Physical state for non-relativistic quantum electrodynamics

Fumio Hiroshima[*]
Department of Mathematics
Kyushu University

Akito Suzuki[†]
Department of Mathematics
Hokkaido University

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Abstract

A physical subspace and physical Hilbert space associated with asymptotic fields of nonrelativistic quantum electrodynamics are constructed through the Gupta-Bleuler procedure. Asymptotic completeness is shown and a physical Hamiltonian is defined on the physical Hilbert space.

1 Introduction

1.1 The Gupta-Bleuler formalism

Quantization of the electromagnetic field does not cohere with normal postulates such as Lorentz covariance and existence of a positive definite metric on some Hilbert space. This means that we chose to quantize in a manner sacrificing manifest Lorentz covariance; conversely if the electromagnetic field is quantized in a manifestly covariant fashion, the notion of a positive definite metric must be sacrificed and the existence of negative probability arising from the indefinite metric renders invalid a probabilistic interpretation of quantum field theory. One prescription for quantization of the

[*]e-mail: hiroshima@ math.kyushu-u.ac.jp
[†]e-mail: akito@math.sci.hokudai.ac.jp

electromagnetic field in a Lorentz covariant manner is the Gupta-Bleuler procedure [Ble50, Gup50]. This procedure provides a covariant procedure for quantization at the cost of a cogent physical interpretation.

In this paper we will consider the so-called nonrelativistic quantum electrodynamics (NRQED). A significant point is that NRQED is nonrelativistic with respect to the motion of an electron only; the electromagnetic field is always relativistic. Although it is customary to adopt the Coulomb gauge in the theory of NRQED, it can be investigated using the Lorentz gauge by the Gupta-Bleuler approach [Bab82]. This will be rigorously pursued in this paper.

Indefinite metric and Lorentz condition: Let $\mathscr{A}_\mu = \mathscr{A}_\mu(x,t)$, $\mu = 0,1,2,3$, be a quantized radiation field and $\dot{\mathscr{A}}_\mu = \dot{\mathscr{A}}_\mu(x,t)$ its time derivative. $\mathscr{A}_\mu$ and its time derivative $\dot{\mathscr{A}}_\nu$ satisfy the commutation relations

$$[\mathscr{A}_\mu(x,t), \dot{\mathscr{A}}_\nu(x',t)] = -ig_{\mu\nu}\delta(x-x'), \tag{1.1}$$

$$[\mathscr{A}_\mu(x,t), \mathscr{A}_\nu(x',t)] = 0, \tag{1.2}$$

$$[\dot{\mathscr{A}}_\mu(x,t), \dot{\mathscr{A}}_\nu(x',t)] = 0, \tag{1.3}$$

where $g_{\mu\nu}$ is the metric tensor given by (2.9). An inevitable consequence of the commutation relations (1.1)-(1.3) is to introduce an indefinite metric $(\cdot|\cdot)$ onto the state space. This creates problems in physical interpratations and in formulating things in a mathematically well defined way. For example, the Hamiltonian H cannot be defined as a self-adjoint operator and so the time-evolution e^{itH} is not unitary. So we have to investigate questions concerning the domain of e^{itH}.

In addition to the indefinite metric, the Lorentz condition also poses a dilemma. We impose the Lorentz condition:

$$\partial^\mu \mathscr{A}_\mu(x,t) = 0 \tag{1.4}$$

as an operator identity. Here and in what follows $\partial^\mu X_\mu$ is the conventional abbreviation for $\partial^\mu X_\mu = \partial_t X_0 - \partial_{x^1} X_1 - \partial_{x^2} X_2 - \partial_{x^3} X_3$. Under (1.4), as is well known, we find that the conventional Lagrangian formalism is not available.

To resolve this difficulty, in the Gupta-Bleuler procedure mentioned below, we first single out the so-called physical subspace from the Lorentz condition, and it is required that the Lorentz condition is valid only in terms of expectation values on the physical subspace. The sesquilinear form $(\cdot|\cdot)$ restricted to the physical subspace is merely semidefinite. So, we define the physical Hilbert space to be the quotient space of the physical subspace divided by the subspace with zero norm with respect to $(\cdot|\cdot)$. This space has a positive definite form, and a self-adjoint Hamiltonian can also be derived.

Gupta-Bleuler formalism: Here we present an outline of the Gupta-Bleuler formalism in NRQED for the reader's convenience, without mathematical rigor. Let $H_{\rm tot}$ be the full Hamiltonian for NRQED with form factor φ . Note that $H_{\rm tot}$ is not self-adjoint. Let X be an operator. Generally, a solutions $X(t)$ to the Heisenberg equation:

$$\frac{d}{dt}X(t) = i[H_{\rm tot}, X(t)], \quad X(0) = X, \tag{1.5}$$

is called a Heisenberg operators of X associated with $H_{\rm tot}$. Since $H_{\rm tot}$ is, however, not self-adjoint, intuitively a solution to (1.5) is possibly not unique. In order to ensure uniqueness we give an alternative definition of Heisenberg operators in Definition 3.10.

Let p and q be the momentum and position operators respectively of an electron, and $\mathscr{A}(f) = (\mathscr{A}_0(f), \vec{\mathscr{A}}(f))$ the smeared electromagnetic field, i.e.,

$$\mathscr{A}(f) = \int f(x)\mathscr{A}(x)dx.$$

Let $p(t)$, $q(t)$ and $\mathscr{A}(f,t) = (\mathscr{A}_0(f,t), \vec{\mathscr{A}}(f,t))$ be the Heisenberg operators of p, q and $\mathscr{A}(f)$, respectively. We denote $\mathscr{A}(f,t)$ by

$$\mathscr{A}(f,t) = \int f(x)\mathscr{A}(x,t)dx.$$

Then formally the equations

$$\Box\vec{\mathscr{A}}(x,t) = \vec{J}(x,t), \tag{1.6}$$

$$\Box\mathscr{A}_0(x,t) = \rho(x,t) \tag{1.7}$$

can be derived. Here ρ and $\vec{J}$ are the charge and the current density of the electron, respectively, given by

$$\rho(x,t) = e\varphi(x - q(t)), \tag{1.8}$$

$$\vec{J}(x,t) = \frac{e}{2}\Big(\varphi(x - q(t))\vec{v}(t) + \vec{v}(t)\varphi(x - q(t))\Big) \tag{1.9}$$

where e denotes the charge on an electron and $\vec{v}(t)$ the velocity:

$$\vec{v}(t) = \dot{q}(t) = \frac{1}{m}\left(p(t) - e\int \vec{\mathscr{A}}(z,t)\varphi(z - q(t))dz\right).$$

It can be seen from (1.8) and (1.9) that the 4-current $j = (\rho, \vec{J}) = (j^0, j^1, j^2, j^3)$ satisfies the continuity equation

$$\partial^\mu j_\mu = 0. \tag{1.10}$$

By this, together with (1.6) and (1.7), the kernel $\mathscr{A}(x,t)$ automatically satisfies that the condition

$$\Box \partial^\mu \mathscr{A}_\mu(x,t) = 0. \tag{1.11}$$

Equation (1.11) tells us that $\partial^\mu \mathscr{A}_\mu$ is a free field and hence formally, it can be described in terms of some annihilation operator $c(k)$ and the creation operator $c^\dagger(k)$ by

$$\partial^\mu \mathscr{A}_\mu(x,t) = \int \left(c(k) e^{-i|k|t+ikx} + c^\dagger(k) e^{i|k|t-ikx} \right) dk. \tag{1.12}$$

The term including the factor $e^{-i|k|t}$ in (1.12) is called the positive frequency part of $\partial^\mu \mathscr{A}_\mu(x,t)$ and written as $[\partial^\mu \mathscr{A}_\mu]^{(+)}(x,t)$. On the other hand the negative frequency part $[\partial^\mu \mathscr{A}_\mu]^{(-)}(x,t)$ is defined by the term including $e^{+i|k|t}$. As is mentioned above the Lorentz condition (1.4) is not valid as an operator identity. We may demand that some state Ψ should satisfy $\partial^\mu \mathscr{A}_\mu(x,t)\Psi = 0$. This is however too severe a condition to demand, since $[\partial^\mu \mathscr{A}_\mu]^{(+)}(x,t)\Psi + [\partial^\mu \mathscr{A}_\mu]^{(-)}(x,t)\Psi = 0$ and the negative frequency part contains creation operators, so not even the vacuum could satisfy this identity. However, since the positive frequency part contains the annihilation operator, we could adopt the less demanding requirement

$$[\partial^\mu \mathscr{A}_\mu]^{(+)}(x,t)\Psi = 0. \tag{1.13}$$

The state Ψ in (1.13) is called the physical state, and (1.13) is called the Gupta-Bleuler subsidiary condition. The set of physical states is denoted by $\mathscr{V}_{\rm phys}$ and is called the physical subspace. Moreover the Lorentz condition is realized as the expectation value on the physical subspace:

$$(\Psi | \partial^\mu A_\mu \Psi) = 0, \quad \Psi \in \mathscr{V}_{\rm phys}.$$

In much of the physical literature little attention is paid to the existence of a nontrivial physical subspace. The absence of a physical subspace was, however, recently pointed out in [Suz07]. In this paper we want to derive sufficient conditions for the existence of a physical subspace and characterize such a subspace in the NRQED framework.

1.2 Main results and plan of the paper

Our main concern in this paper is to develop the Gupta-Bleuler formalism for NRQED, and to characterize the physical subspace rigorously. The physical subspace, however, can be trivial because of the infrared singularity [Suz07]. The difficulty in construction of the physical subspace of our system is due to the fact that $H_{\rm tot}$ is η-self-adjoint but not self-adjoint on a Klein space. Therefore one cannot realize the solution of the Heisenberg equation (1.5) as $e^{itH_{\rm tot}}\mathscr{A}e^{-itH_{\rm tot}}$.

In this paper we introduce a dipole approximation to $H_{\rm tot}$ to reduce this difficulty. Let H denote the Hamiltonian with a dipole approximation. Even so, although the Hamiltonian H is η-self-adjoint, it is not yet self-adjoint. However, thanks to the dipole approximation, we can construct the Heisenberg operators $\mathscr{A}_0(f,t)$ and $\vec{\mathscr{A}}(f,t)$ exactly. See Theorem 3.12.

On the other hand, there is a disadvantage in using the dipole approximation. Unfortunately, with this approximation, the system does not conserve the 4-current $j_{\rm dip} = (\rho_{\rm dip}, \vec{J}_{\rm dip})$. In fact, the 4-current in the dipole approximation turns out to be

$$\rho_{\rm dip}(x,t) = e\varphi(x), \tag{1.14}$$

$$\vec{J}_{\rm dip}(x,t) = \frac{e}{2}\left(\varphi(x)\vec{v}_{\rm dip}(t) + \vec{v}_{\rm dip}(t)\varphi(x)\right) \tag{1.15}$$

where

$$\vec{v}_{\rm dip}(t) = \frac{1}{m}\left(p(t) - e\int \vec{\mathscr{A}}(z,t)\varphi(z)dz\right)$$

and

$$\partial^\mu j_{{\rm dip}_\mu} \neq 0. \tag{1.16}$$

Hence $\partial^\mu \mathscr{A}_\mu$ is not a free field in the sense of (1.11), and we lose the method of defining the positive frequency part $[\partial^\mu \mathscr{A}_\mu]^{(+)}$. Therefore, in the dipole approximation, the physical subspace cannot be defined in the usual way.

Nevertheless the asymptotic field provides a tool for employing the Gupta-Bleuler formalism. Decompose H with respect to the spectrum of the electron momentum:

$$H = \int_{\mathbb{R}^3}^{\oplus} H_P dP. \tag{1.17}$$

We shall generally consider H_P for an arbitrary fixed $P \in \mathbb{R}^3$ throughout this paper.

The main results of this paper are

(i) Asymptotic completeness of H_P based on the LSZ method (Theorem 4.3);

(ii) Characterization of the physical subspace (Theorems 5.8 and 5.9) and the physical Hilbert space (6.5);

(iii) Construction of the physical scattering operator (Theorem 6.4);

(iv) Construction of the physical self-adjoint Hamiltonian (Theorem 6.11).

(i) The explicit form of the Heisenberg operator with respect to H_P allows us to construct the asymptotic fields $\mathscr{A}_\mu^{\mathrm{out/in}}(f,t,P)$ exactly and we prove the asymptotic completeness in Theorem 4.3. As far as we know, the asymptotic completeness of NRQED with the dipole approximation was proven initially by Arai [Ara83a, Ara83b] but for the model without both a scalar and a longitudinal component. See also Spohn [Sup97]. We extend this to our case.

(ii) $\mathscr{A}_\mu^{\mathrm{out/in}}(f,t,P)$ is a free field defined in terms of asymptotic annihilation and creation operators, therefore so is $\partial^\mu\mathscr{A}_\mu^{\mathrm{out/in}}(f,t,P)$. Therefore one can define the non-trivial physical subspace $\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{out/in}}$ associated with $\partial^\mu\mathscr{A}_\mu^{\mathrm{out/in}}(f,t,P)$ by the Gupta-Bleuler subsidiary condition

$$[\partial^\mu\mathscr{A}_\mu^{\mathrm{out/in}}]^{(+)}(f,t,P)\Psi=0. \tag{1.18}$$

We characterize $\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{out/in}}$ and prove that $\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{out/in}}$ is positive semi-definite in Theorem 5.8. Moreover, in Theorem 5.9, we show that

$$\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{out}}\neq\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{in}}$$

which cannot occur in the case where the 4-current is conserved [Sun58, IZ80]. The physical subspace is decomposed as the direct sum: $\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{out/in}}=\mathscr{V}_{P}^{\mathrm{out/in}}[\dot{+}]\mathscr{V}_{P,\mathrm{null}}^{\mathrm{out/in}}$, where $\mathscr{V}_{P,\mathrm{null}}^{\mathrm{out/in}}$ is the null space with respect to an indefinite metric and the Hamiltonian leaves it invariant. Then the physical Hilbert space is given as the quotient space

$$\mathscr{H}_{P,\mathrm{phys}}^{\mathrm{out/in}}=\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{out/in}}/\mathscr{V}_{P,\mathrm{ull}}^{\mathrm{out/in}}.$$

See [KO79, Nak72].

(iii) Next we determine the physical scattering operator. Consider the scattering operator

$$S_P:\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{out}}\to\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{in}}$$

as a unitary operator; namely $S_P\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{out}}=\mathscr{V}_{P,\mathrm{phys}}^{\mathrm{in}}$. We can check that S_P leaves the null space invariant and define the physical scattering operator $S_{P,\mathrm{phys}}$ by

$$S_{P,\mathrm{phys}}[\Psi]_{\mathrm{out}}:=[S_P\Psi]_{\mathrm{in}}$$

for $[\Psi]_{\rm out/in} \in \mathscr{H}^{\rm out/in}_{P,\rm phys}$. It can be shown that this is also a unitary operator from $\mathscr{H}^{\rm out}_{P,\rm phys}$ to $\mathscr{H}^{\rm in}_{P,\rm phys}$ in Theorem 6.4.

(iv) It can be seen from Lemma 6.10 that

$$H^{\rm out/in}_{P,\rm phys} = \left[H_P \lceil_{D(H_P)\cap\mathscr{V}^{\rm ex}_{P,\rm phys}} P^{\rm ex} \right]_{\rm ex}$$

is a well defined operator on $\mathscr{H}^{\rm ex}_{P,\rm phys}$, where $P^{\rm ex}$ denotes the projection onto $\mathscr{V}^{\rm ex}_P$. We call this the physical Hamiltonian. It is proven in Theorem 6.11 that $H^{\rm out/in}_{P,\rm phys}$ is a *self-adjoint operator* on $\mathscr{H}^{\rm out/in}_{P,\rm phys}$. Note that the physical Hamiltonian $H^{\rm out/in}_{P,\rm phys}$ is self-adjoint, whereas our Hamiltonian H_P is *not* self-adjoint,

This paper is organized as follows. In Section 2 we define NRQED. In Section 3 we present the explicit form of the Heisenberg operators. In Section 4 we construct the asymptotic fields $\mathscr{A}^{\rm out/in}_\mu(f,t,P)$ based on the LSZ formalism and define the scattering operator S_P. In section 5 we define physical subspaces in an abstract way, and characterize the physical subspace at time t and for $t=\pm\infty$. In Section 6 we define the physical Hamiltonian on the quotient space $\mathscr{H}^{\rm out/in}_{P,\rm phys}$.

2 NRQED in the Lorentz gauge

2.1 Boson Fock space

We begin by defining elements of a Boson Fock space. The Boson Fock space over the Hilbert space $\oplus^4 L^2(\mathbb{R}^3)$ is given by the infinite direct sum of the n-fold symmetric tensor product of $\oplus^4 L^2(\mathbb{R}^3)$:

$$\mathscr{F} := \mathscr{F}_{\rm b}(\oplus^4 L^2(\mathbb{R}^3)) = \bigoplus_{n=0}^\infty \left(\bigotimes_s^n \left(\oplus^4 L^2(\mathbb{R}^3)\right) \right). \tag{2.1}$$

Here $\otimes_s^n$ denotes the symmetric tensor product and we set $\otimes_s^0(\oplus^4 L^2(\mathbb{R}^3)) = \mathbb{C}$. We denote the scalar product on $\mathscr{F}$ by

$$(\Phi,\Psi)_{\mathscr{F}} := \sum_{n=0}^\infty (\Phi^{(n)},\Psi^{(n)})_{\otimes^n(\oplus^4 L^2(\mathbb{R}^3))} \tag{2.2}$$

for $\Psi = \{\Psi^{(n)}\}_{n=0}^\infty$ and $\Phi = \{\Phi^{(n)}\}_{n=0}^\infty \in \mathscr{F}$, which is anti-linear in Φ and linear in Ψ. Then $\mathscr{F}$ becomes a Hilbert space with scalar product given by (2.2).

The creation operator $a^*(F) : \mathscr{F} \to \mathscr{F}$ with a smeared function $F \in \oplus^4 L^2(\mathbb{R}^3)$ is defined by

$$(a^*(F)\Psi)^{(n+1)} = \sqrt{n+1} S_{n+1}(F \otimes \Psi^{(n)}), \quad n \geq 0, \tag{2.3}$$

with domain

$$D(a^*(F)) = \left\{ \{\Psi\}_{n=0}^{\infty} \in \mathscr{F} \,\middle|\, \sum_{n=0}^{\infty}(n+1)\|S_{n+1}(F \otimes \Psi^{(n)})\|^2 < \infty \right\},$$

where S_n denotes the symmetrizer defined by $S_n(F_1 \otimes \cdots \otimes F_n) = (n!)^{-1}\sum_{\pi \in S_n} F_{\pi(1)} \cdots \otimes F_{\pi(n)}$ with S_n the set of permutations of degree n. The annihilation operator $a(F)$ is defined by the adjoint of $a^*(\bar{F})$ with respect to the scalar product (2.2), i.e., $a(F) = \big(a^*(\bar{F})\big)^*$. We can identify $\mathscr{F}$ as

$$\mathscr{F} \cong \mathscr{F}_1 \otimes \mathscr{F}_2 \otimes \mathscr{F}_3 \otimes \mathscr{F}_0, \tag{2.4}$$

where $\mathscr{F}_\mu = \mathscr{F}_{\rm b}(L^2(\mathbb{R}^3))$, $\mu = 0, 1, 2, 3$. Hereinafter we make this identification without further notice, and under this identification we set

$$a(f,\mu) := \begin{cases} a(f,1) = a(f) \otimes 1 \otimes 1 \otimes 1, \\ a(f,2) = 1 \otimes a(f) \otimes 1 \otimes 1, \\ a(f,3) = 1 \otimes 1 \otimes a(f) \otimes 1, \\ a(f,0) = 1 \otimes 1 \otimes 1 \otimes a(f). \end{cases}$$

We also define $a^*(f,\mu)$ in a similar manner and formally write

$$a^\sharp(f,\mu) = \int a^\sharp(k,\mu) f(k) dk, \qquad a^\sharp = a, a^*,$$

with the informal kernel $a^\sharp(k)$.

$\Omega \in \mathscr{F}$ denotes the Fock vacuum defined by $\Omega = \{1, 0, 0, ...\}$. The Fock vacuum is the unique vector such that $a(f,\mu)\Psi = 0$ for all $f \in L^2(\mathbb{R}^3)$ and $\mu = 0, 1, 2, 3$. Let $\Omega_\mu \in \mathscr{F}_\mu$ be the Fock vacuum. Then $\Omega = \Omega_1 \otimes \Omega_2 \otimes \Omega_3 \otimes \Omega_0$ follows. The set of vectors

$$\mathscr{F}_{\rm fin} := \text{L.H.} \left\{ \prod_{i=1}^{n} a^*(f_i,\mu_i)\Omega,\ \Omega \,\middle|\, f_j \in L^2(\mathbb{R}^3), \mu_j = 0, 1, 2, 3 \right\}$$

is called the finite particle subspace and it is dense in $\mathscr{F}$. The annihilation and creation operators leave $\mathscr{F}_{\rm fin}$ invariant and satisfy the canonical commutation relations:

$$[a(f,\mu), a^*(g,\nu)] = \delta_{\mu\nu}(\bar{f}, g), \quad [a^\sharp(f,\mu), a^\sharp(g,\nu)] = 0, \quad \mu,\nu = 0, 1, 2, 3, \tag{2.5}$$

on $\mathscr{F}_{\rm fin}$.

Next we define the second quantization. Let $\mathscr{C}(\mathcal{K})$ denote the set of contraction operators on Hilbert space $\mathcal{K}$. The functor $\Gamma : \mathscr{C}(\oplus^4 L^2(\mathbb{R}^3)) \to \mathscr{C}(\mathscr{F})$ is given by

$$\Gamma(T) \prod_{i=1}^{n} a^*(F_i)\Omega = \prod_{i=1}^{n} a^*(TF_i)\Omega$$

and $\Gamma(T)\Omega = \Omega$ for $T \in \mathscr{C}(\oplus^4 L^2(\mathbb{R}^3))$, which is called the second quantization of T. Let

$$\omega(k) = |k|, \quad k \in \mathbb{R}^3. \tag{2.6}$$

The second quantization of the one-parameter multiplicative unitary group $e^{-it\omega}$ on $L^2(\mathbb{R}^3)$ induces the one-parameter unitary group $\{\Gamma(\oplus^4 e^{-it\omega})\}_{t\in\mathbb{R}}$ on $\mathscr{F}$. Its self-adjoint generator is denoted by $H_{\rm f}$, i.e.,

$$\Gamma(\oplus^4 e^{-it\omega}) = e^{-itH_{\rm f}}, \qquad t \in \mathbb{R}, \tag{2.7}$$

and it is formally written as

$$H_{\rm f} = \sum_{\mu=0}^{3} \int \omega(k) a^*(k,\mu) a(k,\mu) dk. \tag{2.8}$$

Replacing $\omega(k)$ with the multiplication by the identity 1 in (2.8), we define the number operator $N_{\rm f}$ of $\mathscr{F}$. Furthermore let

$$N_{\rm f}^0 = \int a^*(k,0) a(k,0) dk.$$

This is the number operator on $\mathscr{F}_0$.

2.2 Indefinite metric

Let g be the 4×4 matrix $g = (g_{\mu\nu})_{\mu,\nu=0,1,2,3}$ given by

$$g_{\mu\nu} = \left\{ \begin{array}{rl} 1, & \mu=\nu=0, \\ -1, & \mu=\nu\neq 0, \\ 0, & \mu\neq\nu. \end{array} \right. \tag{2.9}$$

Now we introduce the indefinite-metric on $\mathscr{F}$. Let $[g]$ be the linear operator induced from the metric tensor g:

$$[g] = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} : \oplus^4 L^2(\mathbb{R}^3) \to \oplus^4 L^2(\mathbb{R}^3),$$

and define $\eta : \mathscr{F} \to \mathscr{F}$ by the second quantization of $-[g]$, i.e.,

$$\eta := \Gamma(-[g]) = (-1)^{N_{\rm f}^0}. \tag{2.10}$$

From the definition,

$$\eta^2 = 1. \tag{2.11}$$

By using η we introduce an indefinite metric on $\mathscr{F}$ by

$$(\Psi|\Phi) := (\Psi, \eta\Phi)_{\mathscr{F}}. \tag{2.12}$$

In order to define the adjoint with respect to the indefinite metric (2.12) we introduce the η-adjoint of $a(f,\mu)$ by

$$a^\dagger(f,\mu) := \eta a^*(f,\mu)\eta. \tag{2.13}$$

Then $(\Psi|a^\dagger(f,\mu)\Phi) = (a(\bar{f},\mu)\Psi|\Phi)$ and

$$a^\dagger(f,\mu) = \begin{cases} \ \ a^*(f,j), & \mu = j = 1,2,3, \\ -a^*(f,0), & \mu = 0 \end{cases} \tag{2.14}$$

hold. Hence we have the commutation relations:

$$[a(f,\mu), a^\dagger(g,\nu)] = -g_{\mu\nu}(\bar{f}, g), \qquad [a^\dagger(f,\mu), a^\dagger(g,\nu)] = 0. \tag{2.15}$$

Let us define the quantized radiation field $\mathscr{A}_\mu(f,x)$, $x \in \mathbb{R}^3$, $\mu = 0,1,2,3$, for a test function $f \in L^2(\mathbb{R}^3)$. Let $e^j(k) \in \mathbb{R}^3$, $k \in \mathbb{R}^3$, $j = 1,2,3$, be unit vectors such that $e^3(k) = k/|k|$, and let three vectors $e^1(k)$, $e^2(k)$ and $e^3(k)$ form a right-handed system for each $k \in \mathbb{R}^3$. We fix them. The quantized radiation field,

$$\Big(\mathscr{A}_0(f,x), -\mathscr{A}_1(f,x), -\mathscr{A}_2(f,x), -\mathscr{A}_3(f,x)\Big) = \Big(\mathscr{A}^0(f,x), \vec{\mathscr{A}}(f,x)\Big), \tag{2.16}$$

smeared by the test function $f \in L^2(\mathbb{R}^3)$ at time zero is defined by

$$\vec{\mathscr{A}}(f,x) = \frac{1}{\sqrt{2}} \sum_{j=1}^3 \int dk \frac{e^j(k)}{\sqrt{\omega(k)}} \left(a^\dagger(k,j)\hat{f}(k)e^{-ikx} + a(k,j)\hat{f}(-k)e^{ikx}\right),$$

$$\mathscr{A}_0(f,x) = \frac{1}{\sqrt{2}} \int dk \frac{1}{\sqrt{\omega(k)}} \left(a^\dagger(k,0)\hat{f}(k)e^{-ikx} + a(k,0)\hat{f}(-k)e^{ikx}\right)$$

and its derivative by

$$\dot{\vec{\mathscr{A}}}(g,x) = \frac{i}{\sqrt{2}} \sum_{j=1}^3 \int dk e^j(k)\sqrt{\omega(k)} \left(a^\dagger(k,j)\hat{g}(k)e^{-ikx} - a(k,j)\hat{g}(-k)e^{ikx}\right),$$

$$\dot{\mathscr{A}}_0(g,x) = \frac{i}{\sqrt{2}} \int dk \sqrt{\omega(k)} \left(a^\dagger(k,0)\hat{g}(k)e^{-ikx} - a(k,0)\hat{g}(-k)e^{ikx}\right).$$

$\mathscr{A}^0$ is a scalar potential and $\vec{\mathscr{A}}$ a vector potential. Conventionally the vector potential $\vec{\mathscr{A}}$ is decomposed as $\vec{\mathscr{A}} = \mathscr{A}^\perp + \mathscr{A}^\parallel$, where $\mathscr{A}^\perp$ is the transversal part and $\mathscr{A}^\parallel$ the longitudinal part given by

$$\mathscr{A}^\perp(f,x) = \frac{1}{\sqrt{2}} \sum_{j=1,2} \int dk \frac{e^j(k)}{\sqrt{\omega(k)}} \left(a^\dagger(k,j)\hat{f}(k)e^{-ikx} + a(k,j)\hat{f}(-k)e^{ikx} \right),$$

$$\mathscr{A}^\parallel(f,x) = \frac{1}{\sqrt{2}} \int dk \frac{e^3(k)}{\sqrt{\omega(k)}} \left(a^\dagger(k,3)\hat{f}(k)e^{-ikx} + a(k,3)\hat{f}(-k)e^{ikx} \right).$$

Note that $\sum_{l=1}^3 \partial_{x_l} \mathscr{A}_l^\perp(f,x) = 0$. Set

$$\mathscr{A}_\mu(f) := \mathscr{A}_\mu(f,0), \qquad \mu = 0,1,2,3. \tag{2.17}$$

By the canonical commutation relations (2.5) and (2.15) we have

$$[\mathscr{A}_\mu(f), \dot{\mathscr{A}}_\nu(g)] = -ig_{\mu\nu}(\bar{f}, g) \tag{2.18}$$

and

$$[\mathscr{A}_\mu(f), \mathscr{A}_\nu(g)] = 0, \quad [\dot{\mathscr{A}}_\mu(f), \dot{\mathscr{A}}_\nu(g)] = 0 \tag{2.19}$$

for *all* $f, g \in L^2(\mathbb{R}^3)$. It can also be seen that

$$[H_{\rm f}, a^\dagger(f,\mu)] = a^\dagger(\omega f, \mu), \quad [H_{\rm f}, a(f,\mu)] = -a(\omega f, \mu), \tag{2.20}$$

by which we have

$$[H_{\rm f}, \mathscr{A}_\mu(f)] = -i\dot{\mathscr{A}}_\mu(f), \quad [H_{\rm f}, \dot{\mathscr{A}}_\nu(f)] = i\mathscr{A}_\mu(-\Delta f). \tag{2.21}$$

We introduce notions of η-self-adjointness and η-unitarity [Bog73] below.

Definition 2.1 *(1) A densely defined linear operator X is η-self-adjoint if and only if $\eta X^* \eta = X$.*

(2) A densely defined linear operator X is η-unitary if and only if X is injective and $X^{-1} = \eta X^* \eta$.

The next lemma immediately follows from the definition of η-self-adjointness.

Lemma 2.2 *(1) X is η-self-adjoint if and only if ηX is self-adjoint. (2) Let X be η-self-adjoint. Then X is closed on $D(X)$. (3) Let X be η-self-adjoint and ηX is essentially self-adjoint on D. Then D is a core of X.*

For real-valued f, note that the closures of $\mathscr{A}_j(f,x)$ and $\dot{\mathscr{A}}_j(f,x)$, $j = 1,2,3$, are self-adjoint and η-self-adjoint for each $x \in \mathbb{R}^3$. However the closure of $\mathscr{A}_0(f,x)$ and $\dot{\mathscr{A}}_0(f,x)$ for real-valued f are η-self-adjoint but not even symmetric. Moreover the free Hamiltonian $H_{\rm f}$ is self-adjoint and η-self-adjoint.

2.3 Definition of NRQED in the Lorentz gauge

The Hilbert space of our system consisting of one electron coupled with photons is given by the tensor product of $L^2(\mathbb{R}^3)$ and $\mathscr{F}$:

$$\mathscr{H} := L^2(\mathbb{R}^3) \otimes \mathscr{F}, \tag{2.22}$$

where $L^2(\mathbb{R}^3)$ describes the state space of one electron and $\mathscr{F}$ the photon field. The full Hamiltonian of our system is defined by

$$H_{\mathrm{tot}} := \frac{1}{2m}\left(p \otimes 1 - e\vec{\mathscr{A}}(\hat{\varphi}, \cdot)\right)^2 + 1 \otimes H_{\mathrm{f}} + e1 \otimes \mathscr{A}_0 \tag{2.23}$$

for a given fixed test function $\hat{\varphi}$ on $\mathbb{R}^3$ which satisfies some conditions mentioned later. Let $m > 0$ and $e \in \mathbb{R}$ denote the mass and charge of the electron, respectively, and $p = -i\vec{\nabla}_x$ denote the momentum operator of the electron. Instead of this full Hamiltonian in this paper we take the dipole approximation; namely we replace $\mathscr{A}(\hat{\varphi}, \cdot)$ in H_{tot} by $1 \otimes \mathscr{A}(\hat{\varphi})$. We set

$$\mathscr{A}_\mu := \mathscr{A}_\mu(\hat{\varphi}). \tag{2.24}$$

We make the following assumptions about $\hat{\varphi}$ throughout this paper.

Assumption 2.3 (Assumptions for η-self-adjointness). *$\hat{\varphi}/\omega, \hat{\varphi}/\sqrt{\omega}, \sqrt{\omega}\hat{\varphi} \in L^2(\mathbb{R}^3)$ and $\hat{\varphi}(-k) = \overline{\hat{\varphi}(k)}$.*

Then our Hamiltonian is given by

$$H := \frac{1}{2m}\left(p \otimes 1 - e1 \otimes \vec{\mathscr{A}}\right)^2 + 1 \otimes H_{\mathrm{f}} + e1 \otimes \mathscr{A}_0 \tag{2.25}$$

with domain

$$D(H) := D(-\Delta \otimes 1) \cap D(1 \otimes H_{\mathrm{f}}). \tag{2.26}$$

Proposition 2.4 *H is η-self-adjoint and ηH is essentially self-adjoint on any core of $-\Delta \otimes 1 + 1 \otimes H_{\mathrm{f}}$. In particular H is closed and an arbitrary core of $-\Delta \otimes 1 + 1 \otimes H_{\mathrm{f}}$ is also a core of H.*

Proof: Set $H' = H - e1 \otimes \mathscr{A}_0$. Let $L = -\Delta \otimes 1 + 1 \otimes H_{\mathrm{f}} + 1$. Then we have

$$|(L\Psi, H'\Phi) - (H'\Psi, L\Phi)| \leq C\|L^{1/2}\Phi\|\|L^{1/2}\Psi\|$$

for some constant C by the fundamental inequality $\|a^\sharp(f)\Psi\| \le C'\|(H_{\rm f}+1)^{1/2}\Psi\|$. Thus by the Nelson commutator theorem, H' is self-adjoint on $D(-\Delta\otimes 1)\cap D(1\otimes H_{\rm f})$. We can also see that

$$\|\eta\mathscr{A}_0\Psi\| \le C'(\|(H_{\rm f}^0)^{1/2}\Psi\| + \|\Psi\|) \tag{2.27}$$

and $[H',\eta]=0$, which implies that

$$\|\eta\mathscr{A}_0\Psi\| \le C'(\|(H')^{1/2}\Psi\| + \|\Psi\|) \le \epsilon\|\eta H'\Psi\| + b_\epsilon\|\Psi\|$$

for arbitrary $\epsilon>0$. Since $\mathscr{A}_0$ is skew symmetric and $\{\mathscr{A}_0,\eta\}=0$, we have $(\eta H)^* = H^*\eta \supset \eta H$, which yields the result that ηH is symmetric. Then we can see by the Kato-Rellich theorem that ηH is self-adjoint on $D(-\Delta\otimes 1)\cap D(1\otimes H_{\rm f})$. This completes the proof. **qed**

We divide $\mathscr{H}$ into a scalar part and a vector part. Let $\mathscr{H}_0 := \mathscr{F}_0$, $\mathscr{F}_{\rm TL} = \mathscr{F}_1\otimes\mathscr{F}_2\otimes\mathscr{F}_3$ and $\mathscr{H}_{\rm TL} := L^2(\mathbb{R}^3)\otimes\mathscr{F}_{\rm TL}$. Then $\mathscr{H}$ can be realized as the tensor product of the scalar part and the vector part:

$$\mathscr{H} \cong \mathscr{H}_{\rm TL}\otimes\mathscr{H}_0. \tag{2.28}$$

We use this identification without further notice through this paper. This identification is inherited by the Hamiltonian H and we have

$$H = H_{\rm TL}\otimes 1 + 1\otimes H_0, \tag{2.29}$$

where $H_{\rm TL}$ is the vector component of H:

$$H_{\rm TL} := \frac{1}{2m}(p\otimes 1 - e1\otimes\vec{\mathscr{A}})^2 + 1\otimes H_{\rm f}^{\rm TL} \tag{2.30}$$

defined on $\mathscr{H}_{\rm TL} = L^2(\mathbb{R}^3)\otimes\mathscr{F}_{\rm TL}$, and H_0 the scalar component:

$$H_0 := e\mathscr{A}_0 + H_{\rm f}^0 \tag{2.31}$$

defined on $\mathscr{H}_0$. Here $H_{\rm f}^{\rm TL}$ denotes the free Hamiltonian in $\mathscr{F}_{\rm TL}$:

$$H_{\rm f}^{\rm TL} = \sum_{j=1}^3\int\omega(k)a^*(k,j)a(k,j)dk = \sum_{j=1}^3\int\omega(k)a^\dagger(k,j)a(k,j)dk$$

and $H_{\rm f}^0$ in $\mathscr{F}_0$:

$$H_{\rm f}^0 = \int\omega(k)a^*(k,0)a(k,0)dk = -\int\omega(k)a^\dagger(k,0)a(k,0)dk.$$

Proposition 2.5 *(1) $H_{\rm TL}$ is self-adjoint on $D(-\Delta\otimes 1)\cap D(1\otimes H_{\rm f}^{\rm TL})$ and essentially self-adjoint on any core of $-\Delta\otimes 1+1\otimes H_{\rm f}^{\rm TL}$. (2) H_0 is η-self-adjoint on $D(H_{\rm f}^0)$. In particular H_0 is closed on $D(H_{\rm f}^0)$ and an arbitrary core of $H_{\rm f}^0$ is also a core of H_0.*

Proof: (1) has been proven in the proof of Proposition 2.4. By (2.27), ηH_0 is self-adjoint on $D(H_{\rm f}^0)$. Hence the proof is complete. **qed**

3 Heisenberg equations

In this section we first diagonalize the total Hamiltonian by making use of a certain η-unitary operator, and solve the Heisenberg equation exactly. The first rigorous results on the diagonalization of NRQED are in Arai [Ara83a, Ara83b], where the electromagnetic field is quantized with respect to the Coulomb gauge and then there is no scalar potential $\mathscr{A}_0$ nor longitudinal potential $\mathscr{A}^{\|}$.

In addition to Assumption 2.3, from now on we make the following assumption.

Assumption 3.1 *We assume (1)-(5).*

(1) $\int_{\mathbb{R}^3}|\hat\varphi(k)|^2/\omega(k)^3dk<\infty$,

(2) *there exists $\epsilon>0$ such that $\|e^{+\epsilon\omega}\hat\varphi\|_\infty<\infty$,*

(3) *there exists a function ρ on $[0,\infty)$ such that $\hat\varphi(k)=\rho(|k|)$,*

(4) $\rho(s)>0$ *for $s\neq 0$,*

(5) $F(s):=\rho(\sqrt{s})^2\sqrt{s}\in L^p([0,\infty);ds)$ *for some $1<p$, and there exists $0<\alpha<1$ such that $|F(s+h)-F(s)|\le K|h|^\alpha$ for all s and $0<h\le 1$.*

We explain Assumption 3.1.

(1) This condition is called the infrared regular condition, which is used to construct η-unitary operators V_0 in Section 3.1 and U_P in Section 3.2.

(2) This ensures that $\|\omega\hat\varphi\|_\infty<\infty$, $\|\sqrt{\omega}\hat\varphi\|_\infty<\infty$ and $\|\hat\varphi\|_\infty<\infty$. Then the operators T and $W_\pm^{ij}$ introduced in Section 3.2 can be defined as bounded operators. Furthermore we can construct the Heisenberg operators defined by Definition 3.10 by (2), where we need analytic continuation of $e^{-it\omega}\hat\varphi$ with respect to t.

(3) This means that $\hat\varphi$ is rotation invariant.

In Section 3.2 we introduce the function

$$D_\pm(s) = m - \frac{e^2}{2}4\pi\left\{\lim_{\epsilon\to 0}\int_{|s-r|>\epsilon, r>0}\frac{\rho(\sqrt{r})^2\sqrt{r}}{s-r}dr \mp 2\pi i\rho(\sqrt{s})^2\sqrt{s}\right\} \tag{3.1}$$

and define

$$Q(k) = \frac{\hat{\varphi}(k)}{D_+(\omega(k)^2)}. \tag{3.2}$$

Conditions (4) and (5) are used to ensure that Q is well defined.

(4) This condition implies that the imaginary part of $D_\pm$ is strictly positive for all $s > 0$, in particular it is non-zero except for $s = 0$.

(5) Note that

$$HF(s) = (2\pi i)^{-1}\lim_{\epsilon\to 0}\int_{|s-r|>\epsilon, r>0}\frac{F(s)}{s-r}dr$$

is the Hilbert transform of $F(s)$. By the Lipshitz condition (5) the real part of $D_\pm$ is also Lipshitz continuous with the same order α as $F(s)$ and belongs to $L^p(\mathbb{R})$. See e.g., [Tit36, p.145, THEOREM 106]. This yields the result that the real part of $D_\pm(s) \to 0$ as $s \to \infty$.

Thus (4) and (5), together with $D_\pm(0) > 0$, ensure that there exists $c > 0$ such that

$$|D_\pm(s)| > c, \quad \forall s \geq 0 \tag{3.3}$$

and hence Q is well defined.

Assumption (4), however, seems to be unusual. We note that, as mentioned above, assumptions (4) and (5) are sufficient to allow the definition of Q. It is possible to choose an alternative ρ so that Q is well defined. In particular, one can choose ρ satisfying (5) but not (4). For example suppose that $\rho(s)$ has compact support $|s| < N$. Then in order to define Q it is enough to assume further that $\mathrm{Re}D_+(s) = m - (2\pi e^2)(2\pi i)HF(s) > \delta > 0$ for all $|s| > N - 1$ for some $\delta > 0$. Notice that this assumption is satisfied, because $HF(s) \to 0$ as $s \to \infty$ and $m > 0$. We omit the detail.

3.1 Scalar potential

Let us begin by discussing the scalar part of the Hamiltonian. The scalar part H_0 of H can be easily diagonalized by an η-unitary (but not unitary) operator. Let

$$V_0 = \exp\left(\frac{e}{\sqrt{2}}\left(a^*\left(\frac{\hat{\varphi}}{\omega^{3/2}}, 0\right) + a\left(\frac{\hat{\varphi}}{\omega^{3/2}}, 0\right)\right)\right). \tag{3.4}$$

This is unbounded η-unitary on $\mathscr{F}_0$. It can be seen that the finite particle subspace $\mathscr{F}_{0,\text{fin}}$ of $\mathscr{F}_0$ contains analytic vectors of V_0. Then

$$V_0\Psi = \sum_{n=0}^{\infty} \frac{1}{n!}\left(a^*\left(\frac{\hat{\varphi}}{\omega^{3/2}}, 0\right) + a\left(\frac{\hat{\varphi}}{\omega^{3/2}}, 0\right)\right)^n \Psi \tag{3.5}$$

for $\Psi \in \mathscr{F}_{0,\text{fin}}$. By the commutation relations and (3.5), we have

$$(H_0^*\Phi, V_0\Psi) = (\Phi, V_0(H_\text{f}^0 + E_0)\Psi)$$

for $\Psi, \Phi \in \mathscr{F}_{0,\text{fin}}$, where

$$E_0 := \frac{e^2}{2}\|\hat{\varphi}/\omega\|^2. \tag{3.6}$$

Thus $V_0\Psi \in D(H_0)$ and $H_0V_0\Psi = V_0(H_\text{f}^0 + E_0)\Psi$; furthermore $H_0V_0\Psi \in D(V_0^{-1})$. Then we have

$$V_0^{-1}H_0V_0 = H_\text{f}^0 + E_0 \tag{3.7}$$

on $\mathscr{F}_{0,\text{fin}}$. Since $\mathscr{F}_{0,\text{fin}}$ is a core of H_f^0, we have

$$\overline{V_0^{-1}H_0V_0\lceil_{\mathscr{F}_{0,\text{fin}}}} = H_\text{f}^0 + E_0 \tag{3.8}$$

on $D(H_\text{f}^0)$. From (3.7), we can see that $V_0\Omega_0$ is an eigenvector of H_0 associated with eigenvalue E_0:

$$H_0V_0\Omega_0 = E_0V_0\Omega_0. \tag{3.9}$$

Define

$$b(f, 0) := a(f, 0) - \frac{e}{\sqrt{2}}(\hat{\varphi}/\omega^{3/2}, f), \tag{3.10}$$

$$b^\dagger(f, 0) := a^\dagger(f, 0) - \frac{e}{\sqrt{2}}(\hat{\varphi}/\omega^{3/2}, f). \tag{3.11}$$

These operators satisfy the canonical commutation relations:

$$[b(f, 0), b^\dagger(g, 0)] = -(\bar{f}, g), \quad [b(f, 0), b(g, 0)] = 0 = [b^\dagger(f, 0), b^\dagger(g, 0)] \tag{3.12}$$

and

$$[H_0, b^\dagger(f, 0)] = b^\dagger(\omega f, 0), \quad [H_0, b(f, 0)] = -b(\omega f, 0). \tag{3.13}$$

Thus the quadruple

$$(\mathscr{F}_0, V_0\Omega_0, \{b^\dagger(f, 0), b(f, 0) | f \in L^2(\mathbb{R}^3)\}, H_0) \tag{3.14}$$

corresponds to the free case $(\mathscr{F}_0, \Omega_0, \{a(f, 0), a^*(f, 0) | f \in L^2(\mathbb{R}^3)\}, H_\text{f}^0)$, but H_0 is not self-adjoint.

3.2 Vector potential

In this subsection we investigate the vector part $H_{\rm TL}$ of H. $H_{\rm TL}$ is quadratic and can also be diagonalized by a Bogoliubov transformation.

$H_{\rm TL}$ is self-adjoint on $D(-\Delta\otimes 1)\cap D(1\otimes H_{\rm f})$ and essentially self-adjoint on any core of $(-1/2)\Delta\otimes 1+1\otimes H_{\rm f}$. This can be proven by virtue of the Nelson commutator theorem as stated in the proof of Lemma 2.4. Since $H_{\rm TL}$ commutes with p_j, $j=1,2,3$, $H_{\rm TL}$ and $\mathscr{H}_{\rm TL}$ are decomposable with respect to the spectrum of p_j and are given by

$$\mathscr{H}_{\rm TL}=\int_{\mathbb{R}^3}^{\oplus}\mathscr{H}_{{\rm TL},P}dP$$

and

$$H_{\rm TL}=\int_{\mathbb{R}^3}^{\oplus}H_{{\rm TL},P}dP,$$

where $\mathscr{H}_{{\rm TL},P}=\mathscr{F}_{\rm TL}$ and $H_{{\rm TL},P}$ is the self-adjoint operator on $\mathscr{F}_{\rm bTL}$, given by

$$H_{{\rm TL},P}=\frac{1}{2m}(P-e\vec{\mathscr{A}})^2+H_{\rm f}^{\rm TL},\quad P\in\mathbb{R}^3. \tag{3.15}$$

The fiber Hamiltonian $H_{{\rm TL},P}$ is, indeed, self-adjoint on $D(H_{\rm f}^{\rm TL})$ for all $(P,e)\in\mathbb{R}^3\times\mathbb{R}$ and bounded from below. In the similar way as Proposition 2.4 this can also be proven by virtue of the Nelson commutator theorem with the conjugate operator L replaced by $N_{\rm TL}+1$, where $N_{\rm TL}$ denotes the number operator on $\mathscr{F}_{\rm TL}$. Now for each $(P,e)\in\mathbb{R}^3\times\mathbb{R}$, let us construct a quadruple (3.16) relevant to the free case $(\mathscr{F}_{\rm TL},\Omega_{\rm TL},\{a(f,j),a^*(f,j)|f\in L^2(\mathbb{R}^3),j=1,2,3\},H_{\rm f}^{\rm TL})$:

$$\big(\mathscr{F}_{\rm TL},\Omega_{{\rm TL},P},\{b_P(f,j),b_P^*(f,j)|f\in L^2(\mathbb{R}^3),j=1,2,3\},H_{{\rm TL},P}\big) \tag{3.16}$$

such that

(1) $b_P(f,j)$ and $b_P^*(g,j)$ satisfy the canonical commutation relations,

$$[b_P(f,j),b_P^*(g,i)]=\delta_{ij}(\bar{f},g),\qquad [b_P(f,j),b_P(g,i)]=0=[b_P^*(f,j),b_P^*(g,i)],$$

(2) $[H_{{\rm TL},P},b_P(f,j)]=-b_P(\omega f,j)$ and $[H_{{\rm TL},P},b_P^*(f,j)]=b_P^*(\omega f,j)$,

(3) $\Omega_{{\rm TL},P}$ is the unique vector such that $b_P(f,j)\Omega_{{\rm TL},P}=0$ and is the ground state of $H_{{\rm TL},P}$.

From (1) to (3) above we will be able to infer the unitary equivalences: $\Omega_{\mathrm{TL},P} \cong \Omega$, $b_P^\sharp(f,j) \cong a^\sharp(f)$ and $H_{\mathrm{TL},P} \cong H_{\mathrm{f}}^{\mathrm{TL}} + E_{\mathrm{TL}}(P)$ for each P, where $E_{\mathrm{TL}}(P) = \inf \mathrm{Sp}(H_{\mathrm{TL},P})$ is given explicitly.

In order to construct $b_P^\sharp$ we make explicit the relationship between $a^\sharp$ and $\vec{\mathscr{A}}$. It can be seen that the creation operator and the annihilation operator can be expressed as

$$a(f,l) = \frac{1}{\sqrt{2}} \sum_{j=1}^{3} \left(\hat{\mathscr{A}}_j(e_j^l \sqrt{\omega} f) + i \hat{\dot{\mathscr{A}}}_j(e_j^l \frac{1}{\sqrt{\omega}} f) \right), \tag{3.17}$$

$$a^*(f,l) = \frac{1}{\sqrt{2}} \sum_{j=1}^{3} \left(\hat{\mathscr{A}}_j(\tilde{e}_j^l \sqrt{\omega} \tilde{f}) - i \hat{\dot{\mathscr{A}}}_j(\tilde{e}_j^l \frac{1}{\sqrt{\omega}} \tilde{f}) \right), \tag{3.18}$$

where $\hat{\mathscr{A}}(f) := \mathscr{A}(\hat{f})$ and $\hat{\dot{\mathscr{A}}}(g) := \dot{\mathscr{A}}(\hat{g})$, and $\tilde{f}(k) = f(-k)$. Note that $\hat{\hat{f}} = \tilde{\tilde{\tilde{f}}} = \tilde{f}$. Modifying the right-hand side of (3.17) and (3.18), we can construct $b^\sharp$ in (3.16). Let

$$G_\epsilon f(k) := \int_{\mathbb{R}^3} \frac{f(k')}{(\omega(k)^2 - \omega(k')^2 + i\epsilon)\omega(k)^{1/2}\omega(k')^{1/2}} dk', \quad \epsilon > 0.$$

Then G_ϵ is bounded and skew-symmetric on $L^2(\mathbb{R}^3)$. Moreover the strong limit $G := \lim_{\epsilon\downarrow 0} G_\epsilon$ exists as a bounded skew-symmetric operator.

Let

$$D(z) := m - e^2 \int_{\mathbb{R}^3} \frac{|\hat{\varphi}(k)|^2}{z - \omega(k)^2} dk, \tag{3.19}$$

which is analytic on $\mathbb{C} \setminus [0,\infty)$. Let $D_\pm(s) := \lim_{\epsilon\downarrow 0} D(s \pm i\epsilon)$ for $s \in [0,\infty)$; then we see that $|D_\pm(s)| > c$ for some $c > 0$ by (4) and (5) of Assumption 3.1. See (3.3) and (3.1) for the explicit form of $D_\pm$. Then we can define $Q(k) := \hat{\varphi}(k)/D_+(\omega(k)^2)$. Operator $T : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ is given by

$$Tf := f + e^2 Q \sqrt{\omega} G \sqrt{\omega} \hat{\varphi} f. \tag{3.20}$$

Since G is skew-symmetric, we have $T^* f = f - e^2 \hat{\varphi} \sqrt{\omega} G \sqrt{\omega} \bar{Q} f$.

Lemma 3.2 *T satisfies the following algebraic relations:*

(1) *T is unitary on $L^2(\mathbb{R}^3)$ and bounded on $L^2(\mathbb{R}^3, \omega^n dk)$, $n = \pm 1$;*

(2) $T^* \frac{1}{\omega^2} Q = \frac{\hat{\varphi}}{m_{\mathrm{eff}} \omega^2}$, *where $m_{\mathrm{eff}} := D(0) = m + e^2 \|\hat{\varphi}/\omega\|^2$;*

(3) $[\omega^2, T^*] f = -e^2 (Q, f) \hat{\varphi}, \quad [\omega^2, T] f = +e^2 (\hat{\varphi}, f) Q$;

(4) $T\hat{\varphi} = mQ$.

Proof: This is a slight modification of [Ara83a, Ara83b]. We omit the proof. **qed**

Now, for $f \in L^2(\mathbb{R}^3)$, we define

$$b_P(f,l) := \frac{1}{\sqrt{2}}\sum_{j=1}^{3}\left(\hat{\mathscr{A}}_j(T^* e_j^l \sqrt{\omega} f) + i\dot{\hat{\mathscr{A}}}_j(T^* e_j^l \frac{1}{\sqrt{\omega}} f) - P_j\left(\frac{e e_j^l Q}{\omega^{3/2}}, f\right)\right), \quad (3.21)$$

$$b_P^*(f,l) := \frac{1}{\sqrt{2}}\sum_{j=1}^{3}\left(\hat{\mathscr{A}}_j(\bar{T}^* \tilde{e}_j^l \sqrt{\omega} \tilde{f}) - i\dot{\hat{\mathscr{A}}}_j(\bar{T}^* \tilde{e}_j^l \frac{1}{\sqrt{\omega}} \tilde{f}) - P_j\left(\frac{e e_j^l \bar{Q}}{\omega^{3/2}}, f\right)\right) \quad (3.22)$$

and set $b^\sharp(F) := \sum_{l=1}^3 b^\sharp(F_l, l)$ for $F \in \oplus^3 L^2(\mathbb{R}^3)$.

Lemma 3.3 *It follows that* $(b_P(f,j))^* = b_P^*(\bar{f}, j)$*, and the commutation relations below hold:*

$$[b_P(f,i), b_P^*(g,j)] = \delta_{ij}(\bar{f}, g), \quad [b_P(f,j), b_P(g,i)] = 0 = [b_P^*(f,j), b_P^*(g,i)], \quad (3.23)$$

$$[H_{\mathrm{TL},P}, b_P(f,j)] = -b_P(\omega f, j), \quad [H_{\mathrm{TL},P}, b_P^*(f,j)] = b_P^*(\omega f, j). \quad (3.24)$$

Proof: By the definition of $b_P^\sharp$ we have

$$b_P(f,j) = \sum_{i=1}^{3}\left(a^*(W_-^{ij} f, i) + a(W_+^{ij} f, i) + \sum_{l=1}^{3}(P_l L_l^j, f)\right),$$

$$b_P^*(f,j) = \sum_{i=1}^{3}\left(a^*(\bar{W}_+^{ij} f, i) + a(\bar{W}_-^{ij} f, i) + \sum_{l=1}^{3}(P_l \bar{L}_l^j, f)\right),$$

where $\bar{X} f = \overline{X\bar{f}}$, $L_l^j = e\frac{1}{\sqrt{2}}\frac{e_l^j Q}{\omega^{3/2}}$ and $W_{P,\pm}^{ij} : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ is defined by

$$W_+^{ij} f := \frac{1}{2}\sum_{l=1}^{3} e_l^i \left(\frac{1}{\sqrt{\omega}} T^* \sqrt{\omega} + \sqrt{\omega} T^* \frac{1}{\sqrt{\omega}}\right) e_l^j f,$$

$$W_-^{ij} f := \frac{1}{2}\sum_{l=1}^{3} e_l^i \left(\frac{1}{\sqrt{\omega}} T^* \sqrt{\omega} - \sqrt{\omega} T^* \frac{1}{\sqrt{\omega}}\right) \tilde{e}_l^j \tilde{f}.$$

Then $W_\pm = \left(W_\pm^{ij}\right)_{1 \le i,j \le 3} : \oplus^3 L^2(\mathbb{R}^3) \to \oplus^3 L^2(\mathbb{R}^3)$ has the symplectic structure (3.26) below. Let

$$\mathbb{W} = \begin{bmatrix} W_+ & \bar{W}_- \\ W_- & \bar{W}_+ \end{bmatrix} : \bigoplus^2 [\oplus^3 L^2(\mathbb{R}^3)] \to \bigoplus^2 [\oplus^3 L^2(\mathbb{R}^3)]. \quad (3.25)$$

Using (4) and (5) of Lemma 3.2, it can be determined that $\mathbb{W}$ satisfies

$$\mathbb{W}^* J \mathbb{W} = \mathbb{W} J \mathbb{W}^* = J, \tag{3.26}$$

where

$$J := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbb{W}^* := \begin{bmatrix} W_+^* & W_-^* \\ \bar{W}_-^* & \bar{W}_+^* \end{bmatrix}.$$

This is equivalent to (3.23). Next we show (3.24). Note that

$$[\mathscr{A}_j, b_P(f,l)] = -m\frac{1}{\sqrt{2}}\left(\frac{e_j^l Q}{\sqrt{\omega}}, f\right), \quad [\mathscr{A}_j, b_P^*(f,l)] = +m\frac{1}{\sqrt{2}}\left(\frac{e_j^l \bar{Q}}{\sqrt{\omega}}, f\right), \quad j,l = 1,2,3,$$

and

$$[H_{\mathrm{f}}, b_P(f,l)] = \frac{1}{\sqrt{2}}\sum_{j=1}^3\left(-\hat{\mathscr{A}}_j\left(\omega^2 T^* e_j^l \frac{1}{\sqrt{\omega}} f\right) - i\hat{\dot{\mathscr{A}}}_j\left(T^* e_j^l \sqrt{\omega} f\right)\right),$$

$$[H_{\mathrm{f}}, b_P^*(f,l)] = \frac{1}{\sqrt{2}}\sum_{j=1}^3\left(\hat{\mathscr{A}}_j\left(\omega^2 \bar{T}^* \tilde{e}_j^l \frac{1}{\sqrt{\omega}} \tilde{f}\right) - i\hat{\dot{\mathscr{A}}}_j\left(\bar{T}^* \tilde{e}_j^l \sqrt{\omega} \tilde{f}\right)\right).$$

Then we have

$$\begin{aligned}
&[H_{\mathrm{TL},P}, b_P(f,l)] \\
&= -\frac{e}{m}\sum_{j=1}^3 P_j[\mathscr{A}_j, b_P(f,l)] + \frac{e^2}{m}\sum_{j=1}^3 \mathscr{A}_j[\mathscr{A}_j, b_P(f,l)] + [H_{\mathrm{f}}, b_P(f,l)] \\
&= \sum_{j=1}^3\left(-\frac{e}{m}P_j\frac{1}{\sqrt{2}}(-m)\left(\frac{e_j^l Q}{\sqrt{\omega}}, f\right) + \frac{e^2}{m}\mathscr{A}_j(-m)\frac{1}{\sqrt{2}}\left(\frac{e_j^l Q}{\sqrt{\omega}}, f\right)\right. \\
&\qquad\left. + \frac{1}{\sqrt{2}}\left(-\hat{\mathscr{A}}_j\left(\omega^2 T^* e_j^l \frac{f}{\sqrt{\omega}}\right) - i\hat{\dot{\mathscr{A}}}_j\left(T^* e_j^l\sqrt{\omega} f\right)\right)\right) \\
&= \frac{1}{\sqrt{2}}\sum_{j=1}^3\left(-\hat{\mathscr{A}}_j\left(T^* e_j^l \sqrt{\omega}\omega f\right) - i\hat{\dot{\mathscr{A}}}_j\left(T^* e_j^l \frac{1}{\sqrt{\omega}}\omega f\right) + P_j\left(\frac{e e_j^l Q}{\omega^{3/2}}, \omega f\right)\right) \\
&= -b_P(\omega f, l).
\end{aligned}$$

Here we used the fact that $\omega^2 T^* e_j^l \frac{1}{\sqrt{\omega}} f = T^* e_j^l \sqrt{\omega}\omega f - e^2\left(\frac{e_j^l Q}{\sqrt{\omega}}, f\right)\hat{\varphi}$. See (2) of Lemma 3.2. Then (3.24) follows. **qed**

Lemma 3.4 *There exists a unitary operator $U_P : \mathscr{F}_{\mathrm{TL}} \to \mathscr{F}_{\mathrm{TL}}$ such that*

$$U_P^{-1} b_P^\sharp(f,j) U_P = a^\sharp(f,j), \quad f \in L^2(\mathbb{R}^3). \tag{3.27}$$

Proof: Since W_- is a Hilbert-Schmidt operator on $\oplus^3 L^2(\mathbb{R}^3)$, there exists a canonical linear transformation $U(\mathbb{W})$ associated with $\mathbb{W}$ [Rui78] such that for $F = (F_1, F_2, F_3) \in \oplus^3 L^2(\mathbb{R}^3)$, $U(\mathbb{W})^{-1} B^\sharp(F) U(\mathbb{W}) = a^\sharp(F)$, where

$$\begin{bmatrix} B(F) \\ B^*(F) \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^3 \sum_{j=1}^3 \left(a(W_+^{ij} F_j, i) + a^*(W_-^{ij} F_j, i) \right) \\ \sum_{i=1}^3 \sum_{j=1}^3 \left(a(\bar{W}_-^{ij} F_j, i) + a^*(\bar{W}_+^{ij} F_j, i) \right). \end{bmatrix}$$

Since

$$\begin{bmatrix} b_P(F) \\ b_P^*(F) \end{bmatrix} = \begin{bmatrix} B(F) \\ B^*(F) \end{bmatrix} + \begin{bmatrix} \sum_{j=1}^3 \sum_{l=1}^3 (P_l L_l^j, F_j) \\ \sum_{j=1}^3 \sum_{l=1}^3 (P_l \bar{L}_l^j, F_j) \end{bmatrix},$$

we see that

$$U_P := S(P) U(\mathbb{W}) \tag{3.28}$$

satisfies (3.27), where $S(P)$ is the unitary operator given by

$$S(P) := \exp\left(\frac{e}{\sqrt{2}} \sum_{j=1}^3 \sum_{l=1}^3 \frac{P_j}{m_{\text{eff}}} \left(a\left(\frac{e_j^l \hat{\varphi}}{\omega^{3/2}}, l \right) - a^*\left(\frac{e_j^l \hat{\varphi}}{\omega^{3/2}}, l \right) \right) \right). \tag{3.29}$$

Hence the lemma is complete. **qed**

Let

$$\Omega_{\text{TL},P} := U_P \Omega_{\text{TL}} \in \mathscr{F}_{\text{TL}}, \tag{3.30}$$

where $\Omega_{\text{TL}} = \Omega_1 \otimes \Omega_2 \otimes \Omega_3 \in \mathscr{F}_{\text{TL}}$.

Lemma 3.5 *(1) It follows that U_P maps $D(H_{\text{f}}^{\text{TL}})$ onto $D(H_{\text{TL},P})(= D(H_{\text{f}}^{\text{TL}}))$ and*

$$U_P^{-1} H_{\text{TL},P} U_P = H_{\text{f}}^{\text{TL}} + E_{\text{TL}}(P), \tag{3.31}$$

where

$$E_{\text{TL}}(P) = \frac{1}{2m_{\text{eff}}} |P|^2 + \frac{3}{2\pi} \int_{-\infty}^{\infty} \frac{e^2 s^2 \|\hat{\varphi}/(s^2+\omega^2)\|^2}{m + e^2 \|\hat{\varphi}/\sqrt{s^2+\omega^2}\|^2} ds. \tag{3.32}$$

(2) $\Omega_{\text{TL},P}$ is the unique ground state of $H_{\text{TL},P}$. (3) $\Omega_{\text{TL},P}$ is the unique vector such that $b_P(f,j)\Psi = 0$, $j = 1,2,3$, for all $f \in L^2(\mathbb{R}^3)$.

Proof: (3.32) is a minor modification of [HS01]. Suppose that $b_P(f,j)\Psi = 0$ for all $f \in L^2(\mathbb{R}^3)$ and $j = 1,2,3$. Then we have $U_P a(f,j) U_P^{-1} \Psi = 0$ and $U_P^{-1}\Psi = \alpha \Omega_{\text{TL}}$, $\alpha \in \mathbb{C}$. Hence (3) follows. By the commutation relation $[H_{\text{TL},P}, b_P(f,j)] = -b_P(\omega f, j)$

we can see that $b_P(f,j)e^{itH_{\mathrm{TL},P}}\Omega_{\mathrm{TL},P} = e^{itH_{\mathrm{TL},P}}b_P(e^{it\omega}f,j)\Omega_{\mathrm{TL},P} = 0$ for all $f \in L^2(\mathbb{R}^3)$. Then there exists a real number c such that $e^{itH_{\mathrm{TL},P}}U_P\Omega_{\mathrm{TL}} = e^{itc}\Omega_{\mathrm{TL},P}$ and

$$U_P^{-1}e^{itH_{\mathrm{TL},P}}U_P\prod_{i=1}^n a^*(f_i,j_i)\Omega_{\mathrm{TL}} = e^{itc}\prod_{i=1}^n a^*(e^{it\omega}f_i,j_i)\Omega_{\mathrm{TL}}.$$

Since the linear hull of $\prod_{i=1}^n a^*(f_i,j_i)\Omega_{\mathrm{TL}}$ is dense in $\mathscr{F}_{\mathrm{TL}}$,

$$U_P^{-1}e^{itH_{\mathrm{TL},P}}U_P = e^{it(H_{\mathrm{f}}^{\mathrm{TL}}+c)}$$

and $c = E_{\mathrm{TL}}(P)$ follows. Then (1) is valid. (2) follows from (1). **qed**

3.3 Total Hamiltonian

In the previous sections we diagonalized $H_{\mathrm{TL},P}$ and H_0. Thus we can also diagonalize the total Hamiltonian. Define

$$H_P := H_{\mathrm{TL},P}\otimes 1 + 1\otimes H_0 \tag{3.33}$$

with domain

$$D(H_P) = D(H_{\mathrm{f}}) \tag{3.34}$$

for $P \in \mathbb{R}^3$ on $\mathscr{F} = \mathscr{F}_{\mathrm{TL}}\otimes\mathscr{F}_0$.

Proposition 3.6 *H_P is η-self-adjoint. In particular H_P is closed and an arbitrary core of H_{f} is also a core of H_P.*

Proof: The proof is similar to that of Proposition 2.4. **qed**

We have already shown that H_P can be diagonalized by making use of the η-unitary $U_P\otimes V_0$. We summarize with a proposition. Let

$$\Psi_P := \Omega_{\mathrm{TL},P}\otimes V_0\Omega_0. \tag{3.35}$$

Proposition 3.7 *It follows that*

$$\overline{(U_P\otimes V_0)^{-1}H_P(U_P\otimes V_0)\lceil_{D(H_{\mathrm{f}}^{\mathrm{TL}})\otimes\mathscr{F}_{0,\mathrm{fin}}}} = (H_{\mathrm{f}}^{\mathrm{TL}}+E_{\mathrm{TL}}(P))\otimes 1 + 1\otimes(H_{\mathrm{f}}^0+E_0). \tag{3.36}$$

Moreover

$$H_P\Psi_P = (E_0+E_{\mathrm{TL}}(P))\Psi_P. \tag{3.37}$$

Proof: On $D(H_{\rm f}^{\rm TL})\otimes\mathscr{F}_{0,\rm fin}$ it follows that

$$(U_P\otimes V_0)^{-1}H_P(U_P\otimes V_0)=(H_{\rm f}^{\rm TL}+E_{\rm TL}(P))\otimes 1+1\otimes(H_{\rm f}^0+E_0). \tag{3.38}$$

Since $D(H_{\rm f}^{\rm TL})\otimes\mathscr{F}_{0,\rm fin}$ is a core of the right hand side of (3.38), the proposition follows.
qed

Remark 3.8 *The operator $U_P\otimes V_0$ is η-unitary.*

Next we will indicate the diagonalization of Hamiltonian H. Note that

$$H=\left(\int_{\mathbb{R}^3}^{\oplus}H_{{\rm TL},P}dP\right)\otimes 1+1\otimes H_0.$$

Define the η-unitary operator by

$$\mathscr{U}:=\left(\int_{\mathbb{R}^3}^{\oplus}U_Pdp\right)\otimes V_0=U(-i\vec{\nabla})\otimes V_0:\mathscr{H}\to\mathscr{H}. \tag{3.39}$$

Thus we have the proposition.

Proposition 3.9 *$\mathscr{U}$ is η-unitary on $\mathscr{H}$ and*

$$\overline{\mathscr{U}^{-1}H\mathscr{U}\lceil_{D(H_{\rm TL})\otimes\mathscr{F}_{0,\rm fin}}}=-\frac{1}{2m_{\rm eff}}\Delta\otimes 1+1\otimes H_{\rm f}+\frac{3}{2\pi}\int_{-\infty}^{\infty}\frac{e^2s^2\|\hat\varphi/(s^2+\omega^2)\|^2}{m+e^2\|\hat\varphi/\sqrt{s^2+\omega^2}\|^2}ds+E_0. \tag{3.40}$$

Proof: It can be seen that

$$U(-i\vec{\nabla})^{-1}H_{\rm TL}U(-i\vec{\nabla})=H_{\rm f}^{\rm TL}+E_{\rm TL}(-i\nabla). \tag{3.41}$$

Then by (3.7)

$$\mathscr{U}^{-1}H\mathscr{U}=E_{\rm TL}(-i\nabla)\otimes 1+1\otimes H_{\rm f}+E_0 \tag{3.42}$$

follows on $D(H_{\rm TL})\otimes\mathscr{F}_{0,\rm fin}$. Since $D(H_{\rm TL})\otimes\mathscr{F}_{0,\rm fin}$ is the core of the right hand side of (3.42), the proposition follows. **qed**

3.4 Heisenberg operators

In this section we construct a Heisenberg operator $X(t)$ as a solution to the Heisenberg equation

$$\frac{d}{dt}X(t) = i[H, X(t)], \qquad X(0) = X, \tag{3.43}$$

where we notice that H is not self-adjoint but η-self-adjoint. In particular the solution to (3.43) *cannot* always be expressed as $e^{itH}X(0)e^{-itH}$. So care is required in defining the Heisenberg operator associated with the non-self-adjoint operator H.

Set

$$\mathscr{H}_{\mathscr{S}} = \mathscr{S}(\mathbb{R}^3)\hat{\otimes}\mathscr{F}_{\mathscr{S}}, \tag{3.44}$$

where $\hat{\otimes}$ denotes the algebraic tensor product and

$$\mathscr{F}_{\mathscr{S}} = \text{L.H.}\left\{ \prod_{i=1}^{n} a^*(f_i, \mu_i)\Omega, \Omega \,\middle|\, f_i \in \mathscr{S}(\mathbb{R}^3), \mu_i = 0,1,2,3, i = 1, \cdots, n, n \geq 1 \right\}.$$

The dense subspace $\mathscr{H}_{\mathscr{S}}$ is useful to study algebraic computations of operators, since $\mathscr{H}_{\mathscr{S}} \subset D(H^n)$ for all $n \geq 1$.

Definition 3.10 (Heisenberg operators) *$X(t)$, $t \in \mathbb{R}$, is called the Heisenberg operator associated with H with the initial condition $X(0) = X$ if and only if*

(1) For each $t \in \mathbb{R}$, $X(t)$ is closed and $\mathscr{H}_{\mathscr{S}}$ is its core.

(2) For each $\Psi, \Phi \in \mathscr{H}_{\mathscr{S}}$, $H\Phi \in D(X(t))$ and $(\Psi|X(t)\Phi)$ is differentiable with

$$\frac{d}{dt}(\Psi|X(t)\Phi) = i\left((H\Psi|X(t)\Phi) - (\Psi|X(t)H\Phi)\right).$$

(3) For each $\Psi, \Phi \in \mathscr{H}_{\mathscr{S}}$, the function $(\Psi|X(\cdot)\Phi)$ on $\mathbb{R}$ can be analytically continued to some domain $\mathscr{O} \subset \mathbb{C}$, which is also denoted by $(\Psi|X(z)\Phi)$ for $z \in \mathscr{O}$. Furthermore, for all $n \geq 1$, $H^n\Phi \in D(X)$ and

$$\left.\frac{d^n}{dz^n}(\Psi|X(z)\Phi)\right|_{z=0} = i^n(\Psi|\text{ad}^n(H)X\Phi),$$

where $(\Psi|\text{ad}^n(H)X\Phi)$ is defined by

$$(\Psi|\text{ad}^n(H)X\Phi) = \sum_{j=0}^{n} \frac{n!}{j!(n-j)!}(-1)^{n-j}(H^n\Psi|XH^{n-j}\Phi), \quad \Psi, \Phi \in \mathscr{H}_{\mathscr{S}}.$$

(2) of Definition 3.10 is a realization of the Heisenberg equation (3.43) in the weak sense. (3) ensures the uniqueness of the Heisenberg operator. See [Suz08] for the detail.

Now let us consider the Heisenberg operators with the initial conditions $X = p, q, A_\mu(f)$ and $\dot{\mathscr{A}}_\mu(f)$, where $p = -i\nabla$ and $q = x$. Define the operator $b^\sharp(f,j)$ on $\mathscr{H} = L^2(\mathbb{R}^3)\otimes\mathscr{F}_\mathrm{b}$ by $b^\sharp_P(f,j)$ with $P\in\mathbb{R}^3$ replaced by p, i.e.,

$$b(f,l) := \frac{1}{\sqrt{2}}\sum_{j=1}^3\left(\hat{\mathscr{A}_j}\left(T^*e^l_j\sqrt{\omega}f\right) + i\hat{\dot{\mathscr{A}_j}}\left(T^*e^l_j\frac{1}{\sqrt{\omega}}f\right) - p_j\left(\frac{ee^l_jQ}{\omega^{3/2}}, f\right)\right), \tag{3.45}$$

$$b^*(f,l) := \frac{1}{\sqrt{2}}\sum_{j=1}^3\left(\hat{\mathscr{A}_j}\left(\bar{T}^*\tilde{e}^l_j\sqrt{\omega}\tilde{f}\right) - i\hat{\dot{\mathscr{A}_j}}\left(\bar{T}^*\tilde{e}^l_j\frac{1}{\sqrt{\omega}}\tilde{f}\right) - p_j\left(\frac{ee^l_j\bar{Q}}{\omega^{3/2}}, f\right)\right). \tag{3.46}$$

Define the operators $\mathscr{A}_j(f,t)$, $\dot{\mathscr{A}_j}(f,t)$, $\mathscr{A}_0(f,t)$, $\dot{\mathscr{A}_0}(f,t)$, $p_j(t)$ and $q_j(t)$, $j=1,2,3$, by

$$\mathscr{A}_j(f,t) = \frac{1}{\sqrt{2}}\sum_{l=1}^3\left(b^*\left(e^{i\omega t}\frac{1}{\sqrt{\omega}}e^l_j\overline{T}\hat{f}, l\right) + b\left(e^{-i\omega t}\frac{1}{\sqrt{\omega}}e^l_jT\tilde{\hat{f}}, l\right)\right) - \frac{e}{m_\mathrm{eff}}\left(\frac{\hat{\varphi}}{\omega^{3/2}}, \frac{\hat{f}}{\sqrt{\omega}}\right)p_j, \tag{3.47}$$

$$\dot{\mathscr{A}_j}(f,t) = \frac{i}{\sqrt{2}}\sum_{l=1}^3\left(b^*\left(e^{it\omega}\frac{1}{\sqrt{\omega}}e^l_j\overline{T}\omega\hat{f}, l\right) - b\left(e^{-it\omega}\frac{1}{\sqrt{\omega}}e^l_jT\omega\tilde{\hat{f}}, l\right)\right), \tag{3.48}$$

$$\mathscr{A}_0(f,t) = \frac{1}{\sqrt{2}}\left(a^*\left(e^{it\omega}\frac{1}{\sqrt{\omega}}\hat{f}, 0\right) + a\left(e^{-it\omega}\frac{1}{\sqrt{\omega}}\tilde{\hat{f}}, 0\right)\right) - \frac{e}{2}\left(\frac{\hat{\varphi}}{\omega^{3/2}}, (e^{it\omega}-1)\frac{\hat{f}}{\sqrt{\omega}} + (e^{-it\omega}-1)\frac{\tilde{\hat{f}}}{\sqrt{\omega}}\right), \tag{3.49}$$

$$\dot{\mathscr{A}_0}(f,t) = \frac{i}{\sqrt{2}}\left(a^*\left(e^{it\omega}\sqrt{\omega}\hat{f}, 0\right) - a\left(e^{-it\omega}\sqrt{\omega}\tilde{\hat{f}}, 0\right)\right) - \frac{ie}{2}\left(\frac{\hat{\varphi}}{\sqrt{\omega}}, e^{it\omega}\hat{f} - e^{-it\omega}\tilde{\hat{f}}\right), \tag{3.50}$$

$$p_j(t) = p_j, \tag{3.51}$$

$$q_j(t) = q_j + \frac{t}{m}\left(1 + \frac{e^2}{m_\mathrm{eff}}\|\hat{\varphi}/\omega\|^2\right)p_j + e\frac{i}{\sqrt{2}}\sum_{l=1}^3\left\{b^*\left((e^{i\omega t}-1)e^l_j\frac{\bar{Q}}{\omega^{3/2}}, l\right) - b\left((e^{-i\omega t}-1)e^l_j\frac{Q}{\omega^{3/2}}, l\right)\right\}. \tag{3.52}$$

Remark 3.11 *All the operators above are defined on $\mathscr{H} = L^2(\mathbb{R}^3)\otimes\mathscr{F}_\mathrm{b}$, but we omit the tensor notation $\otimes$ for notational convenience. For example we used p_j for $p_j\otimes 1$*

and $a^\sharp(f)$ for $1 \otimes a^\sharp(f)$, etc.

Since the operators $\mathscr{A}_j(f,t)\lceil_{\mathscr{H}_\mathscr{S}}$, $\dot{\mathscr{A}_j}(f,t)\lceil_{\mathscr{H}_\mathscr{S}}$, $\mathscr{A}_0(f,t)\lceil_{\mathscr{H}_\mathscr{S}}$, $\dot{\mathscr{A}_0}(f,t)\lceil_{\mathscr{H}_\mathscr{S}}$, $p_j(t)\lceil_{\mathscr{H}_\mathscr{S}}$ and $q_j(t)\lceil_{\mathscr{H}_\mathscr{S}}$ are closable, we denote their closed extensions simply by $\mathscr{A}_j(f,t)$, $\dot{\mathscr{A}_j}(f,t)$, $\mathscr{A}_0(f,t)$, $\dot{\mathscr{A}_0}(f,t)$, $p_j(t)$ and $q_j(t)$, respectively.

Theorem 3.12 *Let $f \in C_0^\infty(\mathbb{R}^3)$. Then $\mathscr{A}_\mu(f,t)$ (resp. $\dot{\mathscr{A}_\mu}(f,t)$, $p(t)$, $q(t)$) is the Heisenberg operator associated with H with the initial condition $\mathscr{A}_\mu(f,0) = \mathscr{A}_\mu(f)$ (resp. $\dot{\mathscr{A}_\mu}(f,0) = \dot{\mathscr{A}_\mu}(f)$, $p(0) = p$, $q(0) = q$).*

The heuristic idea of the proof of Theorem 3.12 is as follows. We note that $\mathscr{A}_0$ commutes with $H_{\rm TL}$ and $\mathscr{A}_j$, p, q commute with H_0. So the informal solutions to the Heisenberg equation (3.43) for the initial condition $X = q, p, \mathscr{A}_j(f)$ and $\dot{\mathscr{A}_j}(f)$ are given by

$$\widetilde{q}_j(t) := e^{itH_{\rm TL}} q_j e^{-itH_{\rm TL}}, \quad \widetilde{p}_j(t) := e^{itH_{\rm TL}} p_j e^{-itH_{\rm TL}} \tag{3.53}$$

and

$$\widetilde{\mathscr{A}_j}(f,t) := e^{itH_{\rm TL}} \mathscr{A}_j(f) e^{-itH_{\rm TL}}, \quad \widetilde{\dot{\mathscr{A}}}_j(f,t) := e^{itH_{\rm TL}} \dot{\mathscr{A}_j}(f) e^{-itH_{\rm TL}} \tag{3.54}$$

for $j = 1, 2, 3$, respectively.

Moreover since $\mathscr{A}_0(f)$ and $H_{\rm TL}$ commute, in order to construct the Heisenberg operators with initial conditions $\mathscr{A}_0(f)$ and $\dot{\mathscr{A}_0}(f)$, it is enough to find the Heisenberg operators $\widetilde{\mathscr{A}_0}(f,t)$ and $\widetilde{\dot{\mathscr{A}}}_0(f,t)$ associated with H_0 instead of H:

$$\frac{d}{dt}\widetilde{\mathscr{A}_0}(f,t) = i[H_0, \widetilde{\mathscr{A}_0}(f,t)], \quad \frac{d}{dt}\widetilde{\dot{\mathscr{A}}}_0(f,t) = i[H_0, \widetilde{\dot{\mathscr{A}}}_0(f,t)]. \tag{3.55}$$

We will show that $\widetilde{\mathscr{A}_\mu}(f,t) = \mathscr{A}_\mu(f,t)$, $\widetilde{\dot{\mathscr{A}}}_\mu(f,t) = \dot{\mathscr{A}_\mu}(f,t)$, $\widetilde{p}_j(t) = p_j(t)$ and $\widetilde{q}_j(t) = q_j(t)$ on $\mathscr{H}_\mathscr{S}$ and prove that they are the Heisenberg operators.

Proof of Theorem 3.12

By the assumption $f \in C_0^\infty(\mathbb{R}^3)$ and (2) of Assumption 3.1, $\|e^{+\epsilon\omega}\hat{\varphi}\|_\infty < \infty$, it is immediate that $(H\Psi|\mathscr{A}_\mu(f,t)\Phi)$ (resp. $(H\Psi|\dot{\mathscr{A}_\mu}(f,t)\Phi)$, $(H\Psi|p_j(t)\Phi)$ and $(H\Psi|q_j(t)\Phi)$) can be analytically continued to some domain with respect to t. So it is enough to check (2) of Definition 3.10.

We see directly that (3.49) and (3.50) satisfy the Heisenberg equation (3.43).

Next we examine (3.47) and (3.48). The vector potentials $\mathscr{A}_j(f)$ and $\dot{\mathscr{A}}_j(f)$ can be expressed by means of b_P^* and b_P. In fact direct computation shows that

$$\mathscr{A}_j(f) = \frac{1}{\sqrt{2}}\sum_{l=1}^{3}\left(b_P^*\left(\frac{1}{\sqrt{\omega}}e_j^l\overline{T}\hat{f},l\right)+b_P\left(\frac{1}{\sqrt{\omega}}e_j^lT\tilde{\hat{f}},l\right)\right)-eP_j\left(\frac{\hat{\varphi}}{m_{\rm eff}\omega^{3/2}},\frac{\hat{f}}{\sqrt{\omega}}\right), \tag{3.56}$$

$$\dot{\mathscr{A}}_j(f) = \frac{i}{\sqrt{2}}\sum_{l=1}^{3}\left(b_P^*\left(\frac{1}{\sqrt{\omega}}e_j^l\overline{T}\omega\hat{f},l\right)-b_P\left(\frac{1}{\sqrt{\omega}}e_j^lT\omega\tilde{\hat{f}},l\right)\right). \tag{3.57}$$

Note that

$$e^{itH_{\rm TL,\it P}}b_P(f,j)e^{-itH_{\rm TL,\it P}}=b_P(e^{-i\omega t}f,j),\quad e^{itH_{\rm TL,\it P}}b_P^*(f,j)e^{-itH_{\rm TL,\it P}}=b_P^*(e^{i\omega t}f,j).$$

Then $\mathscr{A}_j(f,t,P)=e^{itH_{\rm TL,\it P}}\mathscr{A}_j(f)e^{-itH_{\rm TL,\it P}}$ is given by

$$\mathscr{A}_j(f,t,P)=\frac{1}{\sqrt{2}}\sum_{l=1}^{3}\left(b^*\left(e^{i\omega t}\frac{1}{\sqrt{\omega}}e_j^l\overline{T}\hat{f},l\right)+b\left(e^{-i\omega t}\frac{1}{\sqrt{\omega}}e_j^lT\tilde{\hat{f}},l\right)\right) -eP_j\left(\frac{\hat{\varphi}}{m_{\rm eff}\omega^{3/2}},\frac{\hat{f}}{\sqrt{\omega}}\right). \tag{3.58}$$

Thus (3.47) satisfies the Heisenberg equation (3.43).

Finally we analyze (3.51) and (3.52). By the dipole approximation, p and $e^{itH_{\rm TL}}$ commute. Then $e^{itH_{\rm TL}}p_je^{-itH_{\rm TL}}=p_j$. Thus it is trivial to see that p_j is the Heisenberg operator. We see that

$$\begin{aligned} q_j(t)\Psi &= \int_0^t ie^{isH_{\rm TL}}[H_{\rm TL},q_j]e^{-isH_{\rm TL}}\Psi ds+q_j\Psi \\ &= \frac{1}{m}\int_0^t e^{isH_{\rm TL}}(p_j-e\mathscr{A}_j)e^{-isH_{\rm TL}}\Psi ds+q_j\Psi \\ &= \frac{t}{m}p_j\Psi+q_j\Psi-\frac{e}{m}\int_0^t\mathscr{A}_j(\varphi,s)\Psi ds. \end{aligned}$$

By (3.47) we can compute $\frac{e}{m}\int_0^t\mathscr{A}_j(\varphi,s)\Psi ds$ as

$$\begin{aligned} &\frac{e}{m}\int_0^t\mathscr{A}_j(\varphi,s)\Psi ds \\ &=\frac{e}{m}\frac{i}{\sqrt{2}}\sum_{l=1}^{3}\left\{b^*\left((e^{i\omega t}-1)e_j^l\frac{\bar{Q}}{\omega^{3/2}},l\right)-b\left((e^{-i\omega t}-1)e_j^l\frac{Q}{\omega^{3/2}},l\right)\right\}+\frac{t}{m}\frac{e^2}{m_{\rm eff}}\|\hat{\varphi}/\omega\|^2p_j. \end{aligned}$$

Then (3.52) satisfies the Heisenberg equation (3.43). **qed**

We utilize (3.53)-(3.55), Maxwell's equations and Newton's equation of motion for NRQED. For all $f \in \mathscr{S}(\mathbb{R}^3)$,

$$\frac{d^2}{dt^2}\vec{\mathscr{A}}(f,t) - \vec{\mathscr{A}}(\Delta f,t) = \int_{\mathbb{R}^3} \vec{J}(x,t)f(x)dx,$$
$$\frac{d^2}{dt^2}\vec{\mathscr{A}_0}(f,t) - \vec{\mathscr{A}_0}(\Delta f,t) = \int_{\mathbb{R}^3} \rho(x,t)f(x)dx,$$

and

$$\frac{d^2}{dt^2}q(t) = -e\dot{\vec{\mathscr{A}}}(\varphi,t),$$

where

$$\vec{J}(x,t) = \frac{e}{2m}\left(\varphi(x)(p(t)-e\vec{\mathscr{A}}(\varphi,t)) + (p(t)-e\vec{\mathscr{A}}(\varphi,t))\varphi(x)\right),$$
$$\rho(x,t) = e\varphi(x).$$

4 LSZ formalism and asymptotic completeness

We shall construct the asymptotic field $a^*_{P,\pm}(f,\mu)$ by the LSZ method in this section. Let

$$a_{P,t}(f,j) := i\sum_{l=1}^{3}(\dot{\mathscr{A}}_l(f_t^{l,j},t,P) - \mathscr{A}_l(\dot{f}_t^{l,j},t,P)), \quad j=1,2,3, \tag{4.1}$$
$$a_{P,t}(f,0) := i(\dot{\mathscr{A}}_0(f_t^0,t) - \mathscr{A}_0(\dot{f}_t^0,t)), \tag{4.2}$$

for $f \in L^2(\mathbb{R}^3)$, where both $\mathscr{A}_0(f,t)$ and $\dot{\mathscr{A}}_0(f,t)$ are regarded as operators in $\mathscr{F}$, $\mathscr{A}_l(f,t,P) = e^{itH_{\mathrm{TL},P}}\mathscr{A}_l(f)e^{-itH_{\mathrm{TL},P}}$, $\dot{\mathscr{A}}_l(f,t,P) = e^{itH_{\mathrm{TL},P}}\dot{\mathscr{A}}_l(f)e^{-itH_{\mathrm{TL},P}}$ and

$$f_t^0 = F^{-1}\left(\frac{e^{it\omega}}{\sqrt{2\omega}}\tilde{f}\right), \quad f_t^{l,j}(k) = F^{-1}\left(\frac{e^{+it\omega}}{\sqrt{2\omega}}\tilde{e}_l^j\tilde{f}\right), \quad j=1,2,3, \tag{4.3}$$
$$\dot{f}_t^0 = F^{-1}\left(i\omega\frac{e^{it\omega}}{\sqrt{2\omega}}\tilde{f}\right), \quad \dot{f}_t^{l,j}(k) = F^{-1}\left(i\omega\frac{e^{+it\omega}}{\sqrt{2\omega}}\tilde{e}_l^j\tilde{f}\right), \tag{4.4}$$

and F^{-1} denotes the inverse Fourier transformation of $L^2(\mathbb{R}^3)$. We also set

$$a^\dagger_{P,t}(f,\mu) = \begin{cases} \left(a_{P,t}(\bar{f},\mu)\right)^*, & \mu=j=1,2,3, \\ -\left(a_{P,t}(\bar{f},0)\right)^*, & \mu=0. \end{cases}$$

From the expression of (3.17) and (3.18) it can be seen that

$$a_{P,t}(h,j) = e^{itH_{\mathrm{TL},P}}e^{-itH_{\mathrm{f}}^{\mathrm{TL}}}a(h,j)e^{itH_{\mathrm{f}}^{\mathrm{TL}}}e^{-itH_{\mathrm{TL},P}} \tag{4.5}$$

for $j = 1, 2, 3$ and

$$a_{P,t}(f, 0) = a(f, 0) - \frac{e}{\sqrt{2}} \left(\frac{\hat{\varphi}}{\omega^{3/2}}, (1 - e^{it\omega}) f \right). \tag{4.6}$$

From (4.6), the strong limit of $a^{\sharp}_{P,t}(f, 0)$ as $t \to \pm\infty$ is easily obtained. In order to have an explicit form for $a^{\sharp}_{P,t}(h, j)$, $j = 1, 2, 3$, it is enough to obtain explicit forms for $\mathscr{A}_l(f, t)$ and $\dot{\mathscr{A}}_l(f, t)$. Fortunately this can be done using (3.47) and (3.48). In the next lemma we show that the strong limits of $a^{\sharp}_{P,t}(f, \mu)$ can be represented by $b^{\sharp}_P(f, \mu)$ defined in (3.10),(3.11), (3.21) and (3.22).

Lemma 4.1 *Let $\Psi \in \mathscr{F}_{\rm fin}$. Then the strong limits*

$$a_{P,{\rm out/in}}(h, \mu)\Psi = s - \lim_{t\to\pm\infty} a_{P,t}(h, \mu)\Psi, \tag{4.7}$$

$$a^{\dagger}_{P,{\rm out/in}}(h, \mu)\Psi = s - \lim_{t\to\pm\infty} a^{\dagger}_{P,t}(h, \mu)\Psi \tag{4.8}$$

exist where "out", "in" stand for $t \to +\infty$, $t \to -\infty$ respectively, and are given explicitly by

$$a_{P,{\rm in}}(h, j) = b_P(h, j), \tag{4.9}$$

$$a^{\dagger}_{P,{\rm in}}(h, j) = b^*_P(h, j), \tag{4.10}$$

$$a_{P,{\rm out}}(h, j) = \sum_{i=1}^{3} b_P(L^{ij} h, i), \tag{4.11}$$

$$a^{\dagger}_{P,{\rm out}}(h, j) = \sum_{i=1}^{3} b^*_P(\bar{L}^{ij} h, i), \tag{4.12}$$

$$a_{P,{\rm out}}(h, 0) = b(h, 0) = a_{P,{\rm in}}(h, 0), \tag{4.13}$$

$$a^{\dagger}_{P,{\rm out}}(h, 0) = b^{\dagger}(h, 0) = a^{\dagger}_{P,{\rm in}}(h, 0), \tag{4.14}$$

where $L^{ij} h = \delta_{ij} h - i\pi e^2 Q \hat{\varphi} \omega \sum_{l=1}^{3} e^i_l [e^j_l h]$ and $[f](k) := \int_{S_2} f(|k|S) dS$, $dS = \sin\theta d\theta d\phi$, $0 \le \theta \le 2\pi$, $0 \le \phi \le \pi$.

Proof: The proof is parallel with [Ara83b]. (4.13) and (4.14) can be proven by the Riemann-Lebesgue lemma. We shall prove (4.9)-(4.12). By Theorem 3.12 we have

$$i \sum_{l=1}^{3} (\dot{\mathscr{A}}_l(h^{l,j}_t, t, P) - \mathscr{A}_l(\dot{h}^{l,j}_t, t, P))$$

$$= \sum_{i=1}^{3} \left(b^*_P(e^{-it\omega} (\bar{W}^{ji}_-)^* e^{+it\omega} \hat{h}, i) + b_P(e^{-it\omega} (W^{ji}_+)^* e^{+it\omega} \hat{h}, i) \right) + const.$$

Since we can see that W_-^{ji} is an integral operator with kernel in $L^2(\mathbb{R}^3\times\mathbb{R}^3)$, it is a Hilbert-Schmidt operator. Then $\|(\bar{W}_-^{ji})^* e^{it\omega}h\|\to 0$ as $t\to\pm\infty$. Hence $b_P^*(e^{-it\omega}(\bar{W}_-^{ji})^* e^{it\omega}\hat{h},i)\to 0$ as $t\to\pm\infty$. Next we shall estimate $b_P(e^{-it\omega}(W_+^{ji})^* e^{it\omega}\hat{h},i)$. Let $X_{ij}(t)=e^{-it\omega}(W_+^{ji})^* e^{it\omega}h$. Then

$$\begin{aligned}\frac{d}{dt}X_{ij}(t) &= \frac{-i}{2}\sum_{l=1}^3 e^{-it\omega}e_l^i\left[\omega,\frac{1}{\sqrt{\omega}}T\sqrt{\omega}+\sqrt{\omega}T\frac{1}{\sqrt{\omega}}\right]e_l^j e^{it\omega}h\\ &= \frac{-i}{2}\sum_{l=1}^3 e^{-it\omega}e_l^i[\omega^2,T]e_l^j e^{it\omega}h\\ &= \frac{-ie^2}{2}\sum_{l=1}^3\frac{e^{-it\omega}e_l^iQ}{\sqrt{\omega}}\left(\frac{e_l^j e^{-it\omega}\hat{\varphi}}{\sqrt{\omega}},h\right) := \frac{-ie^2}{2}\varrho_{ij}(t,\cdot).\end{aligned}$$

Then

$$X_{ij}(t)=(W_+^{ji})^*h+\frac{-ie^2}{2}\int_0^t ds\varrho_{ij}(s,\cdot). \tag{4.15}$$

Since $\left|\left(\frac{e_l^j e^{-is\omega}\hat{\varphi}}{\sqrt{\omega}},h\right)\right|\le$ const.$/s^2$, the integral of the right-hand side of (4.15) as $t\to\pm\infty$ is well defined. First we investigate the case $t\to-\infty$. Then

$$\begin{aligned}&\frac{-ie^2}{2}\int_0^{-\infty}ds\varrho_{ij}(s,k)\\ &=\frac{ie^2}{2}\sum_{l=1}^3\lim_{\epsilon\downarrow 0}\int_{-\infty}^0 ds\int dk' e^{-is(\omega(k)-\omega(k')+i\epsilon)}\frac{e_l^i(k)e_l^j(k')Q(k)\hat{\varphi}(k')h(k')}{\sqrt{\omega(k)}\sqrt{\omega(k')}}\\ &=-\frac{e^2}{2}\sum_{l=1}^3\lim_{\epsilon\downarrow 0}\int dk'\frac{e_l^i(k)e_l^j(k')Q(k)\hat{\varphi}(k')h(k')}{(\omega(k)-\omega(k')+i\epsilon)\sqrt{\omega(k)}\sqrt{\omega(k')}}\\ &=-\frac{e^2}{2}\sum_{l=1}^3\lim_{\epsilon\downarrow 0}\int dk'\frac{(\omega(k)+\omega(k'))e_l^i(k)e_l^j(k')Q(k)\hat{\varphi}(k')h(k')}{(\omega(k)^2-\omega(k')^2+i\epsilon)\sqrt{\omega(k)}\sqrt{\omega(k')}}\\ &=-(W_+^{ji})^*h(k)+\delta_{ij}h(k).\end{aligned}$$

Hence $\lim_{t\to-\infty}X_{ij}(t)h=\delta_{ij}h$ and (4.9), i.e., $a_{\rm in}(h,j)=b_P(h,j)$ follows. Next we show that

$$\lim_{t\to+\infty}X_{ij}(t)h=\delta_{ij}h-ie^2\pi Q\hat{\varphi}\omega e_\mu^i[he_j^l]. \tag{4.16}$$

We have

$$\lim_{t\to+\infty}X_{ij}(t)h=(W_+^{ji})^*h+\frac{-ie^2}{2}\int_0^\infty ds\varrho_{ij}(s,\cdot)=\frac{-ie^2}{2}\int_{-\infty}^\infty ds\varrho_{ij}(s,\cdot)+\delta_{ij}h.$$

Since, by the Fourier transformation, we have

$$\frac{-ie^2}{2}\sum_{l=1}^{3}\int_{-\infty}^{\infty}\frac{e^{-is\omega}e_l^iQ}{\sqrt{\omega}}\left(\frac{e_l^je^{-is\omega}\hat{\varphi}}{\sqrt{\omega}},h\right)ds=-ie^2\pi Q\hat{\varphi}\omega\sum_{l=1}^{3}e_l^i[he_l^j],$$

(4.16) and then (4.11) follows. (4.12) is similarly proven. Then the proof is complete. **qed**

In what follows "ex" stands for "out" or "in". Next we consider the asymptotic field $\mathscr{F}_P^{\rm ex}$ and construct the scattering operator S connecting $\mathscr{F}_P^{\rm in}$ and $\mathscr{F}_P^{\rm out}$. We denote by $\mathscr{F}_{P,{\rm fin}}^{\rm ex}=\mathscr{F}_{P,{\rm fin}}^{\rm ex}$ the linear hull of the set

$$\left\{\prod_{i=1}^{n}a_{P,{\rm ex}}^{\dagger}(h_i,\mu_i)\Psi_P,\Psi_P\,\middle|\,h_i\in\mathscr{S}(\mathbb{R}^3),\mu_i=0,1,2,3,\ i=1,\cdots n,\ n\geq 1\right\}$$

and by $\mathscr{F}_P^{\rm ex}$ the closure of $\mathscr{F}_{P,{\rm fin}}^{\rm ex}$ in $\mathscr{F}$. In the next lemma, commutation relations are established.

Lemma 4.2 *The following commutation relations hold for* $\mathscr{F}_{P,{\rm fin}}^{\rm ex}$*:*

$$[a_{P,{\rm ex}}(h,\mu),a_{P,{\rm ex}}^{\dagger}(g,\nu)]=-g_{\mu\nu}(\bar{h},g), \tag{4.17}$$

$$[a_{P,{\rm ex}}(h,\mu),a_{P,{\rm ex}}(g,\nu)]=0=[a_{P,{\rm ex}}^{\dagger}(h,\mu),a_{P,{\rm ex}}^{\dagger}(g,\nu)], \tag{4.18}$$

$$[H_P,a_{P,{\rm ex}}(h,\mu)]=-a_{P,{\rm ex}}(\omega h,\mu), \tag{4.19}$$

$$[H_P,a_{P,{\rm ex}}^{\dagger}(h,\mu)]=a_{P,{\rm ex}}^{\dagger}(\omega h,\mu) \tag{4.20}$$

and $a_{P,{\rm ex}}(h,\mu)\Psi_P=0$ *for all* $h\in L^2(\mathbb{R}^3)$.

Proof: (4.19) and (4.20) follow directly from the commutation relations between H_P and $b^\sharp$. The commutation relations in (4.17) for $\mu=0$ or $\nu=0$ are obtained by direct computation. Other commutation relations can be proven by $a_{P,{\rm ex}}(h,j):=\lim_{t\to\pm\infty}a_{P,t}(h,j)=e^{itH_{{\rm TL},P}}e^{-itH_{\rm f}^{\rm TL}}a(h,j)e^{itH_{\rm f}^{\rm TL}}e^{-itH_{{\rm TL},P}}$ and a limiting argument. **qed**

We constructed the quadruple

$$(\mathscr{F}_P^{\rm ex},H_P,\{a_{P,{\rm ex}}(h,\mu),a_{P,{\rm ex}}^{\dagger}(h,\mu)|h\in L^2(\mathbb{R}^3)\},\Psi_P) \tag{4.21}$$

relevant to (3.16), including the scalar potential.

Theorem 4.3 (Asymptotic completeness) *It follows that* $\mathscr{F}_P^{\rm in}=\mathscr{F}_P^{\rm out}=\mathscr{F}$.

Proof: Let

$$\mathscr{F}^{\rm ex}_{P,{\rm fin},{\rm TL}} = \left\{ \prod_{i=1}^n a^\dagger_{P,{\rm ex}}(h_i, j_i)\Omega_{{\rm TL},P}, \Omega_{{\rm TL},P} \,\middle|\, h_i \in \mathscr{S}(\mathbb{R}^3), j_i = 1,2,3,\ i = 1,\cdots n,\ n \geq 1 \right\}$$

and

$$\mathscr{F}^{\rm ex}_{{\rm fin},0} = \left\{ \prod_{i=1}^n a^\dagger_{P,{\rm ex}}(h_i, 0)V_0\Omega_0, V_0\Omega_0 \,\middle|\, h_i \in \mathscr{S}(\mathbb{R}^3),\ i = 1,\cdots n,\ n \geq 1 \right\}.$$

Since $\mathscr{F}^{\rm ex}_{P,{\rm fin}} = \mathscr{F}^{\rm ex}_{P,{\rm fin},{\rm TL}} \hat{\otimes} \mathscr{F}^{\rm ex}_{{\rm fin},0}$, we need only prove that $\mathscr{F}^{\rm ex}_{P,{\rm fin},{\rm TL}}$ (resp. $\mathscr{F}^{\rm ex}_{{\rm fin},0}$) is dense in $\mathscr{F}_{\rm TL}$ (resp. $\mathscr{F}_0$). We assume that there exists a vector $\Phi \in \mathscr{F}_{\rm TL}$ such that

$$\left(\prod_{i=1}^n a^\dagger_{P,{\rm in}}(h_i, j_i)\Omega_{{\rm TL},P}, \Phi \right) = 0$$

for all h_i and $j_i = 1,2,3$. By Lemma 4.1 and the relations $U_P^{-1} b^\sharp(f,j) U_P = a^\sharp(f,j)$, we have

$$\left(\prod_{i=1}^n a^\dagger(h_i, j_i)\Omega_{\rm TL}, U_P^{-1}\Phi \right) = 0$$

for all h_i and $j_i = 1,2,3$. Thus $\Phi = 0$, which yields that $\mathscr{F}^{\rm in}_{P,{\rm fin},{\rm TL}}$ is dense in $\mathscr{F}_{\rm TL}$. Similarly, suppose that $(\prod_{i=1}^n a^\dagger_{P,{\rm out}}(h_i, j_i)\Omega_{{\rm TL},P}, \Phi) = 0$ for all h_i and $j_i = 1,2,3$. Then we have

$$\sum_{i_1,\ldots,i_n=1}^3 \left(\prod_{i=1}^n a^\dagger(\bar{L}^{l_i j_i} h_i, l_i)\Omega_{\rm TL}, U_P^{-1}\Phi \right) = 0. \tag{4.22}$$

Let $L = (L^{ij})_{1\leq i,j\leq 3} \oplus^3 L^2(\mathbb{R}^3) \to \oplus^3 L^2(\mathbb{R}^3)$. We note that, as a consequence, $L = \lim_{t\to+\infty} e^{-it\omega} W_+^* e^{it\omega}$. From the symplectic structure $\mathbb{W}^* J \mathbb{W} = \mathbb{W} J \mathbb{W}^* = J$, it follows that $W_+^* W_+ - W_-^* W_- = 1$. In particular it follows that $e^{-it\omega} W_+^* W_+ e^{it\omega} = e^{-it\omega} W_-^* W_- e^{it\omega} + 1$. Thus

$$LL^* = \lim_{t\to+\infty} e^{-it\omega} W_+^* W_+ e^{it\omega} = 1,$$

since $e^{-it\omega} W_-^* W_- e^{it\omega}$ vanishes as $t \to \pm\infty$. Then L has an inverse as an operator from $\oplus^3 L^2(\mathbb{R}^3)$ to itself and the linear hull of vectors of the form $\prod_{i=1}^n a^\dagger(Lf_i)\Omega_{\rm TL}$ is dense in $\mathscr{F}_{\rm TL}$. Hence (4.22) implies that $\Phi = 0$ and $\mathscr{F}^{\rm out}_{P,{\rm fin},{\rm TL}}$ is dense in $\mathscr{F}_{\rm TL}$.

We prove that $\mathscr{F}^{\rm ex}_{{\rm fin},0}$ is dense in $\mathscr{F}_0$. Denoting by $\mathscr{F}_{{\rm fin},0}$ the linear hull of the set

$$\left\{ \prod_{i=1}^n b^\dagger(h_i, 0)V_0\Omega_0, V_0\Omega_0 \,\middle|\, h_i \in \mathscr{S}(\mathbb{R}^3),\ i = 1,\cdots n,\ n \geq 1 \right\},$$

by Lemma 4.1, we have $\mathscr{F}_{\text{fin},0} = \mathscr{F}^{\text{ex}}_{\text{fin},0}$, and hence we need only prove that $\mathscr{F}_{\text{fin},0}$ is dense in $\mathscr{F}_0$. Setting

$$\mathcal{D}_0 = \left\{ \prod_{i=1}^{n} a^\dagger(h_i, 0)\Omega_0, \Omega_0 \middle| h_i \in \mathscr{S}(\mathbb{R}^3),\ i = 1, \cdots n,\ n \geq 1 \right\},$$

we have the result that the linear hull of $\mathcal{D}_0$ is dense in $\mathscr{F}_0$. Let

$$U_0 = \exp\left(\frac{e}{\sqrt{2}}\left(a^*\left(\frac{\hat{\varphi}}{\omega^{3/2}}, 0\right) - a\left(\frac{\hat{\varphi}}{\omega^{3/2}}, 0\right)\right)\right).$$

Then we observe that U_0 is unitary and that

$$V_0\Omega_0 = e^{e^2/2\|\hat{\varphi}/\omega^{3/2}\|^2} U_0\Omega_0. \tag{4.23}$$

We shall prove $\mathcal{D}_0 \subset U_0^{-1}\mathscr{F}_{\text{fin},0}$ by induction. It is clear from (4.23) that $\Omega_0 \in U_0^{-1}\mathscr{F}_{\text{fin},0}$. Assume that $\prod_{i=1}^{n} a^\dagger(h_i, 0)\Omega_0 \in U_0^{-1}\mathscr{F}_{\text{fin},0}$. Then we have

$$\begin{aligned}
&\prod_{i=1}^{n+1} a^\dagger(h_i, 0)\Omega_0 \\
&= \left(b^\dagger(h_{n+1}, 0) - e(\hat{\varphi}/\omega^{3/2}, h_{n+1})\right) \prod_{i=1}^{n} a^\dagger(h_i, 0)\Omega_0 + e(\hat{\varphi}/\omega^{3/2}, h_{n+1}) \prod_{i=1}^{n} a^\dagger(h_i, 0)\Omega_0 \\
&= U_0^{-1} b^\dagger(h_{n+1}, 0) U_0 \prod_{i=1}^{n} a^\dagger(h_i, 0)\Omega_0 + e(\hat{\varphi}/\omega^{3/2}, h_{n+1}) \prod_{i=1}^{n} a^\dagger(h_i, 0)\Omega_0.
\end{aligned}$$

It follows that $\prod_{i=1}^{n+1} a^\dagger(h_i, 0)\Omega_0 \in U_0^{-1}\mathscr{F}_{\text{fin},0}$ and we have the desired result. **qed**

Let $S_P : \mathscr{F}_P^{\text{out}} \to \mathscr{F}_P^{\text{in}}$ be defined by

$$S_P \prod_{i=1}^{n} a^\dagger_{P,\text{out}}(f_i, \mu_i)\Psi_P := \prod_{i=1}^{n} a^\dagger_{P,\text{in}}(f_i, \mu_i)\Psi_P. \tag{4.24}$$

Then $\|S_P\Phi\| = \|\Phi\|$ for $\Phi \in \mathscr{F}^{\text{out}}_{\text{fin}}$ follows from (4.13) and (4.14) in Lemma 4.1 and the commutation relations (4.17) and (4.18) in Lemma 4.2. Thus S_P can be extended to a unitary operator from $\mathscr{F}_P^{\text{out}}$ to $\mathscr{F}_P^{\text{in}}$. S_P is called the scattering operator.

Theorem 4.4 *S_P is unitary and η-unitary, i.e., $S_P^* = S_P^{-1} = S_P^\dagger$.*

Proof: The unitarity of S_P is already proven. $[S_P, \eta] = 0$ implies that S_P is η-unitary.

5 Physical subspace

5.1 Abstract setting

We begin with an abstract version of physical subspace. Let $\mathcal{K}$ be a Klein space with a metric $(\cdot|\cdot)$. For a densely defined linear operator X on $\mathcal{K}$, we denote by $X^\dagger$ the adjoint of X with respect to $(\cdot|\cdot)$. We denote the set of densely defined operators on $\mathcal{K}$ by $\mathscr{C}(\mathcal{K})$.

Definition 5.1 *The map $F : \mathscr{S}(\mathbb{R}^3) \to \mathscr{C}(\mathcal{K})$ is called an operator valued distribution if and only if there exists a dense subspace $\mathcal{D}$ such that*

(1) $F(\alpha f + \beta g)\Psi = (\alpha F(f) + \beta F(g))\Psi$ for $\alpha, \beta \in \mathbb{C}$, $f, g \in \mathscr{S}(\mathbb{R}^3)$ and $\Psi \in \mathcal{D}$;

(2) the map $\mathscr{S}(\mathbb{R}^3) \ni f \mapsto (\Psi|F(f)\Phi)$ is a tempered distribution for $\Psi, \Phi \in \mathcal{D}$.

Definition 5.2 *Let $B = \{B(\cdot, t)\}_{t\in\mathbb{R}}$ be a family of operator valued distributions. This family is in class $\mathscr{D}(\mathcal{K})$ if and only if*

(1) there exists a dense subspace $\mathcal{D}_B$ in $\mathcal{K}$ such that, for all $t \in \mathbb{R}$ and $f \in \mathscr{S}(\mathbb{R}^3)$, $\mathcal{D}_B \subset D(B(f, t)) \cap D(B(f, t)^\dagger)$ and $B(f, t)^\dagger|_{\mathcal{D}_B} = B(\bar{f}, t)|_{\mathcal{D}_B}$;

(2) for each $\Psi \in \mathcal{D}_B$, $B(f, t)\Psi$ is strongly differentiable in t and its derivative, denoted by $\dot{B}(f, t)\Psi$, is continuous in t.

By Definition 5.2, $\{B(\cdot, t)\}_{t\in\mathbb{R}} \in \mathscr{D}(\mathcal{K})$ implies that $\dot{B}(\cdot, t)$ is also an operator-valued distribution which satisfies (1) of Definition 5.2 with B replaced by $\dot{B}$. We now provide an abstract definition of a free field .

Definition 5.3 *A family of operator valued distributions $\{B(\cdot, t)\}_{t\in\mathbb{R}} \in \mathscr{D}(\mathcal{K})$ is called a free field if and only if $B(f, t)\Psi$ is strongly two-times differentiable in t and*

$$\frac{d^2}{dt^2} B(f, t)\Psi - B(\Delta f, t)\Psi = 0 \tag{5.1}$$

holds for all $f \in \mathscr{S}(\mathbb{R}^3)$ and $\Psi \in \mathcal{D}_B$. The set of free fields is denoted by $\mathscr{D}_{\text{free}}(\mathcal{K})$.

Further to introducing the Gupta-Bleuler subsidiary condition, the positive frequency part of it has to be defined. Let $\{B(\cdot, t)\}_{t\in\mathbb{R}} \in \mathscr{D}(\mathcal{K})$. Then one can automatically construct a free field from $B(\cdot, t)$, as described below. Define

$$c_s(g) := i \left(\dot{B}(g_s, s) - B(\dot{g}_s, s) \right), \tag{5.2}$$

where g_s and $\dot{g}_s$ are defined by

$$g_s = F^{-1}\left(\frac{\tilde{g}}{2\omega}e^{is\omega}\right), \quad \dot{g}_s = \partial_s g_s = F^{-1}\left(i\frac{\tilde{g}}{2}e^{is\omega}\right). \tag{5.3}$$

Note that in (5.2)

$$\dot{B}(g_s, s) = \dot{B}(f, s)\lceil_{f=g_s}.$$

Set $c_s^\dagger(h) := \left(c_s(\bar{h})\right)^\dagger$. Let us define the operator $F(f, s, t) : \mathcal{K} \to \mathcal{K}$ for $f \in \mathscr{S}(\mathbb{R}^3)$ and $s, t \in \mathbb{R}$, by

$$F(f, s, t) := c_s\left(e^{-it\omega}\tilde{\hat{f}}\right) + c_s^\dagger\left(e^{it\omega}\hat{f}\right). \tag{5.4}$$

It can be proven that for each $s \in \mathbb{R}$, $\{F(\cdot, s, t)\}_{t\in\mathbb{R}} \in \mathscr{D}_{\rm free}(\mathcal{K})$. Then we can define the family of maps Θ_s, $s \in \mathbb{R}$,

$$\Theta_s : \mathscr{D}(\mathcal{K}) \to \mathscr{D}_{\rm free}(\mathcal{K}), \quad \{B(\cdot, t)\}_{t\in\mathbb{R}} \mapsto \{F(\cdot, s, t)\}_{t\in\mathbb{R}}.$$

In particular Θ_s leaves $\mathscr{D}_{\rm free}(\mathcal{K})$ invariant. In the next lemma a stronger statement is established.

Lemma 5.4 *Let $B = \{B(\cdot, t)\}_{t\in\mathbb{R}} \in \mathscr{D}$. Then*

(1) $B(f, t) = F(f, t, t)$ holds for all $f \in \mathscr{S}(\mathbb{R}^3)$ and $t \in \mathbb{R}$;

(2) If, in addition, we assume that $B \in \mathscr{D}_{\rm free}(\mathcal{K})$ and that for each $\Psi \in \mathscr{D}_B$, there exists a continuous semi-norm C_Ψ on $\mathscr{S}(\mathbb{R}^3)$ such that

$$\sup_{t\in\mathbb{R}} \|B(f, t)\Psi\| + \sup_{t\in\mathbb{R}} \|\dot{B}(f, t)\Psi\| \le C_\Psi(f), \tag{5.5}$$

then $c_s(h)$ (resp. $c_s^\dagger(h)$) is independent of $s \in \mathbb{R}$ and

$$B(f, t) = c(e^{-it\omega}\tilde{\hat{f}}) + c^\dagger(e^{it\omega}\hat{f}).$$

holds. Here we set $c_s = c$ and $c_s^\dagger = c^\dagger$.

Proof: We have

$$c_s(e^{-it\omega}\tilde{\hat{f}}, t) = i\left(\dot{B}\left(\frac{e^{-i(t-s)\omega}}{2\omega}f, s\right) - iB\left(\frac{e^{-i(t-s)\omega}}{2}f, s\right)\right),$$
$$c_s^\dagger(e^{it\omega}\hat{f}, t) = -i\left(\dot{B}\left(\frac{e^{i(t-s)\omega}}{2\omega}f, s\right) + iB\left(\frac{e^{i(t-s)\omega}}{2}f, s\right)\right).$$

Together with (5.4) we have (1). Let us fix arbitrarily $\Psi, \Phi \in \mathcal{D}_B$ and define the function $\beta(s)$ by $\beta(s) = (\Phi | c_s(h)\Psi)$. Under the assumption of (2), we have

$$\frac{d}{ds}\beta(s) = i\left(\Phi \middle| \left(B(\Delta g_s, s) - B(\partial_s^2 g_s, s)\right)\Psi\right) = 0.$$

Hence, by the arbitrariness of $\Psi \in \mathcal{D}_B$, we obtain the desired results. **qed**

By virtue of the above lemma, we introduce the definition of the positive (resp. negative) frequency part of a given family in the class $\mathscr{D}(\mathcal{K})$.

Definition 5.5 (Positive frequency part and physical subspace)
(1) Let $\{B(\cdot, t)\}_{t\in\mathbb{R}} \in \mathscr{D}_{\mathrm{free}}(\mathcal{K})$ and (5.5) be satisfied. Then we call $c(e^{-it\omega}\tilde{\hat{f}})$ (resp. $c^\dagger(e^{it\omega}\hat{f})$) the positive (resp. negative) frequency part of $B(f,t)$ and denote it by

$$B^{(+)}(f,t) := c(e^{-it\omega}\tilde{\hat{f}}), \quad (resp. B^{(-)}(f,t) := c^\dagger(e^{it\omega}\hat{f})). \tag{5.6}$$

(2) Let $B = \{B(\cdot, t)\}_{t\in\mathbb{R}} \in \mathscr{D}(\mathcal{K})$ and $c_t(h)$ be defined by (5.2). For each $t \in \mathbb{R}$, we define the physical subspace $\mathscr{V}^t$ by

$$\mathscr{V}^t := \{\Psi \in \mathscr{D}_B | c_t(h)\Psi = 0,\ h \in \mathscr{S}(\mathbb{R}^3)\}. \tag{5.7}$$

Remark 5.6 *In the abstract setting the physical subspace $\mathscr{V}^t$ depends on time t. The physical subspace associated with free fields is, however, independent of t. More precisely, assume that $\{B(\cdot, t)\}_{t\in\mathbb{R}} \in \mathscr{D}_{\mathrm{free}}(\mathcal{K})$ and (5.5) is satisfied. Then $\mathscr{V} = \mathscr{V}^t$ is independent of $t \in \mathbb{R}$.*

5.2 Physical subspace at time t

We return to NRQED. Applying the abstract theory explained in the previous section, we shall construct a physical subspace at time $t < \infty$ as the kernel of some operator. First we define an operator valued distribution. Let

$$\mathscr{B}_P(f,t) := \partial^\mu \mathscr{A}_\mu(f,t,P), \tag{5.8}$$
$$\dot{\mathscr{B}}_P(f,t) := \partial^\mu \dot{\mathscr{A}}_\mu(f,t,P). \tag{5.9}$$

More precisely the right-hand side of (5.8) and (5.9) are abbreviations of

$$\partial^\mu \mathscr{A}_\mu(f,t,P) = \partial_t \mathscr{A}_0(f,t) + \mathscr{A}_1(\partial_{x^1} f, t, P) + \mathscr{A}_2(\partial_{x^2} f, t, P) + \mathscr{A}_3(\partial_{x^3} f, t, P), \tag{5.10}$$
$$\partial^\mu \dot{\mathscr{A}}_\mu(f,t,P) = \partial_t \dot{\mathscr{A}}_0(f,t) + \dot{\mathscr{A}}_1(\partial_{x^1} f, t, P) + \dot{\mathscr{A}}_2(\partial_{x^2} f, t, P) + \dot{\mathscr{A}}_3(\partial_{x^3} f, t, P). \tag{5.11}$$

Then $\{\mathscr{B}_P(\cdot,t)\}_{t\in\mathbb{R}} \in \mathscr{D}(\mathscr{F})$. Define the positive frequency part of $\mathscr{B}_P(h,t)$ as

$$c_{P,t}(h) := i\left(\dot{\mathscr{B}}_P(h_t,t) - \mathscr{B}_P(\dot{h}_t,t)\right),$$

where the functions h_t and $\dot{h}_t$ are defined as in (5.3), and the physical subspace is defined as

$$\mathscr{V}^t_{P,\mathrm{phys}} := \{\Psi \in \mathscr{F} | c_{P,t}(h)\Psi = 0,\ h \in \mathscr{S}(\mathbb{R}^3)\}. \tag{5.12}$$

Of course, in general, $\mathscr{V}^t_{\mathrm{phys}}$ is not independent of time t. To characterize $\mathscr{V}^t_{P,\mathrm{phys}}$, we introduce unitary operators. Let $\Gamma([\gamma])$ be a unitary operator defined by the second quantization of the unitary operator

$$[\gamma] := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} : \oplus^4 L^2(\mathbb{R}^3) \to \oplus^4 L^2(\mathbb{R}^3), \tag{5.13}$$

Furthermore we define the unitary operator $\mathcal{W}$ by

$$\mathcal{W} := \exp\left(-\frac{e}{\sqrt{2}}\left(a^*\left(\frac{\hat{\varphi}}{\omega^{3/2}},3\right) - a\left(\frac{\hat{\varphi}}{\omega^{3/2}},3\right)\right)\right)\Gamma([\gamma]). \tag{5.14}$$

Theorem 5.7 *$\mathscr{V}^t_{P,\mathrm{phys}}$ is positive semi-definite and*

$$\mathscr{V}^t_{P,\mathrm{phys}} = e^{itH_{\mathrm{TL},P}} e^{-itH_{\mathrm{f}}^{\mathrm{TL}}} \mathcal{W} \mathscr{F}^{(0)}_{\mathrm{TL}}, \tag{5.15}$$

where $\mathscr{F}^{(0)}_{\mathrm{TL}} = \mathscr{F}_{\mathrm{TL}} \otimes \{\alpha\Omega_0 | \alpha \in \mathbb{C}\}$.

Proof: We notice that

$$c_{P,0}(h) = a(\sqrt{\omega}h,3) - a(\sqrt{\omega}h,0) + \frac{e}{\sqrt{2}}(\bar{h},\hat{\varphi}/\omega), \tag{5.16}$$

and by the definition of $c_{P,t}(h)$ we can observe that

$$c_{P,t}(h) = \frac{i}{\sqrt{2}} e^{itH_{\mathrm{TL},P}} e^{-itH_{\mathrm{f}}^{\mathrm{TL}}} c_0(h) e^{itH_{\mathrm{f}}^{\mathrm{TL}}} e^{-itH_{\mathrm{TL},P}}.$$

Moreover, it follows directly that $\mathcal{W}^{-1}c_{P,0}(h)\mathcal{W} = \sqrt{2}a(\sqrt{\omega}h,0)$, where we have used

$$\begin{aligned} \Gamma([\gamma])a(f,j)\Gamma([\gamma])^{-1} &= a(f,j), \quad j = 1,2, \\ \Gamma([\gamma])a(f,3)\Gamma([\gamma])^{-1} &= \frac{1}{\sqrt{2}}[a(f,3) + a(f,0)], \\ \Gamma([\gamma])a(f,0)\Gamma([\gamma])^{-1} &= \frac{1}{\sqrt{2}}[a(f,3) - a(f,0)]. \end{aligned}$$

Hence (5.15) follows from the equality $\{\Psi \in \mathscr{F} | c_{P,0}(h)\Psi = 0\} = \mathcal{W}\mathscr{F}_{\rm TL}^{(0)}$. Let $\Psi = e^{itH_{{\rm TL},P}} e^{-itH_{\rm f}^{\rm TL}} \mathcal{W}\Phi \in \mathscr{V}^t$, where $\Phi \in \mathscr{F}_{\rm TL}^{(0)}$. Then $(\Psi|\Psi) = (\Gamma([\gamma])\Phi, \eta\Gamma([\gamma])\Phi) = (\Phi, -\Gamma([\gamma g \gamma])\Phi) \geq 0$. Here

$$-[\gamma g \gamma] = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} : \oplus^4 L^2(\mathbb{R}^3) \to \oplus^4 L^2(\mathbb{R}^3)$$

denotes the interchange between the 0th and 3rd components. Then the theorem is complete. **qed**

$\mathcal{W}$ leaves the transversal part $\mathscr{F}_1 \otimes \mathscr{F}_2$ invariant, $\mathscr{F}_0$ and $\mathscr{F}_3$ are, however, mixed together by $\mathcal{W}$. Although the Hamiltonian $H_P = H_{{\rm TL},P} \otimes 1 + 1 \otimes H_0$ is subdivided into a scalar and a vector component , the physical subspace is, however, of a more complicated form.

5.3 Physical subspace at $t = \pm\infty$

In this subsection we consider the physical subspace at $t = \pm\infty$. We have already presented the explicit form of the asymptotic field $a_{P,{\rm ex}}(h, \mu)$, $\mu = 0, 1, 2, 3$, and proven its asymptotic completeness. We can construct the free field in terms of $a_{P,{\rm ex}}(h, \mu)$ and define the physical subspace independent of t.

Formally, we write

$$a^\sharp_{P,{\rm ex}}(h, \mu) = \int h(k) a^\sharp_{P,{\rm ex}}(k, \mu) dk.$$

We now define the smeared field $\mathscr{A}_\mu^{\rm ex}(f, t, P)$ in terms of $a^\sharp_{P,{\rm ex}}$ by

$$\mathscr{A}_j^{\rm ex}(f, t, P) = \sum_{l=1}^3 \int dk \frac{e_j^l(k)}{\sqrt{2\omega(k)}} \left(a^\dagger_{P,{\rm ex}}(k, l) \hat{f}(k) e^{i\omega(k)t} + a_{P,{\rm ex}}(k, l) \hat{f}(-k) e^{-i\omega(k)t} \right), \quad j = 1, 2, 3, \tag{5.17}$$

$$\mathscr{A}_0^{\rm ex}(f, t, P) = \int \frac{dk}{\sqrt{2\omega(k)}} \left(a^\dagger_{P,{\rm ex}}(k, 0) \hat{f}(k) e^{i\omega(k)t} + a_{P,{\rm ex}}(k, 0) \hat{f}(-k) e^{-i\omega(k)t} \right). \tag{5.18}$$

Let us define the operator valued distribution

$$\mathscr{B}_{P,{\rm ex}}(f, t) := \partial^\mu \mathscr{A}_\mu^{\rm ex}(f, t, P), \quad \dot{\mathscr{B}}_{P,{\rm ex}}(f, t) := \partial^\mu \dot{\mathscr{A}}_\mu^{\rm ex}(f, t, P). \tag{5.19}$$

Here the right-hand side of (5.19) is understood as in (5.10) and (5.11) with $\mathscr{A}_\mu$ replaced by $\mathscr{A}_\mu^{\rm ex}$. Then $\{\mathscr{B}_{P,{\rm ex}}(\cdot,t)\}_{t\in\mathbb{R}} \in \mathscr{D}(\mathscr{F})$. In addition, by the definition of $\mathscr{A}_\mu^{\rm ex}$ it is clear that $\{\mathscr{B}_{P,{\rm ex}}(\cdot,t)\}_{t\in\mathbb{R}} \in \mathscr{D}_{\rm free}(\mathscr{H})$. From Lemma 5.4, the positive frequency part

$$c_{P,{\rm ex}}(g) := i\left(\dot{\mathscr{B}}_{P,{\rm ex}}(g_t,t) - \mathscr{B}_{P,{\rm ex}}(\dot{g}_t,t)\right) \tag{5.20}$$

is independent of t, and the physical subspace at time $t = \pm\infty$ is defined by

$$\mathscr{V}_{P,{\rm phys}}^{\rm ex} := \{\Psi \in \mathscr{F} | c_{P,{\rm ex}}(h)\Psi = 0,\ h \in \mathscr{S}(\mathbb{R}^3)\}. \tag{5.21}$$

Let

$$\mathcal{W}_P := U_P \mathcal{W} \tag{5.22}$$

We can characterize the physical subspace $\mathscr{V}_P^{\rm ex}$ in the theorem below.

Theorem 5.8 *Both $\mathscr{V}_{P,{\rm phys}}^{\rm in}$ and $\mathscr{V}_{P,{\rm phys}}^{\rm out}$ are positive semi-definite and*

$$\mathscr{V}_{P,{\rm phys}}^{\rm in} = \mathcal{W}_P \mathscr{F}_{\rm TL}^{(0)}, \tag{5.23}$$

$$\mathscr{V}_{P,{\rm phys}}^{\rm out} = S_P^{-1} \mathcal{W}_P \mathscr{F}_{\rm TL}^{(0)}. \tag{5.24}$$

Proof: Directly, we have

$$c_{P,{\rm ex}}(h) = \frac{i}{\sqrt{2}}\left(a_{P,{\rm ex}}(\sqrt{\omega}h,3) - a_{P,{\rm ex}}(\sqrt{\omega}h,0)\right). \tag{5.25}$$

Here we have used $\sum_{j=1,2}\sum_{l=1}^3 k_l e_l^j = 0$. In particular

$$U_P^{-1} c_{P,{\rm in}}(h) U_P = \frac{i}{\sqrt{2}}\left(a(\sqrt{\omega}h,3) - a(\sqrt{\omega}h,0)\right)$$

follows. Then (5.23) follows. By $a_{P,{\rm in}}^\sharp(h,\mu)S_P = S_P a_{P,{\rm out}}^\sharp(h,\mu)$, (5.24) also follows. Finally the semidefinite property of $\mathscr{V}_{P,{\rm phys}}^{\rm ex}$ can be obtained from the fact that S_P is η unitary and $[U_P,\eta] = 0$. Then the proof is complete. **qed**

By Theorem 5.8, we observe that $\mathscr{V}_{P,{\rm phys}}^{\rm in} = S_P \mathscr{V}_{P,{\rm phys}}^{\rm out}$. We find, however, that $\mathscr{V}_{P,{\rm phys}}^{\rm in}$ is *not* identical to $\mathscr{V}_{P,{\rm phys}}^{\rm out}$.

Theorem 5.9 *We have $\mathscr{V}_{P,{\rm phys}}^{\rm in} \neq \mathscr{V}_{P,{\rm phys}}^{\rm out}$.*

Proof: Let $\Psi = \mathcal{W}_P \Phi \in \mathscr{V}_{P,{\rm phys}}^{\rm in}$ with $\Phi \in \mathscr{F}_{\rm TL}^{(0)}$. Then we have

$$c_{P,{\rm out}}(h)\Psi = \frac{i}{\sqrt{2}} U_P \left(\sum_{l=1}^3 a(L^{l3}\sqrt{\omega}h,l) - a(\sqrt{\omega}h,0)\right)\mathcal{W}\Phi.$$

One can easily find some vector $\Phi \in \mathscr{F}_{\rm TL}^{(0)}$ such that the right-hand side above does not vanish. Then the theorem follows. **qed**

6 Physical Hamiltonian

6.1 Physical Hilbert space and physical scattering operator

We defined $\mathscr{V}^{\rm ex}_{P,{\rm phys}}$ in the previous section and it includes the null space $\mathscr{V}^{\rm ex}_{P,{\rm null}}$ with respect to $(\cdot|\cdot)$. We want to define the physical Hilbert space by $\mathscr{V}^{\rm ex}_{P,{\rm phys}}$ divided by the null space and a self-adjoint physical Hamiltonian on it.

We first of all characterize the null space of $\mathscr{V}^{\rm ex}_{P,{\rm phys}}$. Let $\mathscr{F}_{\rm T}=\mathscr{F}_1\otimes\mathscr{F}_2$ and

$$\mathscr{F}^{(0)}_{\rm T}=\mathscr{F}_{\rm T}\otimes\{\alpha\Omega_3|\alpha\in\mathbb{C}\}\otimes\{\alpha\Omega_0|\alpha\in\mathbb{C}\}. \tag{6.1}$$

Then $\mathscr{F}^{(0)}_{\rm TL}$ can be decomposed as $\mathscr{F}^{(0)}_{\rm TL}=\mathscr{F}^{(0)}_{\rm T}\oplus\left(\mathscr{F}^{(0)\perp}_{\rm T}\cap\mathscr{F}^{(0)}_{\rm TL}\right)$. Let

$$\mathscr{V}^{\rm in}_P:=\mathcal{W}_P\mathscr{F}^{(0)}_{\rm T},\quad \mathscr{V}^{\rm in}_{P,{\rm null}}:=\mathcal{W}_P\left(\mathscr{F}^{(0)\perp}_{\rm T}\cap\mathscr{F}^{(0)}_{\rm TL}\right), \tag{6.2}$$

$$\mathscr{V}^{\rm out}_P:=S_P^{-1}\mathscr{V}^{\rm in}_P,\quad \mathscr{V}^{\rm out}_{P,{\rm null}}:=S_P^{-1}\mathscr{V}^{\rm in}_{P,{\rm null}}. \tag{6.3}$$

Then $\mathscr{V}^{\rm ex}_{P,{\rm phys}}$ is also decomposed as

$$\mathscr{V}^{\rm ex}_{P,{\rm phys}}=\mathscr{V}^{\rm ex}_P\oplus\mathscr{V}^{\rm ex}_{P,{\rm null}}. \tag{6.4}$$

Here $\mathscr{V}^{\rm ex}_P$ is closed, positive definite and satisfies $(\Psi_1|\Psi_1')=(\Psi_1,\Psi_1')$ for $\Psi_1,\Psi_1'\in\mathscr{V}^{\rm ex}_P$, and $\mathscr{V}^{\rm ex}_{P,{\rm null}}$ is closed, neutral and

$$\mathscr{V}^{\rm ex}_{P,{\rm null}}=\{\Psi_0\in\mathscr{V}^{\rm ex}_{P,{\rm phys}}|(\Psi_0|\Psi_0)=0\}.$$

Definition 6.1 *For subspaces Y, Z and X in $\mathscr{F}$, we use the notation*

$$X=Y\ [\dot{+}]\ Z$$

if and only if (1) for all $x\in X$, there exist unique vectors $y\in Y$ and $z\in Z$ such that $x=y+z$, (2) $(y|z)=0$ holds for all $y\in Y$ and $z\in Z$.

Lemma 6.2 *It follows that $\mathscr{V}^{\rm ex}_{P,{\rm phys}}=\mathscr{V}^{\rm ex}_P\ [\dot{+}]\ \mathscr{V}^{\rm ex}_{P,{\rm null}}$.*

Proof: Since $\mathscr{V}^{\rm ex}_{P,{\rm phys}}$ is positive semi-definite with respect to the metric $(\cdot|\cdot)$, we have, by the Schwartz inequality, $|(\Psi_1|\Psi_0)|^2\le(\Psi_1|\Psi_1)(\Psi_0|\Psi_0)=0$ for $\Psi_1\in\mathscr{V}^{\rm ex}_P$ and $\Psi_0\in\mathscr{V}^{\rm ex}_{P,{\rm null}}$. Hence $(\Psi_1|\Psi_0)=0$. Then the lemma follows. **qed**

We define the physical Hilbert space in terms of the quotient Hilbert space

$$\mathscr{H}^{\rm ex}_{P,{\rm phys}}:=\mathscr{V}^{\rm ex}_{P,{\rm phys}}/\mathscr{V}^{\rm ex}_{P,{\rm null}}. \tag{6.5}$$

We denote by $[\Psi]_{\rm ex}$ the element of $\mathscr{H}^{\rm ex}_{P,{\rm phys}}$ associated with $\Psi \in \mathscr{V}^{\rm ex}_{P,{\rm phys}}$ and the induced scalar product on $\mathscr{H}^{\rm ex}_{P,{\rm phys}}$ is denoted by $(\cdot,\cdot)_{\rm ex}$, i.e., $([\Psi]_{\rm ex},[\Phi]_{\rm ex})_{\rm ex} = (\Psi,\Phi)$. Furthermore let $\pi_{\rm ex} : \mathscr{V}^{\rm ex}_p \to \mathscr{H}^{\rm ex}_{P,{\rm phys}}$ be the natural onto map defined by $\pi_{\rm ex}(\Phi) := [\Phi]_{\rm ex}$. Thus $\pi_{\rm ex}$ is an isometry and so is a unitary operator between $\mathscr{V}^{\rm ex}_p$ and $\mathscr{H}^{\rm ex}_{P,{\rm phys}}$.

We have already defined the scattering operator S_P. This operator maps the null space $\mathscr{V}^{\rm out}_{P,{\rm null}}$ into the null space $\mathscr{V}^{\rm in}_{P,{\rm null}}$. Now we can define the physical scattering operator.

Definition 6.3 *The physical scattering operator* $S_{P,{\rm phys}} : \mathscr{H}^{\rm out}_{P,{\rm phys}} \longrightarrow \mathscr{H}^{\rm in}_{P,{\rm phys}}$ *is defined by*

$$S_{P,{\rm phys}}[\Psi]_{\rm out} := [S_P\Psi]_{\rm in}. \tag{6.6}$$

Theorem 6.4 (Physical scattering operator) $S_{P,{\rm phys}}$ *is unitary.*

Proof: Since S_P is a unitary operator from $\mathscr{V}^{\rm out}_P$ to $\mathscr{V}^{\rm in}_P$, the theorem follows. **qed**

6.2 Physical Hamiltonian

In the previous section we defined the physical Hilbert space. Next we define the physical Hamiltonian $H^{\rm ex}_{P,{\rm phys}}$ on $\mathscr{H}^{\rm ex}_{P,{\rm phys}}$ and prove its self-adjointness.

We define

$$P^{\rm in} := \mathcal{W}_P P_{\rm TL} \mathcal{W}_P^{-1}, \quad P^{\rm out} := S^{-1}\mathcal{W}_P P_{\rm TL}\mathcal{W}_P^{-1} S.$$

Here $P_{\rm TL} = 1\otimes 1\otimes 1\otimes P_{\Omega_0}$ is the orthogonal projection onto $\mathscr{F}^{(0)}_{\rm TL}$, where P_{Ω_0} is the orthogonal projection onto $\{\alpha\Omega_0|\alpha\in\mathbb{C}\}$. Then $P^{\rm ex}$ is the orthogonal projection onto $\mathscr{V}^{\rm ex}_{P,{\rm phys}}$. We have to say something about relationships between the domain of H_P and $\mathscr{V}^{\rm ex}_{P,{\rm phys}}$.

Lemma 6.5 *(1)* $P^{\rm ex}$ *leaves* $D(H_P)$ *invariant, i.e.,* $P^{\rm ex}D(H_P)\subset D(H_P)$.

(2) H_P *leaves* $\mathscr{V}^{\rm ex}_{P,{\rm phys}}$ *invariant, i.e.,* $H_P(D(H_P)\cap\mathscr{V}^{\rm ex}_{P,{\rm phys}})\subset\mathscr{V}^{\rm ex}_{P,{\rm phys}}$.

Proof: Let us define the operator

$$\tilde{H}_P := H_{\rm f} - a^*(\hat\varphi/\sqrt{\omega},3) - a(\tilde{\hat\varphi}/\sqrt{\omega},0) + E_{\rm TL}(P) + E_0$$

with domain $D(\tilde{H}_P) = D(H_{\rm f})$. Since $-a^*(\hat\varphi/\sqrt{\omega},3) - a(\tilde{\hat\varphi}/\sqrt{\omega},0)$ is infinitesimally small with respect to $H_{\rm f}$, we have $\|H_{\rm f}\Psi\| \le C(\|\tilde{H}_P\Psi\| + \|\Psi\|)$ for some constant C.

Then $\tilde{H}_P$ is closed. Furthermore by $\|\tilde{H}_P\Psi\| \le c(\|H_{\rm f}\Psi\|+\|\Psi\|)$ for some constant c, an arbitrary core of $H_{\rm f}$ is also a core of $\tilde{H}_P$. Thus both H_P and $\tilde{H}_P$ are closed and have the same domain $D(H_P) = D(H_{\rm f}) = D(\tilde{H}_P)$; moreover have the common core

$$\mathscr{F}_{\rm fin}(\omega) := {\rm L.H.}\left\{\prod_{i=1}^n a^*(f_i,\mu_i)\Omega, \Omega \middle| f_i \in D(\omega), \mu_i = 0,1,2,3, i=1,...,n, n\ge 1\right\}.$$

It is immediate that $\mathcal{W}_P^{-1}H_P\mathcal{W}_P = \tilde{H}_P$ on the common core $\mathscr{F}_{\rm fin}(\omega)$. Then $\mathcal{W}_P D(H_P) \subset D(H_P)$ and we have the operator equation $\mathcal{W}_P^{-1}H_P\mathcal{W}_P = \tilde{H}_P$. Since, by $P_{\rm TL}H_{\rm f} \subset H_{\rm f}P_{\rm TL}$, $P_{\rm TL}$ leaves $D(H_P)$ invariant, we have

$$\begin{aligned} &P^{\rm in}D(H_P) \subset \mathcal{W}_P P_{\rm TL} D(H_P) \subset \mathcal{W}_P D(H_P) \subset D(H_P), \\ &P^{\rm out}D(H_P) \subset S_P^{-1}\mathcal{W}_P P_{\rm TL} D(H_P) \subset S_P^{-1}\mathcal{W}_P D(H_P) \subset D(H_P), \end{aligned}$$

where we have used the intertwining property $S_P H_P = H_P S_P^{-1}$. Thus the first half of the lemma is proven. For $\Psi \in D(H_P)\cap \mathscr{V}_{P,\rm phys}^{\rm in}$, we have

$$\begin{aligned} H_P\Psi &= H_P P^{\rm in}\Psi = \mathcal{W}_P\tilde{H}_P P_{\rm TL}\mathcal{W}_P^{-1}\Psi \\ &= \mathcal{W}_P P_{\rm TL}\left(H_{\rm f} - a^*(\hat{\varphi}/\sqrt{\omega},3) + E_{\rm TL}(P) + E_0\right)\mathcal{W}_P^{-1}\Psi \in \mathscr{V}_{P,\rm phys}^{\rm in}. \end{aligned} \tag{6.7}$$

Then for $\Psi \in D(H_P)\cap \mathscr{V}_{P,\rm phys}^{\rm out}$,

$$\begin{aligned} H_P\Psi &= S_P^{-1}H_P P^{\rm out}\Psi = \mathcal{W}_P\tilde{H}_P P_{\rm TL}\mathcal{W}_P^{-1}S_P\Psi \\ &= S_P^{-1}\mathcal{W}_P P_{\rm TL}\left(H_{\rm f} - a^*(\hat{\varphi}/\sqrt{\omega},3) + E_{\rm TL}(P) + E_0\right)\mathcal{W}_P^{-1}S_P\Psi \in \mathscr{V}_{P,\rm phys}^{\rm out}. \end{aligned} \tag{6.8}$$

Hence the proof is complete. **qed**

Let $K_P^{\rm ex}$ be the restriction of H_P to $D(H_P)\cap\mathscr{V}_{P,\rm phys}^{\rm ex}$:

$$K_P^{\rm ex} := H_P\lceil_{D(H_P)\cap\mathscr{V}_{P,\rm phys}^{\rm ex}}. \tag{6.9}$$

By Lemma 6.5 $K_P^{\rm ex}$ is a densely defined closed operator on $\mathscr{V}_{P,\rm phys}^{\rm ex}$. Note that $\mathscr{V}_{P,\rm phys}^{\rm ex}$ is closed. In order to study $K_P^{\rm ex}$ we introduce the operator

$$\hat{H}_P := H_{\rm f} - a^*(\hat{\varphi}/\sqrt{\omega},3) + E_{\rm TL}(P) + E_0$$

with domain $D(\hat{H}_P) = D(H_{\rm f})$. In a similar way as in the proof that $\tilde{H}_p$ is closed, one can determine that $\hat{H}_P$ is closed. By (6.7) and (6.8), we have, for all $\Psi \in D(K_P^{\rm ex})$,

$$K_P^{\rm in}\Psi = \mathcal{W}_P\hat{H}_P\mathcal{W}_P^{-1}\Psi, \tag{6.10}$$

$$K_P^{\rm out}\Psi = S_P^{-1}\mathcal{W}_P\hat{H}_P\mathcal{W}_P^{-1}S_P\Psi. \tag{6.11}$$

Lemma 6.6 *(1) $K_P^{\rm in}$ is reduced by $\mathscr{V}_{P,\rm phys}^{\rm in}$, i.e., $P^{\rm in}K_P^{\rm in} \subset K_P^{\rm in}P^{\rm in}$.*

(2) $K_P^{\rm ex}$ leaves $\mathscr{V}_{P,\rm null}^{\rm ex}$ invariant, i.e., $K_P^{\rm ex}(D(K_P^{\rm ex}) \cap \mathscr{V}_{P,\rm null}^{\rm ex}) \subset \mathscr{V}_{P,\rm null}^{\rm ex}$.

Proof: (1) follows from (6.10), (6.11) and the fact that $\hat{H}_P$ is reduced by $\mathscr{F}_{\rm TL}^{(0)}$, i.e., $P_{\rm TL}\hat{H}_P \subset \hat{H}_P P_{\rm TL}$. Let $\Psi_0 \in D(K_P^{\rm in}) \cap \mathscr{V}_{P,\rm null}^{\rm in}$ and set $\Phi_0 = \mathcal{W}_P^{-1}\Psi_0 \in D(\hat{H}_P)$. Then $\Phi_0 \in \mathscr{F}_{\rm T}^{(0)\perp} \cap \mathscr{F}_{\rm TL}^{(0)}$. Since $\hat{H}_P\Phi_0 \in \mathscr{F}_{\rm T}^{(0)\perp} \cap \mathscr{F}_{\rm TL}^{(0)}$, we have $K_P^{\rm in}\Psi_0 = \mathcal{W}_P\hat{H}_P\Phi_0 \in \mathscr{V}_{P,\rm null}^{\rm in}$. Thus $K_P^{\rm in}$ leaves $\mathscr{V}_{P,\rm null}^{\rm in}$ invariant. Similarly, one can prove that $K_P^{\rm out}$ leaves $\mathscr{V}_{P,\rm null}^{\rm out}$ invariant. **qed**

We denote by $\rho(X)$ the resolvent set of a linear operator X. By (6.10) and (6.11) it follows that $\rho(\hat{H}_P) \subset \rho(K_P^{\rm ex})$ and for $z \in \rho(\hat{H}_P)$,

$$(K_P^{\rm in} - z)^{-1} = \mathcal{W}_P(\hat{H}_P - z)^{-1}\mathcal{W}_P^{-1}, \tag{6.12}$$

$$(K_P^{\rm out} - z)^{-1} = S_P^{-1}\mathcal{W}_P(\hat{H}_P - z)^{-1}\mathcal{W}_P^{-1}S_P. \tag{6.13}$$

Let us now define the physical Hamiltonian $H_{P,\rm phys}^{\rm ex}$ on the physical Hilbert space $\mathscr{H}_{P,\rm phys}^{\rm ex}$. In order to define the domain $D(H_{\rm phys}^{\rm ex})$ consistently, we first consider the resolvent of $K_P^{\rm ex}$.

Let

$$\mathcal{R} = \left\{ z \in \rho\left(H_{\rm f} + E_{\rm TL}(P) + E_0\right) \middle| 2\epsilon + \frac{\|\hat{\varphi}/\omega\|^2/(2\epsilon) + \|\hat{\varphi}/\sqrt{\omega}\|/\sqrt{2}}{|E_{\rm TL}(P) + E_0 - z|} < 1 \text{ for some } \epsilon > 0 \right\}.$$

Since $\|a^*(\hat{\varphi}/\sqrt{\omega}, 3)(H_{\rm f} + E_{\rm TL}(P) + E_0 - z)^{-1}\| < 1$ for $z \in \mathcal{R}$, for all $z \in \mathcal{R}$, the Neumann expansion is valid and

$$(\hat{H}_P - z)^{-1} = \sum_{n=0}^{\infty}(H_{\rm f} + E_{\rm TL}(P) + E_0 - z)^{-1}\left(a^*(\hat{\varphi}/\sqrt{\omega}, 3)(H_{\rm f} + E_{\rm TL}(P) + E_0 - z)^{-1}\right)^n. \tag{6.14}$$

Let us fix $z \in \mathcal{R}$. Then, by (6.12) and (6.13), $z \in \rho(K_P^{\rm ex})$ and the resolvent

$$R_P^{\rm ex}(z) := (K_P^{\rm ex} - z)^{-1} \tag{6.15}$$

is bijective on $\mathscr{V}_{P,\rm phys}^{\rm ex}$.

Lemma 6.7 *$R_P^{\rm ex}(z)$ is reduced by $\mathscr{V}_{P,\rm phys}^{\rm ex}$ and leaves $\mathscr{V}_{P,\rm null}^{\rm ex}$ invariant, i.e., $P^{\rm ex}R_P^{\rm ex}(z) = R_P^{\rm ex}(z)P^{\rm ex}$ and $R_P^{\rm ex}(z)\mathscr{V}_{P,\rm null}^{\rm ex} \subset \mathscr{V}_{P,\rm null}^{\rm ex}$.*

Proof: The first half of this lemma has already been proven via Lemma 6.6 (1). We prove the second half. Let $\Psi_0 \in \mathscr{V}^{\rm in}_{P,\rm null}$ and set $\Phi_0 = \mathcal{W}_P^{-1}\Psi_0$. Then $\Phi_0 \in \mathscr{F}_{\rm T}^{(0)\perp} \cap \mathscr{F}_{\rm TL}^{(0)}$. By (6.12), (6.13) and (6.14), we observe that

$$R_P^{\rm in}(z)\Psi_0 = \mathcal{W}_P(\hat{H}_P - z)^{-1}\Phi_0 \in \mathcal{W}_P(\mathscr{F}_{\rm T}^{(0)\perp} \cap \mathscr{F}_{\rm TL}^{(0)}) = \mathscr{V}^{\rm in}_{P,\rm null}. \tag{6.16}$$

Thus $R_P^{\rm in}(z)$ leaves $\mathscr{V}^{\rm in}_{P,\rm null}$ invariant. Similarly one can prove that $R_P^{\rm out}(z)$ also leaves $\mathscr{V}^{\rm out}_{P,\rm null}$ invariant. **qed**

Since $R_P^{\rm in}(z)$ leaves the null space invariant, the following operator, $[R_P^{\rm ex}(z)]_{\rm ex}$, on $\mathscr{H}^{\rm ex}_{P,\rm phys}$ is well-defined:

$$[R_P^{\rm ex}(z)]_{\rm ex}[\Psi]_{\rm ex} := [R_P^{\rm ex}(z)\Psi]_{\rm ex}.$$

It is clear that $[R_P^{\rm ex}(z)]_{\rm ex}$ is bounded and $\|[R_P^{\rm ex}(z)]_{\rm ex}\|_{\rm ex} \le \|R_P^{\rm ex}(z)\|$ holds.

Lemma 6.8 *$[R_P^{\rm ex}(z)]_{\rm ex}$ is injective and $[R_P^{\rm ex}(z)]_{\rm ex}^{-1}$ is closed.*

Proof: By the boundedness of $[R_P^{\rm ex}(z)]_{\rm ex}$, $[R_P^{\rm ex}(z)]_{\rm ex}^{-1}$ is closed if $[R_P^{\rm ex}(z)]_{\rm ex}$ is injective. Let $[R_P^{\rm ex}(z)]_{\rm ex}[\Psi]_{\rm ex} = 0$. Then $R_P^{\rm ex}(z)\Psi \in \mathscr{V}_{P,\rm null}$. It follows from Lemma 6.6 (2) that $\Psi = (K_P^{\rm ex} - z)R_P^{\rm ex}(z)\Psi \in \mathscr{V}^{\rm ex}_{P,\rm null}$. Thus $[\Psi]_{\rm ex} = 0$ and $[R_P^{\rm ex}(z)]_{\rm ex}$ is injective. **qed**

Definition 6.9 *We define the physical Hamiltonian $H^{\rm ex}_{P,\rm phys}$ on $\mathscr{H}^{\rm ex}_{P,\rm phys}$ by*

$$H^{\rm ex}_{P,\rm phys} := z + [R_P^{\rm ex}(z)]_{\rm ex}^{-1}. \tag{6.17}$$

By Lemma 6.8, $H^{\rm ex}_{P,\rm phys}$ is closed. We further prove that $H^{\rm ex}_{P,\rm phys}$ is independent of $z \in \mathcal{R}$ and that the domain of $H^{\rm ex}_{P,\rm phys}$ is dense in $\mathscr{H}^{\rm ex}_{P,\rm phys}$. We define $P^{\rm ex}$ by

$$P_1^{\rm in} := \mathcal{W}_P P_{\rm T}\mathcal{W}_P^{-1}, \quad P_1^{\rm out} := S_P^{-1}\mathcal{W}_P P_{\rm T}\mathcal{W}_P^{-1}S_P. \tag{6.18}$$

Here $P_{\rm T} = 1 \otimes 1 \otimes P_{\Omega_3} \otimes P_{\Omega_0}$. Then $P_1^{\rm ex}$ is the orthogonal projection onto $\mathscr{V}_P^{\rm ex}$. We define a linear operator $J_P^{\rm ex}$ on $\mathscr{H}^{\rm ex}_{P,\rm phys}$ by

$$J_P^{\rm ex}[\Psi]_{\rm ex} = [K_P^{\rm ex}P_1^{\rm ex}\Psi]_{\rm ex}, \tag{6.19}$$
$$D(J_P^{\rm ex}) = \left\{[\Psi]_{\rm ex} \in \mathscr{H}^{\rm ex}_{P,\rm phys} | P_1^{\rm ex}\Psi \in D(K_P^{\rm ex})\right\}. \tag{6.20}$$

Note that the domain $D(J_P^{\rm ex})$ is independent of the representative. Indeed if $[\Psi]_{\rm ex} = [\Psi']_{\rm ex}$, then $P_1^{\rm ex}\Psi = P_1^{\rm ex}\Psi'$ because $\Psi - \Psi' \in \mathscr{V}^{\rm ex}_{P,\rm null}$ and $P_1^{\rm ex}\mathscr{V}^{\rm ex}_{P,\rm null} = \{0\}$. Thus the operator $J_P^{\rm ex}$ is well-defined. Moreover since $P_1^{\rm ex}$ leaves $D(K_P^{\rm ex})$ invariant, $D(J_P^{\rm ex})$ is dense in $\mathscr{H}^{\rm ex}_{P,\rm phys}$.

Lemma 6.10 *It follows that*

$$H^{\rm ex}_{P,{\rm phys}} = J^{\rm ex}_P. \tag{6.21}$$

In particular, $H^{\rm ex}_{P,{\rm phys}}$ *is a densely defined closed operator and independent of* $z \in \mathcal{R}$.

Proof: Let $[\Psi]_{\rm ex} \in D(J^{\rm ex}_P)$. Then $P^{\rm ex}_1\Psi \in D(K^{\rm ex}_P)$ and set $\Phi_0 := (K^{\rm ex}_P - z)P^{\rm ex}_1\Psi$. We observe that

$$[\Psi]_{\rm ex} = [P^{\rm ex}_1\Psi]_{\rm ex} = [R^{\rm ex}_P(z)]_{\rm ex}[\Phi_0]_{\rm ex} \in D([R^{\rm ex}_P(z)]^{-1}_{\rm ex})$$

and hence $D(J^{\rm ex}_P) \subset D(H^{\rm ex}_{P,{\rm phys}})$. We show the inverse inclusion. Let $[\Psi]_{\rm ex} \in D(H^{\rm ex}_{P,{\rm phys}})$. Then there exists a vector $[\Phi]_{\rm ex} \in \mathscr{H}^{\rm ex}_{P,{\rm phys}}$ such that $[\Psi]_{\rm ex} = [R^{\rm ex}_P(z)]_{\rm ex}[\Phi]_{\rm ex} = [R^{\rm ex}_P(z)\Phi]_{\rm ex}$. Since $P^{\rm ex}_1$ leaves $D(K^{\rm ex}_P)$ invariant, we have $P^{\rm ex}_1\Psi = P^{\rm ex}_1 R^{\rm ex}_P(z)\Phi \in D(K^{\rm ex}_P)$. Then $D(J^{\rm ex}_P) \supset D(H^{\rm ex}_{P,{\rm phys}})$ follows. Thus

$$D(H^{\rm ex}_{P,{\rm phys}}) = D(J^{\rm ex}_P).$$

For all $[\Psi]_{\rm ex} \in D(H^{\rm ex}_{P,{\rm phys}})$, we see that (1) there exists $[\Phi]_{\rm ex} \in \mathscr{H}^{\rm ex}_{P,{\rm phys}}$ such that $[\Psi]_{\rm ex} = [R^{\rm ex}_P(z)]_{\rm ex}[\Phi]_{\rm ex}$ and (2) $P^{\rm ex}_1\Psi \in D(K^{\rm ex}_P)$. We have

$$H^{\rm ex}_{P,{\rm phys}}[\Psi]_{\rm ex} - J^{\rm ex}_P[\Psi]_{\rm ex} = [z\Psi + \Phi - K^{\rm ex}_P P^{\rm ex}_1\Psi]_{\rm ex}.$$

We need only prove that $z\Psi + \Phi - K^{\rm ex}_P P^{\rm ex}_1\Psi \in \mathscr{V}^{\rm ex}_{P,{\rm null}}$. Together, (1) and (2) imply that $P^{\rm ex}_1\Psi - R^{\rm ex}_P(z)\Phi \in \mathscr{V}^{\rm ex}_{P,{\rm null}} \cap D(K^{\rm ex}_P)$, which, together with Lemma 6.6, yields

$$z\Psi + \Phi - K^{\rm ex}_P P^{\rm ex}_1\Psi = z(1 - P^{\rm ex}_1)\Psi - (K^{\rm ex}_P - z)(P^{\rm ex}_1\Psi - R^{\rm ex}_P(z)\Phi) \in \mathscr{V}^{\rm ex}_{P,{\rm null}}.$$

Thus the lemma follows. **qed**

Now we are in a position to state the main theorem in this section:

Theorem 6.11 $H^{\rm ex}_{\rm phys}$ *is self-adjoint and has a unique ground state with energy* $E_{\rm TL}(P) + E_0$.

Proof: For all $[\Psi]_{\rm ex} \in D(J^{\rm ex}_P)$, we have $J^{\rm ex}_P[\Psi]_{\rm ex} = \pi_{\rm ex}P^{\rm ex}_1 K^{\rm ex}_P P^{\rm ex}_1 \pi^{-1}_{\rm ex}[\Psi]_{\rm ex}$. This equality implies that

$$J^{\rm ex}_P \subset \pi_{\rm ex}P^{\rm ex}_1 H^{\rm ex}_{P,{\rm phys}} P^{\rm ex}_1 \pi^{-1}_{\rm ex}.$$

Conversely if $[\Psi]_{\rm ex} \in D(\pi_{\rm ex}P^{\rm ex}_1 K^{\rm ex}_P P^{\rm ex}_1 \pi^{-1}_{\rm ex})$, then $P^{\rm ex}_1\Psi = P^{\rm ex}_1\pi^{-1}_{\rm ex}[\Psi]_{\rm ex} \in D(K^{\rm ex}_P)$ and henceforth $D(\pi_{\rm ex}P^{\rm ex}_1 H^{\rm ex}_{P,{\rm phys}} P^{\rm ex}_1 \pi^{-1}_{\rm ex}) \subset D(J^{\rm ex}_P)$. Thus we have obtained the result that

$$J^{\rm ex}_P = \pi_{\rm ex}P^{\rm ex}_1 K^{\rm ex}_P P^{\rm ex}_1 \pi^{-1}_{\rm ex}. \tag{6.22}$$

Combining Lemma 6.10 and (6.22), we establish that

$$H^{\rm ex}_{P,{\rm phys}} = \pi_{\rm ex} P_1^{\rm ex} K_P^{\rm ex} P_1^{\rm ex} \pi_{\rm ex}^{-1}.$$

Then $H^{\rm ex}_{P,{\rm phys}}$ is self-adjoint if and only if $P_1^{\rm ex} K_P^{\rm ex} P_1^{\rm ex}$ is self-adjoint. By (6.10), (6.11) and (6.18), we have

$$P_1^{\rm in} K_P^{\rm in} P_1^{\rm in} = \mathcal{W}_P P_{\rm T} \hat{H}_P P_{\rm T} \mathcal{W}_P^{-1} = U_P P_{\rm T} (H_{\rm f}^{\rm T} + E_{\rm TL}(P) + E_0) P_{\rm T} U_P^{-1} \tag{6.23}$$

and, by the intertwining property,

$$\begin{aligned} P_1^{\rm out} K_P^{\rm out} P_1^{\rm out} &= S_P^{-1} \mathcal{W}_P P_{\rm T} \hat{H}_P P_{\rm T} \mathcal{W}_P^{-1} S_P \\ &= S_P^{-1} U_P P_{\rm T} (H_{\rm f}^{\rm T} + E_{\rm TL}(P) + E_0) P_{\rm T} U_P^{-1} S_P, \end{aligned} \tag{6.24}$$

where $H_{\rm f}^{\rm T} = \sum_{j=1,2} \int \omega(k) a^*(k) a(k) dk$. The above equations imply that $P_1^{\rm ex} K_P^{\rm ex} P_1^{\rm ex}$ is self-adjoint and hence we have the desired properties. **qed**

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