

Time in quantum mechanics has been a controversial issue since the advent of quantum theory. Nowadays, it still has theoretical and practical interest.

On the one hand, there exist enough reasons for us to consider time as a dynamical variable or operator: (1) according to the principle of relativity, a position vector *operator* in a reference system would have a temporal component in another reference system; (2) the four-dimensional (4D) angular momentum tensor operator of quantum field theories shows that the time seems to play a twofold role, as both a parameter and an operator; (3) a major conceptual problem in quantum gravity is the issue of what time is, and how it has to be treated in the formalism [1]; (4) another related problem, which still remains controversial today, is concerned with the formal definitions of tunnelling time [2, 3] and traversal time [4–11]. This subtle question, motivated in part by the possible applications of tunnelling in semiconductor technology, has received considerable attention in recent years; (5) in many cases, time is not a mere parameter, but an intrinsic property characterizing the duration of certain physical processes. The lifetime of unstable particles or collision complexes is a well-known example [4]; (6) in signal analysis and signal processing theory [12, 13], as physical quantities time and frequency are treated on a completely equal footing; (7) lack of an appropriate time operator has a number of consequences. In particular, the time–energy uncertainty relation has remained ambiguous over these years and its improper application has led to a great deal of confusion [14–21].

But on the other hand, as is well known according to Pauli's argument [22], the existence of a self-adjoint time operator is incompatible with the semi-bounded character of the Hamiltonian spectrum. By using a different argument based on the time-translation property of the arrival time concept, Allcock has found the same negative conclusion [23–25]. This negative conclusion can also be traced back to the semi-infinite nature of the Hamiltonian spectrum.

A way out of the dilemma set by Pauli's objection is based on the use of positive operator valued measures (POVMs) [26, 27]. Here, we shall propose a different one that emphasizes the need to put time and space on an equal footing. In this work, we apply natural units of measurement ($\hbar = c = 1$).

2. The flaws of Pauli's statement

According to Pauli's statement, let $\hat{H}\psi_E = E\psi_E$ and the *time operator* $\hat{T}$ satisfy $[\hat{H}, \hat{T}] = -\mathrm{i}$, using $[f, \hat{H}] = \mathrm{i}\frac{\partial f}{\partial t}$, we have $\hat{H}\,\mathrm{e}^{\mathrm{i}\alpha\hat{T}}\psi_E = (E+\alpha)\,\mathrm{e}^{\mathrm{i}\alpha\hat{T}}\psi_E$, where α is an arbitrary constant. That is, $\mathrm{e}^{\mathrm{i}\alpha\hat{T}}\psi_E$ is also the eigenstate of the Hamiltonian $\hat{H}$ with the eigenvalue $(E+\alpha)$, which implies that the existence of the time operator contradicts the fact that the Hamiltonian spectrum must be positive.

However, Pauli's (or Allcock's) statement may be criticized according to several arguments:

(1) Pauli's (or Allcock's) demonstration implies a premise that the *time* operator itself is not explicitly *time* dependent: $\frac{\mathrm{d}\hat{T}}{\mathrm{d}t} = \frac{\partial\hat{T}}{\partial t} + \mathrm{i}[\hat{H}, \hat{T}] = \mathrm{i}[\hat{H}, \hat{T}]$. However, studying the conservative property of the 4D angular momentum tensor of a free field (e.g., the Dirac field), we find that, in contradiction to Pauli's (or Allcock's) statement, we have $\frac{\mathrm{d}\hat{T}}{\mathrm{d}t} = \frac{\partial\hat{T}}{\partial t} + \mathrm{i}[\hat{H}, \hat{T}] = \frac{\partial\hat{T}}{\partial t}$ (see appendix A). That is to say, in Heisenberg's picture, the time operator is explicitly time dependent, just as the position operator is explicitly dependent on the position coordinate.

In fact, the 4D angular momentum tensor of a charged field is related to the electromagnetic moment tensor (see appendix B), and has observable effects [28].

(2) As will be shown later, the correctly defined time operator is canonically conjugate to $\mathrm{i}\frac{\partial}{\partial t}$ rather than to $\hat{H}$. Correspondingly, Pauli's (or Allcock's) statement no longer holds and it is now just a matter of choosing a new zero-energy reference surface.

(3) In fact, Galapon [29–31] has shown that Pauli's implicit assumptions are not consistent in a single Hilbert space and that a class of self-adjoint and canonical time of arrival operators can be constructed for a spatially confined particle.

3. The starting point for introducing the time operator

As mentioned above, an important motive for trying to introduce a time operator lies in that the theory of relativity requires that time and space must be treated on an equal footing. However, the traditional theories treat time and space very differently:

(1) The traditional many-particle system theory has a defect: the system contains only one time variable while there are as many position variables as there are particles which is in contradiction with the relativity of simultaneity. As observed in another reference system, all particles in the system would no longer share a common time coordinate, and the original Hamiltonian would no longer correspond to *the total energy*, i.e., the sum of the individual energies of all particles at the same moment of time (note that the energy of a single particle in the system is not necessarily conservative). Historically, in view of this unsatisfactory aspect of the traditional theory, people have introduced the many-time formalism theory [32–34] (being equivalent to the Heisenberg–Pauli theory), where for a system composed of N particles, there corresponds N distinct time and space variables. In this sense, time and space are treated with equality in the many-time formalism [35].

(2) However, even in the many-time formalism of quantum mechanics, for every single particle of a many-particle system, its time and space coordinates are still not equal, namely its space coordinates can be taken as dynamic variables while the time coordinate cannot. This is what we will try to rectify in this paper. In view of what is mentioned above, our discussion would only be limited to the relativistic single-particle and quantum field cases (while the nonrelativistic single-particle theory can be taken as a special case of the former).

Certainly, even in the classical theory of relativity, time and space could not be completely equal because of the law of causality. In other words, in spacetime diagrams, the distribution of the worldline of an arbitrary particle is not symmetrical about the surface of lightcone.

In a word, in order to define a time operator, it is necessary to put the time coordinate on the same footing as position coordinates. For this, we reconstruct the analytical mechanics and the corresponding quantum theories, which are equivalent to the traditional ones.

3.1. The generalized Schrödinger equation

Starting from the usual relativistic quantum mechanics equations, we can obtain the generalized Schrödinger equations as follows:

$$\mathrm{i}\partial_\mu \psi(x) = \hat{H}_\mu \psi(x) \qquad (\mu = 0, 1, 2, 3) \tag{1}$$

where $\hat{H}_\mu$ is the generalized Hamiltonian with $\hat{H}_0 = \hat{H}$ being the usual Hamiltonian.

3.1.1. The generalized Schrödinger form of the Klein–Gordon equation. As for the Klein–Gordon equation

$$(\partial^\mu \partial_\mu + m^2)\phi = 0 \tag{2}$$

it is possible to find a Schrödinger formulation [36] of equation (2), where it is transformed into equation (1) with $\mu = 0$. Now, we will show that equation (2) can also be read as equation (1) with $\mu = l = 1, 2, 3$. Let

$$\left.\begin{aligned} \varphi &= \frac{1}{2}\left(\mathrm{i} - \frac{\mathrm{i}}{m}\frac{\partial}{\partial x^l}\right)\phi \\ \chi &= \frac{1}{2}\left(\mathrm{i} + \frac{\mathrm{i}}{m}\frac{\partial}{\partial x^l}\right)\phi \end{aligned}\right. \qquad (l = 1, 2, 3) \tag{3}$$

(fortunately, the massless spin-0 particle does not exist) and

$$\psi = \begin{pmatrix}\varphi \\ \chi\end{pmatrix} \qquad \tau_2 = \begin{pmatrix}0 & -\mathrm{i} \\ \mathrm{i} & 0\end{pmatrix} \qquad \tau_3 = \begin{pmatrix}1 & 0 \\ 0 & -1\end{pmatrix}. \tag{4}$$

Using equations (3) and (4), we can express equation (2) as equation (1) with $\mu = l = 1, 2, 3$, where

$$\hat{H}_l = -\frac{\mathrm{i}}{2m}(\tau_3 + \mathrm{i}\tau_2)(\partial^\nu\partial_\nu - \partial^l\partial_l) - \mathrm{i}m\tau_3 \tag{5}$$

note that the repeated indices in $\partial^\nu\partial_\nu$ are summed while those in $\partial^l\partial_l$ are not, $\nu = 0, 1, 2, 3$ while l is one of $1, 2, 3$. An operator must satisfy the condition of Hermiticity. Then, similar to reference [36], the scalar product and the expectation value are defined as

$$\begin{aligned}\langle\psi|\psi'\rangle &\equiv \int \mathrm{d}\sigma^l \psi^+\tau_2\psi \\ \langle\hat{L}\rangle &\equiv \int \mathrm{d}\sigma^l \psi^+\tau_2\hat{L}\psi\end{aligned} \qquad (l = 1, 2, 3) \tag{6}$$

respectively, where $\mathrm{d}\sigma^\mu \equiv (\mathrm{d}x^1\,\mathrm{d}x^2\,\mathrm{d}x^3,\ \mathrm{d}t\,\mathrm{d}x^2\,\mathrm{d}x^3,\ \mathrm{d}x^1\,\mathrm{d}t\,\mathrm{d}x^3,\ \mathrm{d}x^1\,\mathrm{d}x^2\,\mathrm{d}t) = (\mathrm{d}\sigma^0, \mathrm{d}\vec{\sigma})$ stands for a 3D hypersurface element, and $\mathrm{d}\sigma^l \equiv (\mathrm{d}t\,\mathrm{d}x^2\,\mathrm{d}x^3,\ \mathrm{d}x^1\,\mathrm{d}t\,\mathrm{d}x^3,\ \mathrm{d}x^1\,\mathrm{d}x^2\,\mathrm{d}t) = (\mathrm{d}\vec{\sigma})$.

3.1.2. The generalized Schrödinger form of the Dirac equation. Substituting

$$\hat{H}_\mu = -\gamma_\mu(\mathrm{i}\gamma^\nu\partial_\nu - \mathrm{i}\gamma^\mu\partial_\mu) + \gamma_\mu m \qquad (\mu = 0, 1, 2, 3) \tag{7}$$

into equation (1), we can obtain the same Dirac equation for $\mu = 0, 1, 2, 3$, where γ^μ are the Dirac matrices, the repeated indices in $\mathrm{i}\gamma^\nu\partial_\nu$ are summed while those in $\mathrm{i}\gamma^\mu\partial_\mu$ are not. In contrast to the case of the Klein–Gordon equation, here the scalar product and the expectation value are defined as the traditional ones.

All mentioned above in section 3.1. also hold in the presence of interactions. For example, one just makes the replacement $\partial_\mu \to \partial_\mu + \mathrm{i}eA_\mu$ for each equation above that contains ∂_μ $(\mu = 0, 1, 2, 3)$.

3.2. The generalized Heisenberg equation

Using equation (1) and the corresponding definitions of expectation value, one can obtain

$$\frac{\mathrm{d}\langle\hat{F}\rangle}{\mathrm{d}x^\mu} = \left\langle\frac{\partial\hat{F}}{\partial x^\mu}\right\rangle + \mathrm{i}\langle[\hat{H}_\mu, \hat{F}]\rangle \tag{8}$$

where $\langle\hat{F}\rangle$ is the expectation value of a dynamical operator $\hat{F}$.

In general, by enlarging t to x^μ, we can arrive at the 4D generalization of the time-evolution operator (say, the spacetime evolution operator). Furthermore, in an analogous procedure, we can arrive at the 4D generalization of Heisenberg's equation

$$\frac{\mathrm{d}\hat{F}}{\mathrm{d}x^\mu} = \frac{\partial\hat{F}}{\partial x^\mu} + \mathrm{i}[\hat{H}_\mu, \hat{F}]. \tag{9}$$

Traditionally, the 4D generalization of Heisenberg's equation is [37]

$$\frac{\partial\hat{F}}{\partial x^\mu} = \mathrm{i}[\hat{P}_\mu, \hat{F}]. \tag{10}$$

However, from equation (10), we can only obtain $\frac{\partial\hat{F}}{\partial x^\mu} = \frac{\partial\hat{F}}{\partial x^\mu}$. That is to say, in contrast to equation (9), equation (10) is only a mathematical identity (without any physical content) rather than a physical equation.

In addition, using equation (9), one can obtain

$$\Delta x_\mu \Delta H_\mu \geqslant \tfrac{1}{2} \tag{11}$$

where $\Delta H_\mu \equiv \sqrt{\langle(\hat{H} - \langle\hat{H}\rangle)^2\rangle}$ is the uncertainty (the mean variation) of $\hat{H}$, and Δx_μ is defined by $\Delta x_\mu \left|\left\langle \frac{\mathrm{d}\hat{F}}{\mathrm{d}x^\mu}\right\rangle\right| = \Delta F$. That is to say, the Mandelstam–Tamm treatment [38] of the time–energy uncertainty relation (as it is presented in most textbooks) has a counterpart in the position–momentum uncertainty relation.

3.3. The generalization in quantum field theory

Before going on, let us introduce the generalized analytical mechanics. Let q be the generalized coordinates of a system, p the generalized momenta, L the Lagrangian, H the Hamiltonian and A the action. *Generalized analytical mechanics* can be obtained by extending t to x^μ (let $\mu = 1$ without loss of generality). For this, we make the following replacements:

$$A = \int L\,\mathrm{d}t \to A = \int L^1\,\mathrm{d}x^1 \quad \text{(from which we define } L^1\text{)} \tag{12}$$

$$q(t) \to q(x^1) \qquad L(q(t), \dot{q}(t)) \to L^1(q(x^1), \partial_1 q(x^1)) \quad \text{(by definition).} \tag{13}$$

Using equations (12) and (13), we have

$$\frac{\partial L}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} = 0 \to \frac{\partial L^1}{\partial q} - \partial^1 \frac{\partial L^1}{\partial \partial^1 q} = 0 \qquad \text{(by the principle of least action).} \tag{14}$$

In fact, equation (14) is a special case of the Whittaker equation [39]. Furthermore,

$$p \equiv \frac{\partial L}{\partial \dot{q}} \to p_{(1)} \equiv \frac{\partial L^1}{\partial \partial^1 q} \qquad \text{(by definition)} \tag{15}$$

$$\dot{p} = \frac{\partial L}{\partial q} \to \partial^1 p_{(1)} = \frac{\partial L^1}{\partial q} \qquad \text{(by equations (14) and (15))} \tag{16}$$

$$H \equiv p\dot{q} - L \to H_1 \equiv p_{(1)}\partial_1 q - L_1 \qquad \text{(by definition)} \tag{17}$$

$$\dot{q} = \frac{\partial H}{\partial p} \qquad \dot{p} = -\frac{\partial H}{\partial q} \to \partial_1 q = \frac{\partial H_1}{\partial p_{(1)}} \qquad \partial_1 p_{(1)} = -\frac{\partial H_1}{\partial q}$$
$$\text{(by equations (12)–(17))} \tag{18}$$

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \{H, f\} \to \frac{\mathrm{d}f}{\mathrm{d}x^1} = \frac{\partial f}{\partial x^1} + \{H_1, f\} \qquad \text{(by equations (18))} \tag{19}$$

where $f = f(q, p_{(1)}, x^1)$ and $\{H_1, f\} = \frac{\partial f}{\partial q}\frac{\partial H_1}{\partial p_{(1)}} - \frac{\partial f}{\partial p_{(1)}}\frac{\partial H_1}{\partial q}$.

Clearly, all the preceding steps are based on first principles and do not resort to any heuristic argument. Then we put t on the same footing as $\vec{x}$ in our analytical mechanics. The correctness of such a formalism can be further shown later.

The generalization mentioned above is also valid for quantum field theory. Let $\mathrm{d}\sigma^\mu$ ($\mu = 0, 1, 2, 3$) stand for a 3D hypersurface element, if the action $A = \int \mathrm{d}^4x\,\Gamma$, where Γ stands for the Lagrange density, using equation (12), we have

$$L^\mu = \int \mathrm{d}\sigma^\mu \Gamma \qquad (\mu = 0, 1, 2, 3). \tag{20}$$

Obviously, $L^0 = L$ is the usual Lagrangian.

We assume that the 3D hypersurface σ^l $(l = 0, 1, 2, 3)$ is divided into small cells of size $\Delta\sigma_i^l$. With each cell, we associate the respective average values of the functions, for example:

$$\phi_i(x^l) = \frac{1}{\Delta\sigma_i^l}\int_{\Delta\sigma_i^l} \phi(\vec{x}, t)\, \mathrm{d}\sigma^l. \tag{21}$$

As $\Delta\sigma_i^l \to 0$, $\phi_i(x^l) \to \phi(\vec{x}, t) \equiv \phi(x)$. By applying equations (12)–(19) and proceeding analogously to the traditional process of canonical quantization, we can obtain the following results. The generalized canonically conjugate field of $\phi(\vec{x}, t)$ is defined as

$$\pi_l(\vec{x}, t) \equiv \frac{\partial\Gamma(x)}{\partial\partial^l\phi(x)} \qquad (l = 0, 1, 2, 3) \tag{22}$$

and the generalized Hamiltonian is

$$H_l(x^l) \equiv \int [\pi_l(x)\partial_l\phi(x) - g_{ll}\Gamma(x)]\, \mathrm{d}\sigma^l \tag{23}$$

where $g_{\mu\nu}$ is the metric tensor with diag$(1, -1, -1, -1)$, the repeated index l is not summed. Obviously, $T_{\mu\nu} = \pi_\mu\partial_\nu\phi - g_{\mu\nu}\Gamma$ is the energy–momentum tensor of a field (see appendix C).

In the case of quantum field theory, however, the condition of microcausality must be taken into account. Traditionally, we first study the plane-wave solutions of a free field equation and obtain $p_0^2 = p_1^2 + p_2^2 + p_3^2 + m^2$ (in general, we can call $w_\mu \equiv \sqrt{p_\mu^2}$ $(\mu = 0, 1, 2, 3)$ the *frequency* or *wave number in* x^μ), and then write the general solution as a linear combination of the $\pm w_0$ solutions. The general solution contains the factors $\mathrm{e}^{\pm\mathrm{i}px}$, where $px = w_0t - p_1x_1 - p_2x_2 - p_3x_3$, $w_0 \geqslant 0$ while $p_1, p_2, p_3 \in (-\infty, +\infty)$. Now, in our case (making the replacement $t \to x^1$ without loss of generality), in order to preserve microcausality, when we obtain $p_0^2 = p_1^2 + p_2^2 + p_3^2 + m^2$, i.e., $p_1^2 = p_0^2 - p_2^2 - p_3^2 - m^2$, we rewrite the general solution as a linear combination of the $\pm w_1 \equiv \pm\sqrt{p_1^2}$ solutions. This time in the factors $\mathrm{e}^{\pm\mathrm{i}px}$, we have $px = p_0t - w_1x_1 - p_2x_2 - p_3x_3$, where $w_1 \equiv \sqrt{p_1^2} \geqslant 0$ while $p_0, p_2, p_3 \in (-\infty, +\infty)$.

In the following, we will take the Klein–Gordon field and the Dirac field for example, while the photon field is analogous to the former.

3.3.1. The Klein–Gordon field. The Lagrange density of the Klein–Gordon field $\phi(\vec{x}, t) = \phi(x)$ reads

$$\Gamma(x) = \partial_\mu\phi^+(x)\partial^\mu\phi(x) - m^2\phi^+(x)\phi(x) \tag{24}$$

where ϕ^+ is the Hermitian adjoint of ϕ. Let $w_\mu \equiv \sqrt{k_\mu^2}$ and $kx = k_lx^l + w_\mu x^\mu$ (the repeated index μ is not summed), where $w_\mu \geqslant 0$ and $k_l \in (-\infty, +\infty)$, $\mu \neq l = 0, 1, 2, 3$. One can easily show that the fields ϕ and ϕ^+ can also be expressed as a linear combination of the $\pm w_\mu$ solutions

$$\phi(x) = \int \mathrm{d}\sigma_k^\mu \left(a_k u_k(x) + b_k^+ u_k^*\right) \tag{25}$$

where $u_k(x) = [2w_1(2\pi)^3]^{-\frac{1}{2}}\, \mathrm{e}^{-\mathrm{i}kx}$, $\mathrm{d}\sigma_k^\mu$ is the μ-component of the 3D hypersurface element in 4-momentum space. As $w_\mu \to 0$, all our final results (in the observable sense) also hold. By defining $a\overleftrightarrow{\partial}b \equiv a\partial_\mu b - (\partial_\mu a)b$, we have

$$\begin{aligned} a_k &= \int \mathrm{d}\sigma^\mu u_k^*(x)\mathrm{i}\overleftrightarrow{\partial}\phi(x) \\ \int \mathrm{d}\sigma^\mu u_{k'}^*(x)\mathrm{i}\overleftrightarrow{\partial}u_k(x) &= \delta^3(k_j - k_j') \qquad (\mu \neq j = 0, 1, 2, 3) \end{aligned} \tag{26}$$

and so on. Using equation (22), we have

$$\pi_\mu(x) = \partial_\mu\phi^+(x) \qquad \pi_\mu^+ = \partial_\mu\phi(x) \tag{27}$$

in view of the fact that what we finally utilize is the canonically conjugate commutators rather than the so-called covariant commutators (the former correspond to the derivative of the latter), and we only discuss the former. Generally, when ϕ and ϕ^+ are expressed as a linear combination of the $\pm w_\mu\big(w_\mu \equiv \sqrt{k_\mu^2}\big)$ solutions, we have

$$[\phi(x), \pi_\mu(y)] = \mathrm{i}\int \mathrm{d}^4k[w_\mu\delta(k^2 - m^2)\,\mathrm{e}^{-\mathrm{i}k(x-y)}] \tag{28}$$

$$[\phi(x), \pi_\mu(y)]|_{x_\mu\to y_\mu} = \mathrm{i}\delta^3(x^l - y^l) \qquad (\mu, l = 0, 1, 2, 3 \quad \mu \neq l) \tag{29}$$

and so on. Using equation (23), we have

$$\begin{aligned} H_\mu &= \int \mathrm{d}\sigma^\mu\big[\pi_\mu\partial_\mu\phi + \pi_\mu^+\partial_\mu\phi^+ + \Gamma\big] \\ &= \int \frac{\mathrm{d}\sigma_k^\mu}{(2\pi)^3} w_\mu(k)[a^+(k)a(k) + b^+(k)b(k) + 1]. \end{aligned} \tag{30}$$

In view of $w_\mu = w_\mu(k) \geqslant 0$ (but not $w_\mu(k) \equiv 0$ for arbitrary k_l, $\mu, l = 0, 1, 2, 3$, $\mu \neq l$), the generalized Hamiltonians H_μ are always positive for the Bose field. On the one hand, $\phi(x)$ is written as a Hilbert space operator, which creates and destroys the particles that are the quanta of field excitation. On the other hand, $\phi(x)$ is written as a linear combination of the $\pm w_\mu$ (μ is one of 0, 1, 2, 3) solutions of the Klein–Gordon equation. Both signs of the x^μ-dependence in the exponential appear, although w_μ is always positive (as mentioned before, our final results hold also for $w_\mu \to 0$). If $\phi(x)$ is a single-particle wavefunction, it would correspond to states of positive- and negative-frequency ($\pm w_\mu$) modes. The connection between the particle creation operators and the waveforms displayed here is always valid for free quantum fields: a negative-frequency solution of the field equation, being the Hermitian conjugate of a positive-frequency solution, has as its coefficient the operator that creates a particle in that positive-frequency single-particle wavefunction. In this way, the fact that the related equations have both positive- and negative-frequency solutions (because of $k_0^2 = k_1^2 + k_2^2 + k_3^2 + m^2$ being always valid) is reconciled with the requirement that a sensible quantum theory contain only positive generalized Hamiltonians.

For the photon field, the zero-point contribution to the generalized Hamiltonians H_μ may lead to *generalized* Casimir effects [40], which may be verified by a different experimental set-up for a different $\mu = 0, 1, 2, 3$ (for $\mu = 1, 2, 3$, the Casimir force is related to the time-varying difference ΔH_μ, which will be discussed in our next paper).

Finally, the Heisenberg equations of motion are

$$\partial_\mu\phi = \mathrm{i}[H_\mu, \phi] \tag{31}$$

$$\partial_\mu\pi_\mu = \mathrm{i}[H_\mu, \pi_\mu] \tag{32}$$

and so on, from which the Klein–Gordon equations can be obtained.

3.3.2. The Dirac field. As for the Dirac field equation, however, its $\pm w_l$ ($l = 1, 2, 3$) solutions are not orthogonal and therefore must be tackled in another manner. According to the traditional procedure of transforming the quantum mechanics description into the quantum field theory one, our discussions can be carried out on the basis of equations (1) and (7).

For this, we reinterpret $\psi(x)$ in equation (1) as a field operator that obeys the canonical anti-commutation rules:

$$\begin{aligned}\{\psi_\alpha(\vec{x},t),\psi_\beta^+(\vec{x}',t)\} &= \delta_{\alpha\beta}\delta^3(\vec{x}-\vec{x}')\\ \{\psi_\alpha(\vec{x},t),\psi_\beta(\vec{x}',t)\} &= \left\{\psi_\alpha^+(\vec{x},t),\psi_\beta^+(\vec{x}',t)\right\} = 0.\end{aligned} \tag{33}$$

The generalized Hamiltonian is

$$H_\mu = \int \psi^+(x)\hat{H}_\mu\psi(x)\,\mathrm{d}^3x \tag{34}$$

where $\hat{H}_\mu$ is given by equation (7). The dynamics of the field operators are determined by the generalized Heisenberg equations of motion

$$\frac{\partial\psi(x)}{\partial x^\mu} = \mathrm{i}[H_\mu, \psi(x)] \tag{35}$$

$$\frac{\partial\psi^+(x)}{\partial x^\mu} = \mathrm{i}[H_\mu, \psi^+(x)] \tag{36}$$

for example, with the help of equation (33), one finds that equation (35) leads back to equation (1) (and hence the Dirac equation). Furthermore, using equation (34), we have

$$H_\mu = \int \mathrm{d}^3p\sum_s p_\mu\left[c^+(p,s)c(p,s) + d^+(p,s)d(p,s) + \tfrac{1}{2}\delta_{\mu0}\right] \tag{37}$$

where c^+, c (d^+, d) are the creator and annihilator of a particle (anti-particle), respectively. p_μ is the four-momentum of a single Fourier mode of the field. Obviously, H_μ is the total four-momentum of the field, which implies that

$$H_\mu = P_\mu = \int \psi^+(x)\hat{P}_\mu\psi(x)\,\mathrm{d}^3x \qquad (\mu = 0,1,2,3) \tag{38}$$

where $\hat{P}_\mu = \mathrm{i}\frac{\partial}{\partial x^\mu}$. However, in spite of equation (38), if we rewrite equation (35) as

$$\frac{\partial\psi(x)}{\partial x^\mu} = \mathrm{i}[P_\mu, \psi(x)] \tag{39}$$

contrary to equation (35), equation (39) gives $\frac{\partial\psi(x)}{\partial x^\mu} = \frac{\partial\psi(x)}{\partial x^\mu}$ instead of leading back to equation (1).

3.3.3. Interacting quantum fields. In the following, we will take quantum electrodynamics (QED) for example, where the Hamilton density describing the interaction is given by

$$H_{\text{int}} = \mathrm{e}\bar{\psi}(x)\gamma^\mu\psi(x)A_\mu(x). \tag{40}$$

In the interaction picture, the field operators $\psi(x)$ and $A_\mu(x)$ are the same as for free fields. Meanwhile, in our formalism, the electromagnetic vector potential $A_\mu(x)$ is written as a linear combination of the $\pm w_1\big(w_1 \equiv \sqrt{k_1^2}\big)$ solutions

$$A_\mu(x) = \frac{1}{\sqrt{(2\pi)^3}}\int \mathrm{d}\sigma_k^1\frac{1}{\sqrt{2w_1}}\sum_\lambda \mathrm{e}_\mu(k,\lambda)\big(a_{k\lambda}\,\mathrm{e}^{-\mathrm{i}kx} + a_{k\lambda}^+\,\mathrm{e}^{\mathrm{i}kx}\big) \tag{41}$$

where $\mathrm{e}_\mu(k,\lambda)$ $(\mu = 0,1,2,3)$ are the polarization four-vectors, $\lambda = 0,1,2,3$, the polarization indices, $kx = k_0t - w_1x_1 - k_2x_2 - k_3x_3$, $w_1 \equiv \sqrt{k_1^2}$ while $k_0, k_1, k_2, k_3 \in (-\infty, +\infty)$. As mentioned before, our final results also hold for $w_1 \to 0$.

To apply Wick's theorem, as for $A_\mu(x)$, we must generalize the definitions of the time-ordering product and the time-evolution operator to the x^μ-*ordering product* and x^μ-*evolution operator*, respectively. For example, the x^1-ordering product is

$$T_1 A_\mu(x) A_\nu(y) \equiv \begin{cases} A_\mu(x) A_\nu(y) & x^1 > y^1 \\ A_\mu(y) A_\nu(x) & x^1 < y^1 \end{cases} \tag{42}$$

and x^1-evolution operator $U(x_1, x_1')$ is defined by

$$|a(x_1)\rangle = U(x_1, x_1')|a(x_1')\rangle. \tag{43}$$

From equations (41) and (42), it can be shown that the x^1-*Feynman propagator* for photons is the same as the usual t-Feynman propagator:

$$\langle 0|T_1 A_\mu(x) A_\nu(y)|0\rangle = \frac{1}{(2\pi)^4} \int \mathrm{d}^4k \frac{-\mathrm{i}g_{\mu\nu}}{k^2 + \mathrm{i}\varepsilon} \mathrm{e}^{-\mathrm{i}k(x-y)}. \tag{44}$$

Furthermore, in the interaction picture, according to our formalism, we have

$$\mathrm{i}\frac{\partial}{\partial x^1}|a\rangle = H_{\mathrm{int}}|a\rangle. \tag{45}$$

Let $S \equiv U(+\infty, -\infty)$, from equations (43) and (45) we have

$$S = T_1 \exp\left[-\mathrm{i}\int \mathrm{d}^4x\ H_{\mathrm{int}}(x)\right]. \tag{46}$$

We define the contraction of $A_\mu(x)$ in the traditional way while all the related definitions for the Dirac field $\psi(x)$ are the same as the traditional ones, except for replacing the time-ordering product with the x^1-ordering product. Correspondingly, in equation (46), we apply the x^1-ordering product and the corresponding contraction for $A_\mu(x)$ while keeping the usual time-ordering product and contraction for $\psi(x)$ (choosing a frame of reference in which $t_i > t_j$ as $x_i^1 > x_j^1$). In this way, the Feynman rules can be obtained, from which we can perform some real calculations such as the particle-scattering process, where the initial state particles come from $(t, x^1) = (-\infty, -\infty)$ and the final state particles go to $(t, x^1) = (+\infty, +\infty)$. The results are the same as the usual ones.

4. Time operator

Up to now, we treat time and space on an equal footing by extending the usual Hamiltonian $\hat{H}$ to the generalized Hamiltonian $\hat{H}_\mu$(with $\hat{H}_0 = \hat{H}$), which will provide the basis for us to discuss the time operator correctly. First, let us refer to the following facts:

(1) From the generalized analytical mechanics to quantum field theory, t is to $\hat{H}_0 = \hat{H}$ as x_j is to $\hat{H}_j$ $(j = 1, 2, 3)$; likewise, t is to $\mathrm{i}\frac{\partial}{\partial t}$ as x_j is to $\mathrm{i}\frac{\partial}{\partial x_j}$.
(2) $\hat{H}_\mu$ is not identically equal to $\hat{P}_\mu$. Otherwise if $\hat{H}_\mu \equiv \mathrm{i}\partial_\mu$, equation (1) becomes a purely mathematical identity $\hat{H}_\mu\psi \equiv \mathrm{i}\partial_\mu\psi$ (where ψ can be arbitrary), with no physical content.
(3) In spite of (2), owing to equation (1), $\mathrm{i}\partial_\mu$ and $\hat{H}_\mu$ have the same spectrum distributions in the same Hilbert space.
(4) Translating the classical mechanics into the relativistic quantum mechanics, we make the replacement $p_\mu \to \hat{P}_\mu \equiv \mathrm{i}\partial_\mu$ rather than $p_\mu \to \hat{H}_\mu$ $(\mu = 0, 1, 2, 3)$.
(5) The generator of translation in x_μ is directly $\hat{p}_\mu$ rather than $\hat{H}_\mu$. Only by making use of equation (1) can we also express the generator as $\hat{H}_\mu$.
(6) Sometimes, one finds that $[\hat{H}_\mu, x_\mu] = 0$ (by equations (5) and (7), for example), whereas $[\hat{p}_\mu, x_\mu] \equiv \mathrm{i}g_{\mu\nu}$.

(7) In the 4D angular momentum tensor $J^{\mu\nu} = \mathrm{i}x^{\mu}\partial^{\nu} - \mathrm{i}x^{\nu}\partial^{\mu}$, x_{μ} ($\mu = 0, 1, 2, 3$) is taken as the dynamics operator.

From (1)–(7), we can draw a conclusion as follows: (1) the defining expression for 4-momentum operator $\hat{p}_{\mu}$ is $\mathrm{i}\partial_{\mu}$ and its form is the same for all fields, while $\hat{H}_{\mu}$, as the calculating expression for 4-momentum $\hat{p}_{\mu}$ (in the quantum field theory case, it is $\sqrt{\hat{p}_{\mu}^{2}}$ instead of $\hat{p}_{\mu}$ for the Bose fields) has a different form for a different field; (2) the 4-vector x_{μ} is canonically conjugate to the 4-vector $\hat{p}_{\mu} = \mathrm{i}\partial_{\mu}$ rather than $\hat{H}_{\mu}$; (3) t can play a twofold role, as a parameter or a dynamic variable.

In other words, just as Dirac thought [41], in the position representation, the time operator $\hat{T}$ is t itself, but in contrast to his viewpoint, the time operator t is canonically conjugate to $\hat{p}_0 = \mathrm{i}\frac{\partial}{\partial t}$ rather than the Hamiltonian $\hat{H}_0 = \hat{H}$. $\mathrm{i}\frac{\partial}{\partial t}$ is the defining expression for the energy operator while $\hat{H}$ corresponds to the calculating expression.

As a consequence, one can readily verify that the existence of a self-adjoint time operator (i.e., t) is NOT incompatible with the semibounded character of the Hamiltonian spectrum.

In fact, let $\mathrm{i}\frac{\partial}{\partial t}\psi_E = \hat{H}\psi_E = E\psi_E$. Similar to Pauli's argument, using $\left[f, \mathrm{i}\frac{\partial}{\partial t}\right] = -\mathrm{i}\frac{\partial f}{\partial t}$, we have

$$\mathrm{i}\frac{\partial}{\partial t}\,\mathrm{e}^{\mathrm{i}\alpha t}\psi_E = (E-\alpha)\,\mathrm{e}^{\mathrm{i}\alpha t}\psi_E, \qquad \text{i.e.,} \left(\mathrm{i}\frac{\partial}{\partial t} - \alpha\right)\psi_E = (\hat{H}-\alpha)\psi_E = \hat{H}'\psi_E = (E-\alpha)\psi_E.$$

Therefore, it is just a matter of the choice of zero-energy reference surface. In contrast to Pauli's argument, here we do not require any additional assumption. As is well known, the signs of $\vec{x}$ and $\vec{p}$ depend on their directions while the signs of t and p_0 depend on the choice of zero-reference-point. Meanwhile, the related observable quantities depend only on the difference, not on their absolute values.

Let $\int_{-\infty}^{+\infty}\psi^{+}(x)\psi(x)\,\mathrm{d}\sigma^{l} = 1$ ($l = 0, 1, 2, 3$). If $\psi^{+}(x)\psi(x)\,\mathrm{d}\sigma^{l}$ is the probability of finding a particle in the 3D hypersurface element $\mathrm{d}\sigma^{l}$ at coordinate x^{l}, then, according to the principle of *probability and statistics*, the expectation value of operator x^{μ} ought to be defined as $\langle x^{\mu}\rangle \equiv \int_{-\infty}^{+\infty}\psi^{+}(x)x^{\mu}\psi(x)\,\mathrm{d}\sigma^{l}(\mu, l = 0, 1, 2, 3, \mu \neq l)$. Especially, in the (1 + 1)-dimensional spacetime (x_1, t), $\mathrm{d}\sigma^{l} = (\mathrm{d}\sigma^{0}, \mathrm{d}\sigma^{1}) = (\mathrm{d}x^{1}, \mathrm{d}t)$, as $\mu = 0$, we have $\langle x^{0}\rangle = \langle t\rangle = \int_{-\infty}^{+\infty}\psi^{+}(x_1, t)t\psi(x_1, t)\,\mathrm{d}t$, which is the average *presence time* [7, 42]. That is to say, in the definition of presence time, it is $x^{0} = t$ that plays the role of the time operator. It is worthwhile to note that, as a physical quantity, we must make a distinction between the unity in its defining expression and the diversity in its calculating expression. That is, the defining expression has the same form for all cases, while the calculating expression may have a different form for different cases.

This paper is intended to lay a foundation and formalism for a different resolution of the time-in-quantum-mechanics conundrum; we will pay attention to its interpretation and physical content more specifically in our forthcoming paper, in which we will give some examples related to time of arrival, tunnelling time, jump time and passage time, etc.

In conclusion, it is reasonable to take $x^{0} = t$ as the time operator conjugating to $\mathrm{i}\partial_0$ rather than $\hat{H}$. As a consequence, Pauli's theorem no longer holds true in this case. Although it is the most appropriate choice to take $x^{0} = t$ as a parameter (because (1) in this case the law of causality is naturally preserved, and (2) time is one-dimensional while space is three-dimensional), $x^{0} = t$ also plays the role of a time operator in quantum mechanics and quantum field theory. In other words, the reasons for choosing time as a parameter lie not so much in ontology as in methodology and epistemology.

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Appendix A. Time operator is time dependent

In fact, for the 4D angular momentum tensor operator $J^{\mu\nu}$ of a free Dirac field, we have

$$\hat{H} = \vec{\alpha}\cdot\hat{p} + \beta m \qquad J^{\mu\nu} = \mathrm{i}x^{\mu}\partial^{\nu} - \mathrm{i}x^{\nu}\partial^{\mu} + S^{\mu\nu} \tag{A1}$$

$$\frac{\mathrm{d}J^{\mu\nu}}{\mathrm{d}t} = \frac{\partial J^{\mu\nu}}{\partial t} + \mathrm{i}[\hat{H}, J^{\mu\nu}] = 0 \tag{A2}$$

where $S^{\mu\nu} = \frac{\mathrm{i}}{4}[\gamma^{\mu}, \gamma^{\nu}]$ is the 4D spin tensor ($\mu, \nu = 0, 1, 2, 3$), $\gamma^{\mu}, \vec{\alpha} = \gamma^0\vec{\gamma}$ and $\beta = \gamma^0$ are the Dirac matrices. Obviously, $x^0 = t$ presenting in the operator $J^{\mu\nu}$ plays the role of a time operator, and then we have $\hat{T} = x^0$. In view of the fact that $[\hat{H}, \mathrm{i}\partial^{\mu}] = 0$, $[\hat{H}, \vec{x}] = -\mathrm{i}\vec{\alpha}$ and $\hat{H}\vec{\alpha} + \vec{\alpha}\hat{H} = -2\mathrm{i}\vec{\partial}$, by using (A2) (let μ or $\nu = 0$), we have $[\hat{H}, x^0] = 0$, which can also be directly derived from (A1). Therefore, (A2) implies that $\frac{\mathrm{d}\hat{T}}{\mathrm{d}t} = \frac{\partial\hat{T}}{\partial t} + \mathrm{i}[\hat{H}, \hat{T}] = \frac{\partial\hat{T}}{\partial t}$.

Appendix B. 4D electromagnetic moment tensor of a charged field

In an analogous manner (see, for example, [43]), we can extend the traditional relation between 3D angular momentum and magnetic moment to the 4D tensor case. As for the electromagnetic vector potential $A_{\mu}(x)$, we have

$$\begin{aligned} A^{\mu}(\vec{x}, t) &= \frac{\mathrm{d}}{\mathrm{d}t'}\int A^{\mu}(\vec{x}, t)\,\mathrm{d}t' = \frac{1}{4\pi}\int \frac{J^{\mu}(\vec{x}', t')}{|\vec{x} - \vec{x}'|}\,\mathrm{d}^3x' \\ &= \frac{1}{|\vec{x}|}\int J^{\mu}(\vec{x}', t')\,\mathrm{d}^3x' + \frac{\vec{x}}{|\vec{x}|^3}\int J^{\mu}(\vec{x}', t')\vec{x}'\,\mathrm{d}^3x' + \cdots \end{aligned} \tag{B1}$$

where $t' = t - \frac{r}{c} = t - r$, $r = |\vec{x} - \vec{x}'|$ ($\hbar = c = 1$), J^{μ} is a localized divergenceless current, which permits simplification and transformation of the expansion (B1). Let $f(x')$ and $g(x')$ be well-behaved functions of x' to be chosen below

$$\int (fJ\Delta g + gJ\Delta f)\,\mathrm{d}^4x = 0 \qquad (\Delta\cdot J = 0) \tag{B2}$$

where Δ denotes the 4D gradient operator. Let $f = x_{\mu}$ and $g = x_{\nu}$, we have

$$\int (x_{\mu}J_{\nu} + x_{\nu}J_{\mu}) = 0 \tag{B3}$$

$$\begin{aligned} \vec{x}\frac{\mathrm{d}}{\mathrm{d}t'}\int J_{\mu}(x')\vec{x}'\,\mathrm{d}^4x' &= \sum_j x_j\frac{\mathrm{d}}{\mathrm{d}t'}\int x_j' J_{\mu}(x')\,\mathrm{d}^4x' \\ &= -\frac{1}{2}\sum_j x_j\frac{\mathrm{d}}{\mathrm{d}t'}\int (x_i'J_{\mu} - x_{\mu}'J_j)\,\mathrm{d}^4x'. \end{aligned} \tag{B4}$$

It is customary to define the electromagnetic moment density

$$m^{\mu\nu} = \tfrac{1}{2}[x^\mu J^\nu - x^\nu J^\mu] \tag{B5}$$

and its integral as the electromagnetic moment

$$M^{\mu\nu} = \frac{1}{2}\int [x'^\mu J^\nu - x'^\nu J^\mu]\,\mathrm{d}^3x'. \tag{B6}$$

Assuming that J^μ is provided by N charged particles with momenta $p_n^\mu = m_0 u_n^\mu$ $(n = 1, 2, \ldots, N)$ and charges e, then $J^\mu(x') = \sum_n e u_n^\mu(t')\delta^3(\vec{x} - \vec{x}'_n)\frac{\mathrm{d}\tau}{\mathrm{d}\tau'}$, where τ, τ' are the proper times. When $t = t'$, we have

$$M^{\mu\nu} = \frac{e}{2m_0}\sum_n \left(x_n^\mu p_n^\nu - x_n^\nu p_n^\mu\right)\frac{\mathrm{d}\tau}{\mathrm{d}t} = \frac{e}{2m}L^{\mu\nu} \tag{B7}$$

where m is the relativistic mass, $L^{\mu\nu}$ is the 4D angular momentum tensor.

Appendix C. Another origin of equation (23)

In fact, equation (23) can be obtained in another manner. If we impose the boundary conditions

$$\phi(x), \partial_\mu\phi(x) \to 0 \qquad \text{as} \quad x^\mu \to \pm\infty \quad \mu = 0, 1, 2, 3 \tag{C1}$$

on the field $\phi(x)$, then an equation of continuity $\frac{\partial j_\mu(x)}{\partial x_\mu} = \partial^\mu j_\mu = 0$ associated with Noether's theorem can be integrated over the 3D hypersurface and the theorem of Gauss can be used:

$$0 = \int_{\sigma^l} \partial^\mu j_\mu\,\mathrm{d}\sigma^l = \int_{\sigma^l} \partial^l j_l\,\mathrm{d}\sigma^l + \oint_{\partial\sigma^l} j_m\,\mathrm{d}S^m \tag{C2}$$

where $m, l = 0, 1, 2, 3$ and $m \neq l$. The value of the integral over the 2D surface $\partial\sigma^l$ vanishes since the fields and their derivatives are assumed to fall off sufficiently. Therefore,

$$\partial^l \int_{\sigma^l} j_l\,\mathrm{d}\sigma^l = 0 \qquad \text{(the index } l \text{ is not summed).} \tag{C3}$$

Namely $G_l \equiv \int_{\sigma^l} j_l\,\mathrm{d}\sigma^l$ is a quantity independent of x^l (we call G_l the *generalized conserved quantity with respect to* x^l). Now, let the current density $j_\mu = T_{\mu\nu}$, where $T_{\mu\nu}$ is the canonical energy–momentum tensor of a field:

$$T_{\mu\nu} = \frac{\partial\Gamma}{\partial\partial^\mu\phi}\partial_\nu\phi - g_{\mu\nu}\Gamma. \tag{C4}$$

Obviously, the corresponding generalized conserved quantity with respect to x^l is the generalized Hamiltonian H_l:

$$G_l = \int \mathrm{d}\sigma^l T_{ll} = H_l. \tag{C5}$$

Which is exactly the same as equation (23).

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