Dirac’s hole theory versus quantum field theory

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Abstract

Dirac’s hole theory and quantum field theory are usually considered equivalent to each other. For models of a certain type, however, the equivalence may not hold as we discuss in this Letter. This problem is closely related to the validity of the Pauli principle in intermediate states of perturbation theory.

Keywords: Hole theory, quantum field theory, vacuum energy

I. INTRODUCTION

Dirac’s hole theory (HT) \cite{1} and quantum field theory (QFT) are usually considered equivalent to each other. This equivalence, however, does not necessarily hold for models of a certain type as noted recently \cite{2}. The purpose of this Letter is to elaborate on this possible inequivalence. We start with the Dirac equation for a particle in a given potential in single particle quantum mechanics. We examine how the energy eigenvalues of the Dirac equation vary when an external perturbation is applied. Then we consider HT and QFT which are based on the same Dirac equation. We focus on the vacuum state and its energy shift caused by an external perturbation.

The possible inequivalence between HT and QFT is closely related to the validity of Feynman’s prescription to disregard the Pauli principle (PP) in intermediate states of perturbation theory \cite{3}. This prescription is based on Feynman’s observation that effects of all virtual processes that violate PP cancel out (at least formally). In HT, however, the PP-violating terms do not necessarily cancel as explicitly illustrated in \cite{4}. In such a case, the result of perturbation calculation differs depending on whether or not PP is enforced in intermediate states. Then the question arises: Should we enforce PP or not?

Cavalcanti \cite{5} found the exact solution of the HT model of \cite{4} in its special case with the particle mass $m = 0$. He pointed out that the exact solution is consistent with the
perturbation calculation in which PP is disregarded throughout but not with the one in which PP is enforced. This was puzzling in view of the usual belief that PP operates in intermediate states. Cavalcanti’s comment was responded by [2] but the above puzzling aspect and the difference between HT and QFT were not fully addressed in it. In this Letter we emphasize that for models of a certain type, including that of [4], HT and QFT are not necessarily equivalent and we explore various aspects of the difference. In QFT, the cancellation of the PP-violating terms in perturbation theory is complete. QFT is free from the puzzling aspect that was found in [4,5].

In Section II we specify the type of the model that we consider. We discuss some difficulties of the HT version of the model. In Section III we examine the QFT version of the model and clarify the difference between HT and QFT. In Section IV we raise a further question regarding HT.

II. THE HOLE THEORY

We start with single-particle relativistic quantum mechanics with the Hamiltonian

\[ H = H_0 + V, \tag{1} \]

where \( H_0 \) is the Dirac Hamiltonian for a particle in a binding potential and \( V \) is an external perturbation. Unperturbed and perturbed systems, respectively, are such that

\[ H_0 \phi_n = \epsilon_n \phi_n, \quad H \psi_n = \eta_n \psi_n. \tag{2} \]

Suffix \( n (= \pm 1, \pm 2, \ldots) \) specifies eigenstates. The energy eigenvalues are labeled such that \( 0 < \epsilon_1 < \epsilon_2 < \ldots, \) and \( 0 > \epsilon_{-1} > \epsilon_{-2} > \ldots, \) and similarly for \( \eta_n. \) We assume that the energy levels are all discrete and non-degenerate and that there is a one-to-one correspondence between unperturbed and perturbed eigenstates. In other words, \( \eta_n \to \epsilon_n \) when \( V \to 0. \) Let us also assume that \( \eta_n \) and \( \epsilon_n \) have the same sign. It is not difficult to relax these restrictions.

We now turn to HT and consider the vacuum in which all negative-energy states are occupied. The unperturbed and perturbed energies of the vacuum are respectively given by \( E_0 = \sum_j \epsilon_{-j} \) and \( E = \sum_j \eta_{-j}. \) We are interested in the energy shift due to the perturbation,

\[ \Delta E = \sum_j (\eta_{-j} - \epsilon_{-j}). \tag{3} \]

Suppose that we start with known \( \epsilon_n \) and attempt to reach \( \eta_n \) by perturbation theory. We follow the standard prescription of perturbation theory including all intermediate states. We treat the system as a one-body system and we do not exclude the intermediate states which are already occupied by other particles. The first order energy shift is given by

\[ \Delta E^{(1)} = \sum_j V_{-j,-j} = \int V(r) \rho_{\text{vac}}(r) dr, \tag{4} \]

where \( V_{-j,-j} = \langle \phi_{-j} | V | \phi_{-j} \rangle \) and \( \rho_{\text{vac}}(r) = \sum_j | \phi_{-j}(r) |^2 \) is the particle density of the unperturbed vacuum. This \( \Delta E^{(1)} \) as such generally diverges because \( \rho_{\text{vac}}(r) \) is actually infinite.
No matter how weak it is, $V$ may cause an infinite energy shift. This difficulty can be avoided by assuming that the density in the perturbed vacuum itself is not an observable quantity and that only the difference between the density of the perturbed vacuum and its unperturbed counterpart is observable. Then the first order energy shift disappears.

We are more interested in the second order energy shift,

$$\Delta E^{(2)} = \sum_j \Delta \epsilon_{-j}^{(2)} = \sum_j \sum_i \frac{|V_{i,-j}|^2}{\epsilon_{-j} - \epsilon_i} + X,$$

(5)

$$X = \sum_j \sum_{k \neq j} \frac{|V_{-k,-j}|^2}{\epsilon_{-j} - \epsilon_k},$$

(6)

where $V_{i,-j} = \langle \phi_i | V | \phi_{-j} \rangle$. Term $X$ is due to the transitions between negative energy states like the one from $-j$ to $-k$. In $\Delta E^{(2)}$, PP has not been considered. If we enforce PP, the transitions between negative energy states are not allowed and we obtain

$$\Delta E_{\text{PP}}^{(2)} = \sum_j \sum_i \frac{|V_{i,-j}|^2}{\epsilon_{-j} - \epsilon_i},$$

(7)

where suffix PP means “with PP enforced”. The $X$ of Eq. (6) is an infinite alternating series. This formally vanishes because the numerator is symmetric with respect to $j \rightarrow k$ while the denominator is antisymmetric. As was illustrated in [4], however, $X$ may not vanish depending on how the calculation is done.

In [4], the one-dimensional bag model with $H_0 = \alpha p + \beta [m + S(x)]$ and perturbation $V(x) = \lambda x$ was considered. Here $m$ is the mass of the particle, $p = -i\hbar d/dx$, $\alpha = \sigma_y$ and $\beta = \sigma_z$ are $2 \times 2$ Dirac matrices. The $S(x)$ is a Lorentz-scalar potential such that $S(x) = 0$ for $|x| < a$ and $S(x) = \infty$ for $|x| > a$. In this model, we obtain $V_{-j,-j} = 0$ and $\Delta E^{(1)} = 0$. The divergence difficulty of $\Delta E^{(1)}$ that we pointed out below (4) does not arise. For the second order energy shift the calculation was done in two ways, methods I and II. In method I, PP is enforced whenever it is applicable. In method II, PP is disregarded throughout. Method I leads to $\Delta E_{\text{PP}}^{(2)}$ and method II to $\Delta E^{(2)}$. The explicit calculations of [4] led to $\Delta E_{\text{PP}}^{(2)} < 0$ and $\Delta E^{(2)} = 0$.

Cavalcanti [5] showed that, if $m = 0$, the perturbed Dirac equation $H \psi_n = \eta_n \psi_n$ for the model of [4] can be solved analytically. This enabled him to obtain the exact energy shift of the model. He showed that $\eta = \epsilon$. The eigenvalue $\eta$ is independent of the perturbation and so is the exact energy of the HT vacuum, that is, $\Delta E = 0$. This is consistent with $\Delta E^{(2)} = 0$ of method II but not with $\Delta E_{\text{PP}}^{(2)} < 0$ of method I. In other words, if one enforces PP in intermediate states, one obtains a wrong energy shift in HT. This is puzzling. According to the spin-statistics theorem (which was proved in QFT), the wave function of a fermion system has to be antisymmetric with respect to interchanges of the particles. This implies PP. The perturbative interaction $V$ is totally symmetric with respect to the interchange of particles. It acts in the same way on all particles. Then the intermediate state that is connected to the antisymmetric initial state through $V$ has to be antisymmetric. Hence PP is expected to hold in the intermediate states. This is also related to the unitarity of the $S$ matrix [6,7]. Recall also that Dirac introduced HT such that the vacuum state is stable. This stability relies on PP.
Cavalcanti solved the Dirac equation by rewriting it as
\[\frac{dw}{dx} \mp \frac{x}{dx} \mp i(\lambda x - \eta)w \pm x = 0,\]
where \(w(x) = u(x) \pm iv(x), u(x)\) and \(v(x)\) being the upper and lower components of \(\psi(x)\), respectively. His solution is of the form of \(w(x) = C_\pm e^{\pm[i(\lambda/2)x^2 - nx]}\) where \(C_\pm\) are constants. His solution can be generalized to the case with an arbitrary potential \(V(x)\) (but still with \(m = 0\)) by replacing his \(w(x)\) with
\[w(x) = C_\pm e^{\pm[i(\lambda/2)x^2 - nx]} \frac{df(x)}{dx} = V(x).\]

The boundary condition for the wave function is \(w_+(\pm a) = -iw_-(\pm a)\), which leads to
\[\eta - \epsilon = \frac{1}{2a} \int_{-a}^{a} V(x) dx,\]
where \(\epsilon = (2n + 1)(\pi/4a)\) with \(n = 0, \pm 1, \pm 2, \ldots\), is the eigenvalue when \(V(x) = 0\). It is remarkable that this exact energy-shift of the single-particle state is first order. The second order and all higher order effects are zero.

If \(V(x)\) is an odd function of \(x\), then \(\eta = \epsilon\). This leads to \(\Delta E = 0\), that is, the exact energy of the HT vacuum is independent of \(V(x)\). If \(V(x)\) contains an even function part, all eigenvalues are shifted exactly by the same amount. The vacuum of HT contains an infinite number of negative-energy particles. If the energy of every particle is shifted by the same amount, the total energy of the vacuum obtains an infinite energy shift. This illustrates what we pointed out below Eq. (4).

III. QUANTUM FIELD THEORY

In QFT the Hamiltonian for the unperturbed system can be expressed as
\[\mathcal{H}_0 = \sum_i \epsilon_i a_\dagger_i a_i + \sum_j \bar{\epsilon}_j b_\dagger_j b_j, \quad \bar{\epsilon}_j = -\epsilon_{-j} > 0.\]
The notation is hopefully self-explanatory. The \(a_i\) (\(a_\dagger_i\)) is the creation (annihilation) operator for the particle in the unperturbed state \(i\). The \(a_i\) creates a particle with energy \(\epsilon_i\) with wave function \(\phi_i(x)\). These operators satisfy the usual anticommutation relations. The \(b_j\) (\(b_\dagger_j\)) is for the antiparticle. No negative-energy particles appear in QFT. Let us emphasize that the Hamiltonian is defined in terms of normal products of the creation and annihilation operators. The unperturbed vacuum contains no particles nor antiparticles. It is the eigenstate of \(\mathcal{H}_0\) with zero eigenvalue.

The interaction Hamiltonian is of the form of
\[\mathcal{V} = \sum_{i,i'} V_{i,i'} a_{i'} a_i + \sum_{i,j} V_{i,-j} a_{i} b_j + \cdots,\]
where, for example, \(a_{i} b_j\) creates a pair of particle and antiparticle. The other terms that are not shown above are of the form of \(ab, a^\dagger b, b^\dagger a\) and \(b^\dagger b\). The number of the particles is conserved with the understanding that an antiparticle has particle number -1. Because \(\mathcal{V}\) consists of normal products, its expectation value in the unperturbed vacuum is zero. Hence we obtain
\[ \Delta \mathcal{E}^{(1)} = 0. \]  

We use notation \( \mathcal{E} \) for the energy of the system in QFT. Equation (12) is in a sharp contrast to Eq. (4). QFT is free from the difficulty of the infinite first-order energy shift of HT that we pointed out below (4). If we did not use the normal products for \( V \), we would obtain (4) for \( \Delta \mathcal{E}^{(1)} \).

Next let us examine the energy shift of the second order. In QFT the vacuum does not contain any particles nor antiparticles. The transitions between negative energy states of HT has no place in QFT. We obtain

\[ \Delta \mathcal{E}^{(2)} = - \sum_j \sum_i \frac{|V_{i,-j}|^2}{\epsilon_i + \bar{\epsilon}_j}, \]

which agrees with \( \Delta E_{\text{PP}}^{(2)} \) of HT. Recall that \( \Delta E_{\text{PP}}^{(2)} \) and \( \Delta E^{(2)} \) may or may not agree with each other in HT.

If the exact solutions of the perturbed Dirac equation are known, they can be used to define the creation and annihilation operators \( c, c^\dagger, d \) and \( d^\dagger \) for the perturbed system. The Hamiltonian for the perturbed system then becomes

\[ \mathcal{H} = \sum_i \eta_i c_i^\dagger c_i + \sum_j \bar{\eta}_j d_j^\dagger d_j, \quad \bar{\eta}_j = -\eta_{-j} > 0. \]

The perturbed vacuum is the eigenstate of \( \mathcal{H} \) with zero eigenvalue. Perturbed vacuum contains no particles nor antiparticles which are defined in terms of \( \{c, c^\dagger, d, d^\dagger\} \).

In the absence of perturbation, the vacuum energy is zero. In the presence of perturbation, if we use \( \mathcal{H} \) given above, the vacuum energy is again zero. This may give the false impression that the perturbation causes no energy shift. Recall that the Hamiltonian is defined as a normal product. The normal product depends on how the creation and annihilation operators are defined. This dependence gives rise to the energy shift. This can be seen as follows. We have two sets of basis functions, \( \{\phi_n\} \) and \( \{\psi_n\} \), each of which forms a complete orthonormal system. The \( \{a, a^\dagger, b, b^\dagger\} \) and \( \{c, c^\dagger, d, d^\dagger\} \) are related by the transformation,

\[ c_i = \sum_{i'} \langle \psi_i | \phi_{i'} \rangle a_{i'} + \sum_j \langle \psi_i | \phi_{-j} \rangle b_j^\dagger, \]

\[ d_j^\dagger = \sum_i \langle \psi_{-j} | \phi_i \rangle a_i + \sum_{j'} \langle \psi_{-j} | \phi_{-j'} \rangle b_{j'}^\dagger, \]

and their hermitian adjoints. If we rewrite \( \mathcal{H}_0 + \mathcal{V} \) in terms of \( \{c, c^\dagger, d, d^\dagger\} \), we expect to obtain

\[ \mathcal{H}_0 + \mathcal{V} = \mathcal{H} + \Delta \mathcal{E}. \]

The \( \Delta \mathcal{E} \) is the expectation value of \( \mathcal{H}_0 + \mathcal{V} \) in the perturbed vacuum. The \( \Delta \mathcal{E} \) is also the negative of the expectation value of \( \mathcal{H} \) in the unperturbed vacuum. If \( \mathcal{V} \to 0 \), then \( \mathcal{H} \to \mathcal{H}_0 \) and \( \Delta \mathcal{E} \to 0 \). Therefore \( \Delta \mathcal{E} \) is the energy shift of the vacuum due to the perturbation \( \mathcal{V} \).
Equation (17) has various interesting implications. Let us first work out $\Delta E$ explicitly. It is somewhat simpler to start with $H$ and rewrite it in terms of $\{a, a^\dagger, b, b^\dagger\}$. The combination $c_i^\dagger c_i$ goes like

$$c_i^\dagger c_i = \left( \sum_{i'} \langle \psi_i | \phi_{i'} \rangle^* a_{i'}^\dagger + \sum_j \langle \psi_i | \phi_{-j} \rangle^* b_j \right) \left( \sum_{i'} \langle \psi_i | \phi_{i'} \rangle a_{i'} + \sum_j \langle \psi_i | \phi_{-j} \rangle b_j^\dagger \right)$$

$$= (\text{normal products of } a, a^\dagger, \ldots) + |\langle \psi_i | \phi_{-j} \rangle|^2,$$  \hspace{1cm} (18)

and similarly for $d_i^\dagger d_i$. If we substitute the above into $H$ and collect the terms of the form of, e.g., $a^\dagger a$, we obtain

$$\sum_{i,i'} \sum_j \eta_i \langle \psi_i | \phi_{i'} \rangle^* \langle \psi_i | \phi_{i'} \rangle - \sum_j \bar{\eta}_j \langle \psi_{-j} | \phi_{i'} \rangle \langle \psi_{-j} | \phi_{i'} \rangle^* a_{i'}^\dagger a_{i'}$$

$$= \sum_{i,i'} \sum_j \langle \phi_i | (H_0 + V) | \phi_{i'} \rangle a_{i'}^\dagger a_{i'} = \sum_i \epsilon_i a_i^\dagger a_i + \sum_{i,i'} V_{i,i'} a_{i'}^\dagger a_i.$$  \hspace{1cm} (19)

In this way the normal products of $a, a^\dagger, \ldots$ altogether become $H_0 + V$ and we obtain

$$\Delta E = -\sum_i \sum_j \left( \eta_i |\langle \psi_i | \phi_{-j} \rangle|^2 + \bar{\eta}_j |\langle \psi_{-j} | \phi_i \rangle|^2 \right).$$  \hspace{1cm} (20)

Equation (20) we believe is new. The $\Delta E$ can vanish only if $V = 0$. Otherwise it is negative. Let us emphasize that this sign of $\Delta E$ is not related to the sign of the single-particle energy-shift $\eta - \epsilon$. Even if $\eta - \epsilon$ is positive for all levels, $\Delta E$ is negative. This does not necessarily mean though that perturbations $V$ and $-V$ lead to the same value of $\Delta E$.

The $\Delta E$ is the exact energy shift. Let us examine its leading term in the perturbation expansion. It is obvious that $\Delta E^{(1)} = 0$. For the matrix elements involved, we obtain in first order

$$\langle \psi_i | \phi_{-j} \rangle = \frac{V_{i,-j}}{\epsilon_i - \epsilon_{-j}}, \quad \langle \psi_{-j} | \phi_i \rangle = \frac{V_{-j,i}}{\epsilon_{-j} - \epsilon_i}.$$  \hspace{1cm} (21)

As far as the leading term of $\Delta E$ is concerned, we can put $\eta_i = \epsilon_i$ and $\bar{\eta}_j = \bar{\epsilon}_j = -\epsilon_{-j}$. Then follows Eq. (13). One can also work out higher order energy shifts $\Delta E^{(3)}$, etc., successively.

The problem regarding PP in intermediate states does not arise in the QFT calculation for the vacuum energy. There is nothing that blocks the particle and antiparticle pair creation in the second-order intermediate states. Because the transitions between negative energy states do not appear in QFT, the perturbation calculation is free from the ambiguity of the kind that was pointed out in [4]. The two methods of calculation I and II lead to exactly the same results in QFT. All the PP-violating effects in method II cancel. One can disregard PP throughout as Feynman advocated.

In HT which is based on the one-dimensional bag model with $m = 0$, there are no second-order and higher order effects in the energy shift. In contrast to this, the exact energy shift of the QFT vacuum is given by $\Delta E$ of Eq. (20). Its first-order part is absent whereas its second-order part is negative definite. The exact energy shift can be explicitly calculated by using the known exact solutions of the Dirac equation of the model.
Let us point out a feature of Eq. (17) which is interesting in relation to Feynman’s prescription. Consider a system that consists of a number of particles and antiparticles together with their vacuum background. The energy shift of this system is simply given by

\[ \sum_i (\eta_i - \epsilon_i) + \sum_j (\bar{\eta}_j - \bar{\epsilon}_j) + \Delta \mathcal{E}, \]

(22)

where the summations are for the particles and antiparticles. The \( \Delta \mathcal{E} \) is the same as that of Eq. (20). In calculating \( \eta_i - \epsilon_i \), for example, one does not have to think about the vacuum background. On the other hand \( \Delta \mathcal{E} \) is the energy shift of the vacuum in the absence of the additional particles and antiparticles. This can be illustrated by using the QFT version of the one-dimensional bag model of [4].

There is another interesting feature of Eq. (17). The energy spectra of the system in the sense of the differences between energy levels are simply determined by the single particle energies \( \eta \)'s and \( \bar{\eta} \)'s. The vacuum energy \( \Delta \mathcal{E} \) is common to all energy levels of the system.

**IV. DISCUSSION**

We started with a problem of single-particle quantum mechanics with the Dirac equation for a particle in a given potential. We then considered the HT and QFT versions of the problem and examined how the vacuum energy shifts when an external perturbation is applied. We discussed a situation such that HT and QFT are not equivalent. In case of such discrepancy we should choose QFT rather than HT.

If HT and QFT are not necessarily equivalent, some of the calculations done in the framework of HT may have to be reexamined. As one of such possible problems, let us mention the fractional fermion number. In HT, an external perturbation causes a change in the density distribution in the vacuum in which all negative energy levels are filled. This may result in fractionalization of the fermion number of the vacuum; See, e.g., [8–11]. In QFT the unperturbed vacuum is empty. When an external perturbation is applied to it, a pair of particle and antiparticle can be created. This process of pair creation, however, does not change the fermion number of the vacuum. It is not clear whether or not this can be compatible with the fermion number fractionalization that occurs in HT.

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