Spectral problems about many-body Dirac operators mentioned by Dereziński

京都大学大学院理学研究科   大鍛治 隆司 [1] Takashi Okaji
Department of Mathematics
Graduate School of Science,
Kyoto University

This is a joint work with H.Kalf[2] and O.Yamada[3].

1   Introduction

In [2], Dereziński mentioned open problems about many-body Dirac operators. These problems are originally formulated by B. Jeziorski who is a chemist from University of Warsaw (cf. J. Sucher [8]). Among them there are spectral problems on Dirac-Coulomb operator H_{DC} for a helium-like ion, which has the form

$$H_{DC} = H(1, Z) + H(2, Z) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}, \qquad (1.1)$$

where

$$H(i, Z) = c\vec{\alpha}\vec{p}_i + mc^2\beta - \frac{Z}{|\mathbf{r}_i|}, \quad i = 1, 2 \qquad (1.2)$$

is the usual Dirac operator for an electron i in the hydrogen-like ion of charge Z and of mass m. In the above notation, $\mathbf{r}_i$ and $\vec{p}_i$, $i = 1, 2$ are a position vector and the momentum operator, respectively, of the i-th electron,

$$\mathbf{r} = (x_1, x_2, x_3), \ \vec{p} = -i\hbar \text{ grad}.$$

The vector $\vec{\alpha}$ is a vector operator whose components $\alpha_1, \alpha_2, \alpha_3$, together with the operator $\beta \equiv \alpha_4$ are Hermitian matrices of order four satisfying the anti-commuting relations

$$\alpha_j \alpha_k + \alpha_k \alpha_j = 2\delta_{jk} \ (j, k = 1, 2, 3, 4).$$

Since the domain of the Dirac operator $H(i, Z)$ is a subspace of four-component wave functions depending on the three coordinates of the i-th electron, we may consider that H_{DC} acts on sixteen-component wave functions, which depend on the six coordinates of two electrons and have the anti-symmetric property due to the Pauli principle.

Mathematically, the operator should be written as

$$H_{DC} = H(Z) \otimes I + I \otimes H(Z) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}, \qquad (1.3)$$

where

$$H(Z) = c\vec{\alpha}\vec{p} + mc^2\beta - \frac{Z}{|\mathbf{r}|} \tag{1.4}$$

is an operator in $\mathcal{H} = L^2(\mathbf{R}^3; \mathbf{C}^4)$. The domain of H_{DC} is a subspace of the antisymmetric tensor product $\mathcal{H} \otimes_A \mathcal{H}$.

In this talk we shall rigorously derive a representation of H_{DC} as a matrix operator of order sixteen and give an answer to its spectral problems, especially essential self-adjointness, continuous (essential) spectrum and absence of eigenvalues. Our method is inspired from a consideration on a simple related operator on $\left[L^2(\mathbf{R}^3) \otimes L^2(\mathbf{R}^3)\right]^4$.

2 Two-electron problems

In the nonrelativistic theory with no effect of spins, Schrödinger's equation for atoms having two electrons is

$$\Delta_1 u + \Delta_2 u + 2(E + \frac{Z}{r_1} + \frac{Z}{r_2} - \frac{1}{r_{12}})u = 0. \tag{2.1}$$

Here, E is the total energy, $Z > 0$, r_1 and r_2 are the distance of the first and second electrons from the nucleus, r_{12} their mutual separation, and u is a function of the six coordinates $(x_1, y_1, z_1) := \mathbf{r}_1$ and $(x_2, y_2, z_2) := \mathbf{r}_2$ which should satisfy the relation

$$u(\mathbf{r}_2, \mathbf{r}_1) = -u(\mathbf{r}_1, \mathbf{r}_2) \tag{2.2}$$

because of the Pauli exclusion principle; these argument, we have used the fact that

$$L^2(\mathbf{R}^3; \mathbf{C})\hat{\otimes}L^2(\mathbf{R}^3; \mathbf{C}) = L^2(\mathbf{R}^6; \mathbf{C}). \tag{2.3}$$

As far as we know, there is no systematic derivation of relativistic systems in the literature in physics and quantum chemistry, so that two-body relativistic systems with which we are concerned seem to be less familiar than nonrelativistic ones. The first relativistic equation for two particles which we find in the book by H.A. Bethe and E.E. Salpeter [1] is the Breit equation, which has been extensively used in the past is a differential equation for a relativistic wave function for two electrons, interacting with each other and with an external electromagnetic field. It is not fully Lorentz invariant and is only an approximation. It reads

$$\left(E - H[1] - H[2] - \frac{e^2}{r_{12}}\right)U = -\frac{e^2}{2r_{12}}\left[\vec{\alpha}_1 \cdot \vec{\alpha}_2 + \frac{(\vec{\alpha}_1 \cdot \mathbf{r}_{12})(\vec{\alpha}_2 \cdot \mathbf{r}_{12})}{r_{12}^2}\right]U, \tag{2.4}$$

where $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$, $r_{12} = |\mathbf{r}_{12}|$ and

$$H[j] = -e\varphi(\mathbf{r}_j) + \beta_j mc^2 + \vec{\alpha}_j \cdot (c\mathbf{p}_j + e\mathbf{A}(\mathbf{r}_j)) \tag{2.5}$$

is the Dirac Hamiltonian and the Dirac matrices $\vec{\alpha}_j$ and β_j operate on the spinor of U (for electron j). The wave function U depends on the positions $\mathbf{r}_1$ and $\mathbf{r}_2$ and has sixteen spinor components.

If we neglect the right hand side of the equation (2.4) with $\mathbf{A} = 0$, then we get the Dirac-Coulomb equation

$$\left(E - H_D[\mathbf{1}] - H_D[\mathbf{2}] - \frac{e^2}{r_{12}} \right) \Psi = 0, \tag{2.6}$$

where $H_D[\mathbf{j}]$ is the usual Dirac operator acting on the j-th electron:

$$H_D \Psi = \left(\begin{array}{cc} (m+V)I_2 & \vec{\sigma} \cdot \vec{p} \\ \vec{\sigma} \cdot \vec{p} & -(m-V)I_2 \end{array} \right) \left(\begin{array}{c} \Psi^\ell \\ \Psi^s \end{array} \right), \text{ with } V = -\frac{Z}{|\mathbf{r}|}. \tag{2.7}$$

Here, $\vec{\sigma}_j = (\sigma_1, \sigma_2, \sigma_3)$ are Pauli matrices

$$\sigma_1 = \left(\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right), \ \sigma_2 = \left(\begin{array}{cc} 0 & -i \\ i & 0 \end{array} \right), \ \sigma_3 = \left(\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right)$$

and

$$\vec{\sigma} \cdot \vec{p} = \sum_{i=1}^{3} \sigma_i p_i.$$

In the relativistic theory, we have to handle a two-fold tensor product space of $\mathbf{C}^4$-valued functions because the usual Dirac operator acts on four-vectors belonging to $L^2(\mathbf{R}^3; \mathbf{C}^4)$. For $\mathcal{H} = L^2(\mathbf{R}^3; \mathbf{C}^4)$, the two-fold tensor product $\mathcal{H}^{\otimes 2} = \mathcal{H} \otimes \mathcal{H}$ can be identified with

$$\mathcal{H} \otimes \mathcal{H} = \left\{ \psi(1,2) = {}^t(\vec{\psi}_{\ell\ell}, \vec{\psi}_{\ell s}, \vec{\psi}_{s\ell}, \vec{\psi}_{ss}) \in L^2(\mathbf{R}^6; \mathbf{C}^{16}) \mid \vec{\psi}_{ij} \in L^2(\mathbf{R}^6; \mathbf{C}^4) \right\}.$$

Here we have identified $L^2(\mathbf{R}^6; \mathbf{C}^4)$ with $L^2(\mathbf{R}^6; \mathbf{C}^2) \otimes \mathbf{C}^2$ in the following way.
For $\mathbf{k} = 1, 2$, let

$$L^2(\mathbf{R}^3; \mathbf{C}^4) \ni \psi(\mathbf{k}) = \left(\begin{array}{c} \psi_1^\ell(\mathbf{r}_k) \\ \psi_2^\ell(\mathbf{r}_k) \\ \psi_1^s(\mathbf{r}_k) \\ \psi_2^s(\mathbf{r}_k) \end{array} \right) = \left(\psi_1^\ell e_1 + \psi_2^\ell e_2 \right) \otimes f_\ell + \left(\psi_1^s e_1 + \psi_2^s e_2 \right) \otimes f_s,$$

where

$$e_1 = {}^t(1,0), \ e_2 = {}^t(0,1), \ f_\ell = {}^t(1,0), \ f_s = {}^t(0,1).$$

In this notation, we see that any product function

$$\psi(1) \otimes \psi(2) = \sum_{a,b \in \{\ell, s\}} \sum_{i=1}^{2} \sum_{j=1}^{2} \psi_{a,b,i,j}(\mathbf{r}_1, \mathbf{r}_2)(e_i \otimes e_j) \otimes (f_a \otimes f_b) \tag{2.8}$$

satisfies

$$\vec{\psi}_{ab}(\mathbf{r}_1, \mathbf{r}_2) = \left(\begin{array}{c} \psi_{a,b,1,1}(\mathbf{r}_1, \mathbf{r}_2) \\ \psi_{a,b,1,2}(\mathbf{r}_1, \mathbf{r}_2) \\ \psi_{a,b,2,1}(\mathbf{r}_1, \mathbf{r}_2) \\ \psi_{a,b,2,2}(\mathbf{r}_1, \mathbf{r}_2) \end{array} \right) = \left(\begin{array}{c} \psi_1^a(\mathbf{r}_1) \\ \psi_2^a(\mathbf{r}_1) \end{array} \right) \otimes \left(\begin{array}{c} \psi_1^b(\mathbf{r}_2) \\ \psi_2^b(\mathbf{r}_2) \end{array} \right) = \left(\begin{array}{c} \psi_1^a(\mathbf{r}_1)\psi_1^b(\mathbf{r}_2) \\ \psi_1^a(\mathbf{r}_1)\psi_2^b(\mathbf{r}_2) \\ \psi_2^a(\mathbf{r}_1)\psi_1^b(\mathbf{r}_2) \\ \psi_2^a(\mathbf{r}_1)\psi_2^b(\mathbf{r}_2) \end{array} \right)$$

for any a, $b \in \{\ell, s\}$.

Now we shall define two subspaces of $\mathcal{H}^{\otimes 2} = \mathcal{H} \otimes \mathcal{H}$, the anti-symmetric space and symmetric space, denoted by $\mathcal{H}^2_A = \mathcal{H} \otimes_A \mathcal{H}$ and $\mathcal{H}^2_S = \mathcal{H} \otimes_S \mathcal{H}$, respectively.

Definition 2.1

$$\mathcal{H}^2_A = \Big\{ \psi(\mathbf{r}_1, \mathbf{r}_2) = {}^t(\vec{\psi}_{11}, \vec{\psi}_{12}, \vec{\psi}_{21}, \vec{\psi}_{22}) \in L^2(\mathbf{R}^6; \mathbf{C}^{16}) \mid \vec{\psi}_{ij} \in L^2(\mathbf{R}^6; \mathbf{C}^4),$$

$$\psi_{ij} = Mat[\vec{\psi}_{ij}] \in L^2(\mathbf{R}^6; M(2, \mathbf{C})), \ \psi_{k,k}(\mathbf{r}_2, \mathbf{r}_1) = -{}^t\psi_{k,k}(\mathbf{r}_1, \mathbf{r}_2), \ k = 1, 2,$$

$$\psi_{1,2}(\mathbf{r}_2, \mathbf{r}_1) = -{}^t\psi_{2,1}(\mathbf{r}_1, \mathbf{r}_2) \Big\},$$

where

$$Mat[\vec{a}] = \begin{pmatrix} a_1 & a_3 \\ a_2 & a_4 \end{pmatrix} \text{ for } \vec{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} \in \mathbf{C}^4 \qquad (2.9)$$

and ${}^tM$ stands for the transposed matrix of the 2×2 matrix M.

Remark 2.1 *The definition 2.1 coincides with the one in the literature on quantum chemistry ([6], [7]), where a slightly different notation from ours is adopted.*

$$\Psi(1, 2) = \begin{pmatrix} \vec{\Psi}^{\ell\ell}(1, 2) \\ \vec{\Psi}^{\ell s}(1, 2) \\ \vec{\Psi}^{s\ell}(1, 2) \\ \vec{\Psi}^{ss}(1, 2) \end{pmatrix} \text{ with } \begin{array}{l} \vec{\Psi}^{\ell\ell}(1, 2) = -\vec{\Psi}^{\ell\ell}(2, 1) \\ \vec{\Psi}^{\ell s}(1, 2) = -\vec{\Psi}^{s\ell}(2, 1) \\ \vec{\Psi}^{ss}(1, 2) = -\vec{\Psi}^{ss}(2, 1). \end{array} \qquad (2.10)$$

Moreover, it should be pointed out that the four components $\vec{\Psi}^{\ell\ell}$, $\vec{\Psi}^{\ell s}$, $\vec{\Psi}^{s\ell}$, $\vec{\Psi}^{ss}$ in (2.10) are not functions from $\mathbf{R}^3 \otimes \mathbf{R}^3$ to $\mathbf{C}^4$, but they are functions from $(\mathbf{R}^3 \times \{\uparrow, \downarrow\}) \otimes (\mathbf{R}^3 \times \{\uparrow, \downarrow\})$ to $\mathbf{C}$.

In a similar way, we can define the symmetric tensor product space which we shall use in proving our main results.

Definition 2.2

$$\mathcal{H}^2_S = \Big\{ \psi(\mathbf{r}_1, \mathbf{r}_2) = {}^t(\vec{\psi}_{11}, \vec{\psi}_{12}, \vec{\psi}_{21}, \vec{\psi}_{22}) \in L^2(\mathbf{R}^6; \mathbf{C}^{16}) \mid \vec{\psi}_{ij} \in L^2(\mathbf{R}^6; \mathbf{C}^4),$$

$$\psi_{ij} = Mat[\vec{\psi}_{ij}] \in L^2(\mathbf{R}^6; M(2, \mathbf{C})), \ \psi_{k,k}(\mathbf{r}_2, \mathbf{r}_1) = {}^t\psi_{1,1}(\mathbf{r}_1, \mathbf{r}_2), \ k = 1, 2,$$

$$\psi_{1,2}(\mathbf{r}_2, \mathbf{r}_1) = {}^t\psi_{2,1}(\mathbf{r}_1, \mathbf{r}_2) \Big\}.$$

In the matrix formulation, we define the standard inner product of $\mathcal{H}^2_A$ or $\mathcal{H}^2_S$ by

$$\langle F, G \rangle = \sum_{i,j=1}^{2} \int_{\mathbf{R}^6} \text{tr}\big(F_{ij}(\mathbf{r}_1, \mathbf{r}_2){}^t\overline{G_{ij}(\mathbf{r}_1, \mathbf{r}_2)}\big) d\mathbf{r}_1 d\mathbf{r}_2. \qquad (2.11)$$

3 Two-electron Dirac-Coulomb Hamiltonian

Let $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and $\beta = \alpha_0$ be 4×4 Hermitian matrices satisfying anti-commuting relations:

$$\alpha_j \alpha_k + \alpha_k \alpha_j = 2\delta_{jk}, \ 0 \leq j, k \leq 3. \tag{3.1}$$

We denote the Dirac operator for one particle by H_D:

$$H_D = \vec{\alpha} \cdot \vec{p} + m\beta + V(\mathbf{r}), \ V(\mathbf{r}) = \frac{k}{|\mathbf{r}|} I_4, \tag{3.2}$$

where $\vec{p} = {}^t(p_1, p_2, p_3)$, $p_j = -i\partial_{\mathbf{r}_j}$, m is a nonnegative number and $k \in \mathbf{R}$. We shall often use the notation

$$H_0 = \vec{\alpha} \cdot \vec{p} + m\beta. \tag{3.3}$$

Let us consider the Dirac-Coulomb Hamiltonian on $\mathcal{H}_A^2$

$$H_{DC} = H_D \otimes Id + Id \otimes H_D + V_0(\mathbf{r}_1, \mathbf{r}_2), \tag{3.4}$$

where $V_0(\mathbf{r}_1, \mathbf{r}_2) = k_0/|\mathbf{r}_1 - \mathbf{r}_2|$.

Lemma 3.1 *Let*

$$M_j = \begin{pmatrix} B & A_j \\ A_j & -B \end{pmatrix} \in M(2, \mathbf{C}), \ j = 1, 2. \tag{3.5}$$

Then it holds that

$$M_1 \otimes I_2 + I_2 \otimes M_2 = \begin{pmatrix} 2B & A_2 & A_1 & 0 \\ A_2 & 0 & 0 & A_1 \\ A_1 & 0 & 0 & A_2 \\ 0 & A_1 & A_2 & -2B \end{pmatrix}. \tag{3.6}$$

Proof: In general, the Kronecker product of two matrices $X = (x_{ij})$ and $Y = (y_{ij})$ is defined by

$$X \otimes Y = \left(x_{ij} Y \right), \tag{3.7}$$

so that $X \otimes Y$ is a matrix of size $mn \times k\ell$ if X and Y are $m \times n$ and $k \times \ell$ type, respectively.

$$M_1 \otimes I_2 = \begin{pmatrix} B & 0 & A_1 & 0 \\ 0 & B & 0 & A_1 \\ A_1 & 0 & -B & 0 \\ 0 & A_1 & 0 & -B \end{pmatrix}, \quad I_2 \otimes M_2 = \begin{pmatrix} B & A_2 & 0 & 0 \\ A_2 & -B & 0 & 0 \\ 0 & 0 & B & A_2 \\ 0 & 0 & A_2 & -B \end{pmatrix}. \tag{3.8}$$

Q.E.D.

In the previous section, we have defined $\mathcal{H}^{\otimes 2} = \mathcal{H} \otimes \mathcal{H}$ as the 2×2 block-wise tensor product, so that we obtain the following representation of H_{DC} which coincides with the operator in the literature on quantum chemistry ([4], [5], [6]).

Theorem 3.2 *Let* $\mathcal{H}^{\otimes 2} \ni \psi = ^t (\vec{\psi}_{11}, \vec{\psi}_{12}, \vec{\psi}_{21}, \vec{\psi}_{22}) \in L^2(\mathbf{R}^6; \ \mathbf{C}^4)^4$. *Then it holds that*

$$(H_0 \otimes I_4 + I_4 \otimes H_0)\psi = \begin{pmatrix} 2mI_4 & h_2 & h_1 & 0 \\ h_2 & 0 & 0 & h_1 \\ h_1 & 0 & 0 & h_2 \\ 0 & h_1 & h_2 & -2mI_4 \end{pmatrix} \begin{pmatrix} \vec{\psi}_{11} \\ \vec{\psi}_{12} \\ \vec{\psi}_{21} \\ \vec{\psi}_{22} \end{pmatrix}, \qquad (3.9)$$

where

$$h_1 = (\vec{\sigma} \cdot \vec{p}_1) \otimes I_2, \quad h_2 = I_2 \otimes (\vec{\sigma} \cdot \vec{p}_2). \qquad (3.10)$$

Proof: Denote f_ℓ and f_s by **i** and **j**, respectively. Let us consider two elements of $\mathcal{H}^{\otimes 2}$

$$\Psi = \Psi_1(\mathbf{r}) \otimes \mathbf{i} + \Psi_2(\mathbf{r}) \otimes \mathbf{j}, \quad \Psi' = \Psi'_1(\mathbf{r}) \otimes \mathbf{i} + \Psi'_2(\mathbf{r}) \otimes \mathbf{j}, \qquad (3.11)$$

where for $k = 1, 2$,

$$\Psi_k(\mathbf{r}) = \begin{pmatrix} \psi_{k1}(\mathbf{r}) \\ \psi_{k2}(\mathbf{r}) \end{pmatrix}, \quad \Psi'_k(\mathbf{r}) = \begin{pmatrix} \psi'_{k1}(\mathbf{r}) \\ \psi'_{k2}(\mathbf{r}) \end{pmatrix}. \qquad (3.12)$$

We can regard Ψ_k $(k = 1, 2)$ as functions of $\mathbf{x} = (\mathbf{r}, \omega)$ as follows.

$$\Psi_k(\mathbf{r}, \omega) = \psi_{k1}(\mathbf{r})\chi_+(\omega) + \psi_{k2}(\mathbf{r})\chi_-(\omega), \qquad (3.13)$$

where $\chi_\pm$ are two orthonormal functions describing the spin of electrons.
Then it holds that

$$\Psi \otimes \Psi' = \Psi_1 \otimes \Psi'_1 \otimes (\mathbf{i} \otimes \mathbf{i}) + \Psi_1 \otimes \Psi'_2 \otimes (\mathbf{i} \otimes \mathbf{j}) + \Psi_2 \otimes \Psi'_1 \otimes (\mathbf{j} \otimes \mathbf{i}) + \Psi_2 \otimes \Psi'_2 \otimes (\mathbf{j} \otimes \mathbf{j}), \qquad (3.14)$$

where

$$\Psi_k \otimes \Psi'_\ell = \begin{pmatrix} \psi_{k1}(\mathbf{r}_1)\psi'_{\ell 1}(\mathbf{r}_2) \\ \psi_{k1}(\mathbf{r}_1)\psi'_{\ell 2}(\mathbf{r}_2) \\ \psi_{k2}(\mathbf{r}_1)\psi'_{\ell 1}(\mathbf{r}_2) \\ \psi_{k2}(\mathbf{r}_1)\psi'_{\ell 2}(\mathbf{r}_2) \end{pmatrix} \cong \begin{pmatrix} \psi_{k1}(\mathbf{r}_1)\psi'_{\ell 1}(\mathbf{r}_2) & \psi_{k2}(\mathbf{r}_1)\psi'_{\ell 1}(\mathbf{r}_2) \\ \psi_{k1}(\mathbf{r}_1)\psi'_{\ell 2}(\mathbf{r}_2) & \psi_{k2}(\mathbf{r}_1)\psi'_{\ell 2}(\mathbf{r}_2) \end{pmatrix}. \qquad (3.15)$$

We see that

$$(H_0 \otimes Id)(\Psi \otimes \Psi') = (H_0\Psi) \otimes \Psi'$$
$$= \left\{ (\vec{\sigma} \cdot \vec{p}\Psi_2 + mI_2\Psi_1)\mathbf{i} + (\vec{\sigma} \cdot \vec{p}\Psi_1 - mI_2\Psi_2)\mathbf{j} \right\} \otimes (\Psi'_1\mathbf{i} + \Psi'_2\mathbf{j})$$
$$= [(\vec{\sigma} \cdot \vec{p}\Psi_2 + mI_2\Psi_1) \otimes \Psi'_1] \otimes (\mathbf{i} \otimes \mathbf{i}) + [(\vec{\sigma} \cdot \vec{p}\Psi_2 + mI_2\Psi_1) \otimes \Psi'_2] \otimes (\mathbf{i} \otimes \mathbf{j})$$
$$+ [(\vec{\sigma} \cdot \vec{p}\Psi_1 - mI_2\Psi_2) \otimes \Psi'_1] \otimes (\mathbf{j} \otimes \mathbf{i}) + [(\vec{\sigma} \cdot \vec{p}\Psi_1 - mI_2\Psi_2) \otimes \Psi'_2] \otimes (\mathbf{j} \otimes \mathbf{j}).$$
$$(3.16)$$

Since the four vectors $\mathbf{i} \otimes \mathbf{i}$, $\mathbf{i} \otimes \mathbf{j}$, $\mathbf{j} \otimes \mathbf{i}$, $\mathbf{j} \otimes \mathbf{j}$ are linearly independent in $\mathcal{H}^{\otimes 2}$, it holds that

$$(H_0 \otimes Id)(\Psi \otimes \Psi') = \begin{pmatrix} (\vec{\sigma} \cdot \vec{p}\Psi_2 + mI_2\Psi_1) \otimes \Psi'_1 \\ (\vec{\sigma} \cdot \vec{p}\Psi_2 + mI_2\Psi_1) \otimes \Psi'_2 \\ (\vec{\sigma} \cdot \vec{p}\Psi_1 - mI_2\Psi_2) \otimes \Psi'_1 \\ (\vec{\sigma} \cdot \vec{p}\Psi_1 - mI_2\Psi_2) \otimes \Psi'_2 \end{pmatrix}$$

$$= \begin{pmatrix} mI_2 & 0 & (\vec{\sigma} \cdot \vec{p}) \otimes I_2 & 0 \\ 0 & mI_2 & 0 & (\vec{\sigma} \cdot \vec{p}) \otimes I_2 \\ (\vec{\sigma} \cdot \vec{p}) \otimes I_2 & 0 & -mI_2 & 0 \\ 0 & (\vec{\sigma} \cdot \vec{p}) \otimes I_2 & 0 & -mI_2 \end{pmatrix} \begin{pmatrix} \Psi_1 \otimes \Psi'_1 \\ \Psi_1 \otimes \Psi'_2 \\ \Psi_2 \otimes \Psi'_1 \\ \Psi_2 \otimes \Psi'_2 \end{pmatrix}. \tag{3.17}$$

Similarly, the identity

$$(Id \otimes H_0)(\Psi \otimes \Psi') = \Psi \otimes (H_0 \Psi') = \left(\Psi_1 \mathbf{i} + \Psi_2 \mathbf{j}\right) \otimes \left\{(\vec{\sigma} \cdot \vec{p}\Psi'_2 + mI_2\Psi'_1)\mathbf{i} + (\vec{\sigma} \cdot \vec{p}\Psi'_1 - mI_2\Psi'_2)\mathbf{j}\right\} \tag{3.18}$$

implies

$$(Id \otimes H_0)(\Psi \otimes \Psi')$$
$$= \begin{pmatrix} mI_2 & I_2 \otimes (\vec{\sigma} \cdot \vec{p}) & 0 & 0 \\ I_2 \otimes (\vec{\sigma} \cdot \vec{p}) & -mI_2 & 0 & 0 \\ 0 & 0 & mI_2 & I_2 \otimes (\vec{\sigma} \cdot \vec{p}) \\ 0 & 0 & I_2 \otimes (\vec{\sigma} \cdot \vec{p}) & -mI_2 \end{pmatrix} \begin{pmatrix} \Psi_1 \otimes \Psi'_1 \\ \Psi_1 \otimes \Psi'_2 \\ \Psi_2 \otimes \Psi'_1 \\ \Psi_2 \otimes \Psi'_2 \end{pmatrix}. \tag{3.19}$$

Q.E.D.

4 Main results

For simplicity we assume that $c = 1$. Instead of the original H_{DC}, we consider a slightly general operator, keeping the same notation H_{DC}, with two real parameters k and k_0 as follows.

$$H_{DC} = H \otimes I + I \otimes H + \frac{k_0}{|\mathbf{r}_1 - \mathbf{r}_2|}, \tag{4.1}$$

where $H = \vec{\alpha} \cdot \vec{p} + m\beta - k/|\mathbf{r}|$.

The spectral properties of the usual Dirac operator H are well investigated (For precise informations, see [9]). Let $m > 0$. Then we know

1. H is essentially selfadjoint on $(C_0^\infty(\mathbf{R}^3)^4)$ if $|k| \le \sqrt{3}/2$.

2. $\sigma_{ess}(H) = \mathbf{R}\backslash(-m, m)$ if $|k| \le \sqrt{3}/2$.

3. If $|k| \le \sqrt{3}/2$, then H has no eigenvalues in $\mathbf{R}\backslash(-m, m)$ and there are countable eigenvalues in $(-m, m)$ whose only accumulating points are $\pm m$.

As for essential self-adjointness, when the scalar potential $k/|\mathbf{r}|$ is replaced by any symmetric matrix potential $V(\mathbf{r})$ satisfying $|V(\mathbf{r})| \leq k/|\mathbf{r}|$, it holds that

4. $\vec{\alpha}\vec{p} + m\beta + V(\mathbf{r})$ is essentially selfadjoint on $(C_0^\infty(\mathbf{R}^3))^4$ if $|k| \leq 1/2$.

Now we shall state our main results for the H_{DC} Hamiltonian. These are just the first attempts to answer the spectral problem.

Theorem 4.1 *Suppose that $|k| < 1/4$. Then for any real k_0, H_{DC} is essentially selfadjoint on $[C_0^\infty(\mathbf{R}^3 \; ; \; \mathbf{C}^4)]^{\otimes 2} \cap \mathcal{H}_A^2$.*

Remark 4.1 *The same conclusion is true if we replace the Coulomb potential $k/|\mathbf{r}|$ by any symmetric matrix potentials $V(\mathbf{r})$ satisfying*

$$|V(\mathbf{r})| \leq k/|\mathbf{r}|. \tag{4.2}$$

The unique self-adjoint extension is denoted by the same symbol H_{DC} again.

Theorem 4.2 *Suppose that $|k| < 1/4$. Then for any real k_0, it holds that*

$$\sigma_{ess}(H_{DC}|_{\mathcal{H}_A^2}) = \mathbf{R}. \tag{4.3}$$

Theorem 4.3 *Suppose that $|k| < 1/4$. If $k_0 \neq 0$, then $H_{DC}|_{\mathcal{H}_A^2}$ has no eigenvalues in $\mathbf{R}$.*

Remark 4.2 *The restriction $|k| < 1/4$ seems to be too strong because $|k| < \sqrt{3}/2$ is sufficient for the essential self-adjointness for the usual Dirac operators with scalar potentials with finite Coulomb singularities.*

Remark 4.3 *In the next section we will show that the operator H_{DC} on the anti-symmetric tensor product has a matrix representation of order sixteen which is not elliptic.*

We also consider the following simple model operator $\mathbb{H}$

$$\mathbb{H} := \alpha p_1 + \alpha p_2 + 2m\beta + \frac{k_1}{|\mathbf{r}_1|} + \frac{k_2}{|\mathbf{r}_2|} + \frac{k_0}{|\mathbf{r}_1 - \mathbf{r}_2|}, \tag{4.4}$$

which is strongly connected to H_{DC} in terms of 2×2 block tensor product. As for the operator $\mathbb{H}$, we can prove better results than for H_{DC} because after making an orthogonal change of variables in $\mathbf{R}^6$, it can be reduced to the Dirac operator with a double-well potential in $L^2(\mathbf{R}^3; \mathbf{C}^4)$.

Theorem 4.4 *If $|k_j| < \sqrt{3}/2$ $(j = 1, 2)$, $\mathbb{H}$ on $C_0^\infty(\mathbf{R}^6)^4$ is essentially self-adjoint for any $k_0 \in \mathbf{R}$.*

Let $\mathbb{H}$ denote the unique self-adjoint extension again.

Theorem 4.5 *Suppose $k_0 \neq 0$. Then the essential spectrum covers the whole line, that is, $\sigma_{ess}(\mathbb{H}) = \mathbf{R}$.*

Theorem 4.6 *Let $k_0 \neq 0$. Then $\mathbb{H}$ has no eigenvalues, that is, $\sigma_p(\mathbb{H}) = \emptyset$.*

Theorem 4.7 *Let $k_0 \neq 0$. Then the spectrum of $\mathbb{H}$ is purely absolutely continuous.*

5 Canonical form of H_{DC} on the anti-symmetric space

We return to the familiar notation $\mathbf{x}_j$ instead of $\mathbf{r}_j$. We may represent H_{DC} as follows.

$$H_{DC}\Psi = \begin{pmatrix} (2m+V)I_4 & h_2 & h_1 & 0 \\ h_2 & VI_4 & 0 & h_1 \\ h_1 & 0 & VI_4 & h_2 \\ 0 & h_1 & h_2 & -(2m-V)I_4 \end{pmatrix} \begin{pmatrix} \vec{\psi}_{1,1}(\mathbf{x}_1,\mathbf{x}_2) \\ \vec{\psi}_{1,2}(\mathbf{x}_1,\mathbf{x}_2) \\ \vec{\psi}_{2,1}(\mathbf{x}_1,\mathbf{x}_2) \\ \vec{\psi}_{2,2}(\mathbf{x}_1,\mathbf{x}_2) \end{pmatrix}, \quad (5.1)$$

$$V(\mathbf{x}_1,\mathbf{x}_2) = V(\mathbf{x}_1) + V(\mathbf{x}_2) + V_0(\mathbf{x}_1,\mathbf{x}_2). \quad (5.2)$$

Proposition 5.1 *Let* $\Psi \in \mathcal{H}^{\otimes 2} = L^2(\mathbf{R}^6; \ M(2,\mathbf{C}))^4$. *Then it holds that*

$$H_{DC}\Psi = \begin{pmatrix} (2m+V)I_2 & (h)_2 & (h)_1 & 0 \\ (h)_2 & VI_2 & 0 & (h)_1 \\ (h)_1 & 0 & VI_2 & (h)_2 \\ 0 & (h)_1 & (h)_2 & -(2m-V)I_2 \end{pmatrix} \begin{pmatrix} \psi_{1,1}(\mathbf{x}_1,\mathbf{x}_2) \\ \psi_{1,2}(\mathbf{x}_1,\mathbf{x}_2) \\ \psi_{2,1}(\mathbf{x}_1,\mathbf{x}_2) \\ \psi_{2,2}(\mathbf{x}_1,\mathbf{x}_2) \end{pmatrix}, \quad (5.3)$$

where

$$(h)_1\psi_{ij}(\mathbf{x}_1,\mathbf{x}_2) = Mat\left[((\vec{\sigma}\cdot\vec{p}_1)\otimes I_2)\vec{\psi}_{ij}(\mathbf{x}_1,\mathbf{x}_2)\right] = \vec{p}_1\psi_{ij}(\mathbf{x}_1,\mathbf{x}_2)\cdot {}^t\vec{\sigma}, \quad (5.4)$$

$$(h)_2\psi_{ij}(\mathbf{x}_1,\mathbf{x}_2) = Mat\left[((I_2\otimes\vec{\sigma}\cdot\vec{p}_2))\vec{\psi}_{ij}(\mathbf{x}_1,\mathbf{x}_2)\right] = \vec{p}_2\cdot\vec{\sigma}\psi_{ij}(\mathbf{x}_1,\mathbf{x}_2). \quad (5.5)$$

Proof: Let

$$\mathrm{vec}\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a \\ c \\ b \\ d \end{pmatrix}. \quad (5.6)$$

It follows that

$$Mat\left[(A\otimes I_2)\mathrm{vec}M\right] = M\,{}^t A, \quad Mat[(I\otimes B)\mathrm{vec}M] = BM \quad (5.7)$$

for any 2×2 matrices A and $M = (\Psi_k \otimes \Psi'_\ell)$, we arrive at the conclusion. Q.E.D.

Proposition 5.2 $\mathcal{H}_A^2$ *is an invariant subspace of* $\mathcal{H}^{\otimes 2} = \mathcal{H}\otimes\mathcal{H}$ *with respect to the operator* H_{DC}.

Proof: If $\psi_{12}(\mathbf{x}_2,\mathbf{x}_1) = -({}^t\psi_{21})(\mathbf{x}_1,\mathbf{x}_2)$, then $(\vec{p}_2\psi_{12})(\mathbf{x}_2,\mathbf{x}_1) = -(\vec{p}_1\,{}^t\psi_{21})(\mathbf{x}_1,\mathbf{x}_2)$. We shall check the first component of $H_{DC}\Psi$. Recall

$$h_1 = (\vec{\sigma}\cdot\vec{p}_1)\otimes I_2, \quad h_2 = I_2\otimes(\vec{\sigma}\cdot\vec{p}_2). \quad (5.8)$$

It holds that

$$\big((h)_2\psi_{12} + (h)_1\psi_{21}\big)(\mathbf{x}_2, \mathbf{x}_1) = \vec{\sigma}\cdot\vec{p}_2\psi_{12}(\mathbf{x}_2, \mathbf{x}_1) + \sum_{j=1}^{3} p_{1,j}\psi_{21}(\mathbf{x}_2, \mathbf{x}_1)({}^t\sigma_j)$$

$$= -\vec{\sigma}\cdot\vec{p}_1({}^t\psi_{21})(\mathbf{x}_1, \mathbf{x}_2) - \sum_{j=1}^{3} p_{2,j}({}^t\psi_{12})(\mathbf{x}_1, \mathbf{x}_2)({}^t\sigma_j)$$

$$= -{}^t\big((h)_1\psi_{21}\big)(\mathbf{x}_1, \mathbf{x}_2) - {}^t\big((h)_2\psi_{12}\big)(\mathbf{x}_1, \mathbf{x}_2)$$

$$= -{}^t\big((h)_2\psi_{12} + (h)_1\psi_{21}\big)(\mathbf{x}_1, \mathbf{x}_2). \tag{5.9}$$

As for the second component, it is seen that

$$\big((h)_2\psi_{11} + (h)_1\psi_{22}\big)(\mathbf{x}_2, \mathbf{x}_1) = \vec{\sigma}\cdot\vec{p}_2\psi_{11}(\mathbf{x}_2, \mathbf{x}_1) + \sum_{j=1}^{3} p_{1,j}\psi_{22}(\mathbf{x}_2, \mathbf{x}_1)({}^t\sigma_j)$$

$$= -\vec{\sigma}\cdot\vec{p}_1({}^t\psi_{11})(\mathbf{x}_1, \mathbf{x}_2) - \sum_{j=1}^{3} p_{2,j}({}^t\psi_{22})(\mathbf{x}_1, \mathbf{x}_2)({}^t\sigma_j)$$

$$= -{}^t\big((h)_1\psi_{11}\big)(\mathbf{x}_1, \mathbf{x}_2) - {}^t\big((h)_2\psi_{22}\big)(\mathbf{x}_1, \mathbf{x}_2)$$

$$= -{}^t\big((h)_2\psi_{11} + (h)_1\psi_{22}\big)(\mathbf{x}_1, \mathbf{x}_2). \tag{5.10}$$

As for the third and fourth components, the similar computations yield

$$\big((h)_1\psi_{11} + (h)_2\psi_{22}\big)(\mathbf{x}_2, \mathbf{x}_1) = -{}^t\big((h)_1\psi_{11} + (h)_2\psi_{22}\big)(\mathbf{x}_1, \mathbf{x}_2) \tag{5.11}$$

and

$$\big((h)_1\psi_{12} + (h)_2\psi_{21}\big)(\mathbf{x}_2, \mathbf{x}_1) = -{}^t\big((h)_1\psi_{12} + (h)_2\psi_{21}\big)(\mathbf{x}_1, \mathbf{x}_2). \tag{5.12}$$

Q.E.D.

We shall make an orthogonal change of coordinates

$$\frac{1}{\sqrt{2}}(\mathbf{x}_1 + \mathbf{x}_2) = \mathbf{y}_1, \quad \frac{1}{\sqrt{2}}(\mathbf{x}_1 - \mathbf{x}_2) = \mathbf{y}_2. \tag{5.13}$$

It holds that

$$V(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{2}k\left(\frac{1}{|\mathbf{y}_2 - \mathbf{y}_1|} + \frac{1}{|\mathbf{y}_2 + \mathbf{y}_1|}\right) + \frac{k_0}{\sqrt{2}|\mathbf{y}_2|}. \tag{5.14}$$

and

$$\vec{p}_{\mathbf{x}_1} = \frac{1}{\sqrt{2}}(\vec{p}_{\mathbf{y}_1} + \vec{p}_{\mathbf{y}_2}), \quad \vec{p}_{\mathbf{x}_2} = \frac{1}{\sqrt{2}}(\vec{p}_{\mathbf{y}_1} - \vec{p}_{\mathbf{y}_2}). \tag{5.15}$$

In the new coordinates $(\mathbf{y}_1, \mathbf{y}_2)$ we have the following representation.

Theorem 5.3 *Let*

$$\widetilde{H}_{DC}\Psi = \begin{pmatrix} V+2m & h_{12} & h_{21} & 0 \\ h_{12} & V & 0 & h_{21} \\ h_{21} & 0 & V & h_{12} \\ 0 & h_{21} & h_{12} & V-2m \end{pmatrix} \begin{pmatrix} \vec{\psi}_{1,1}(\mathbf{y}_1,\mathbf{y}_2) \\ \vec{\psi}_{1,2}(\mathbf{y}_1,\mathbf{y}_2) \\ \vec{\psi}_{2,1}(\mathbf{y}_1,\mathbf{y}_2) \\ \vec{\psi}_{2,2}(\mathbf{y}_1,\mathbf{y}_2) \end{pmatrix} \tag{5.16}$$

with

$$h_{12} = \frac{1}{\sqrt{2}} I_2 \otimes \vec{\sigma} \cdot \vec{p}_{\mathbf{y}_1}, \quad h_{21} = \frac{1}{\sqrt{2}}\vec{\sigma} \cdot \vec{p}_{\mathbf{y}_1} \otimes I_2. \tag{5.17}$$

If $\Psi, \Phi \in \mathcal{H}_A^2$, *then*

$$\langle H_{DC}\Psi, \Phi \rangle = \langle \widetilde{H}_{DC}\Psi, \Phi \rangle. \tag{5.18}$$

The anti-symmetric property implies the following identities.

Lemma 5.4 *Suppose that* $F, G \in \mathcal{H}_A^2$. *Then for any quartet of indices* i, j, k, ℓ,

$$\langle (\vec{\sigma} \cdot \vec{p}_1 \otimes I_2)\vec{F}_{ij}, \vec{G}_{k\ell} \rangle = \langle (I_2 \otimes \vec{\sigma} \cdot \vec{p}_2)\vec{F}_{ji}, \vec{G}_{\ell k} \rangle, \quad \langle V\vec{F}_{ij}, \vec{G}_{ij} \rangle = \langle V\vec{F}_{ji}, \vec{G}_{ji} \rangle \tag{5.19}$$

if V *is a diagonal matrix satisfying*

$$V(\mathbf{x}_1,\mathbf{x}_2) = V(\mathbf{x}_2,\mathbf{x}_1). \tag{5.20}$$

Proof: Let $\mathbf{x}_j = (\mathbf{x}_j^{(1)}, \mathbf{x}_j^{(2)}, \mathbf{x}_j^{(3)})$, $j = 1,2$. Both $\psi \in \mathcal{H}_S^2$ and $\varphi \in \mathcal{H}_A^2$ satisfy that for any $i,j = 1,2$ and $n = 1,2,3$

$$\partial_{\mathbf{x}_2^{(n)}} \vec{\psi}_{ij}(\mathbf{x}_1,\mathbf{x}_2) = \text{vec}[\partial_{\mathbf{x}_1^{(n)}} {}^t\psi_{ji}](\mathbf{x}_2,\mathbf{x}_1), \quad \partial_{\mathbf{x}_2^{(n)}} \vec{\varphi}_{ij}(\mathbf{x}_1,\mathbf{x}_2) = -\text{vec}[\partial_{\mathbf{x}_1^{(n)}} {}^t\varphi_{ji}](\mathbf{x}_2,\mathbf{x}_1). \tag{5.21}$$

Hence for any ψ, $\varphi \in \mathcal{H}_S^2$,

$$\langle (I_2 \otimes \vec{\sigma} \cdot \nabla_{\mathbf{x}_2}\vec{\psi}_{ij})(\mathbf{x}_1,\mathbf{x}_2), \vec{\varphi}_{k\ell}(\mathbf{x}_1,\mathbf{x}_2) \rangle$$

$$= \int_{\mathbf{R}^6} tr\big((\vec{\sigma} \cdot \nabla_{\mathbf{x}_2}\psi_{ij})(\mathbf{x}_1,\mathbf{x}_2) \, {}^t\overline{\varphi}_{k\ell}(\mathbf{x}_1,\mathbf{x}_2)\big) d\mathbf{x}_1 d\mathbf{x}_2$$

$$= \int_{\mathbf{R}^6} tr\big(\vec{\sigma} \cdot \nabla_{\mathbf{x}_1} \, {}^t\psi_{ji}(\mathbf{x}_2,\mathbf{x}_1) \, \overline{\varphi}_{\ell k}(\mathbf{x}_2,\mathbf{x}_1)\big) d\mathbf{x}_1 d\mathbf{x}_2$$

$$= \int_{\mathbf{R}^6} tr\big((\nabla_{\mathbf{x}_1}\psi_{ji}(\mathbf{x}_2,\mathbf{x}_1) \cdot {}^t\sigma) \, {}^t\overline{\varphi}_{\ell k}(\mathbf{x}_2,\mathbf{x}_1)\big) d\mathbf{x}_2 d\mathbf{x}_1$$

$$= \langle \vec{\sigma} \cdot \nabla_{\mathbf{x}_1} \otimes I_2\vec{\psi}_{ji}(\mathbf{x}_1,\mathbf{x}_2), \vec{\varphi}_{\ell k}(\mathbf{x}_1,\mathbf{x}_2) \rangle. \tag{5.22}$$

Here, we have used

$$tr(AB) = tr({}^t(AB)) = tr({}^tB \, {}^tA) = tr({}^tA \, {}^tB). \tag{5.23}$$

Similarly, we see that for any ψ, $\varphi \in \mathcal{H}_A^2$,

$$\langle (I_2 \otimes \vec{\sigma} \cdot \nabla_{\mathbf{x}_2}\vec{\psi}_{ij})(\mathbf{x}_1,\mathbf{x}_2), \vec{\varphi}_{k\ell}(\mathbf{x}_1,\mathbf{x}_2) \rangle$$

$$= \langle \vec{\sigma} \cdot \nabla_{\mathbf{x}_1} \otimes I_2\vec{\psi}_{ji}(\mathbf{x}_1,\mathbf{x}_2), \vec{\varphi}_{\ell k}(\mathbf{x}_1,\mathbf{x}_2) \rangle. \tag{5.24}$$

Proof of Theorem 5.3 We shall calculate delicate terms of the inner product. First, consider the inner product of the first components of $h_{DC}\Psi$ and Φ:

$$\langle h_2\vec{\psi}_{12} + h_1\vec{\psi}_{21}, \vec{\phi}_{11}\rangle = \frac{1}{\sqrt{2}}\Big(\langle I_2 \otimes \vec{\sigma}\cdot\vec{p}_{\mathbf{y}_1}\vec{\psi}_{12}, \vec{\phi}_{11}\rangle + \langle\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_1}\otimes I_2\vec{\psi}_{21}, \vec{\phi}_{11}\rangle\Big)$$

$$+ \frac{1}{\sqrt{2}}\Big(-\langle I_2\otimes\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\vec{\psi}_{12}, \vec{\phi}_{11}\rangle + \langle\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\otimes I_2\vec{\psi}_{21}, \vec{\phi}_{11}\rangle\Big).$$

$$(5.25)$$

By virtue of Lemma 5.4, it holds that

$$-\langle I_2\otimes\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\vec{\psi}_{12}, \vec{\phi}_{11}\rangle + \langle\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\otimes I_2\vec{\psi}_{21}, \vec{\phi}_{11}\rangle = 0. \qquad (5.26)$$

Next consider the sum of the second and the third components of $h_{DC}\Psi$ and Φ:

$$\langle h_2\vec{\psi}_{11} + h_1\vec{\psi}_{22}, \vec{\phi}_{12}\rangle + \langle h_1\vec{\psi}_{11} + h_2\vec{\psi}_{22}, \vec{\phi}_{21}\rangle$$

$$= \frac{1}{\sqrt{2}}\Big(\langle I_2\otimes\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_1}\vec{\psi}_{11}, \vec{\phi}_{12}\rangle + \langle I_2\otimes\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_1}\vec{\psi}_{22}, \vec{\phi}_{21}\rangle$$

$$+ \langle\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_1}\otimes I_2\vec{\psi}_{22}, \vec{\phi}_{12}\rangle + \langle\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_1}\otimes I_2\vec{\psi}_{11}, \vec{\phi}_{21}\rangle\Big)$$

$$+ \frac{1}{\sqrt{2}}\Big(\langle -I_2\otimes\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\vec{\psi}_{11}, \vec{\phi}_{12}\rangle + \langle -I_2\otimes\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\vec{\psi}_{22}, \vec{\phi}_{21}\rangle$$

$$+ \langle\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\otimes I_2\vec{\psi}_{22}, \vec{\phi}_{12}\rangle + \langle\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\otimes I_2\vec{\psi}_{11}, \vec{\phi}_{21}\rangle\Big). \qquad (5.27)$$

By virtue of Lemma 5.4, it holds that

$$\langle -I_2\otimes\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\vec{\psi}_{11}, \vec{\phi}_{12}\rangle + \langle -I_2\otimes\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\vec{\psi}_{22}, \vec{\phi}_{21}\rangle$$

$$+ \langle\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\otimes I_2\vec{\psi}_{22}, \vec{\phi}_{12}\rangle + \langle\vec{\sigma}\cdot\vec{p}_{\mathbf{y}_2}\otimes I_2\vec{\psi}_{11}, \vec{\phi}_{21}\rangle = 0. \qquad (5.28)$$

The fourth components can be calculated by the same manner as for the first components. $\hspace{2cm}$ Q.E.D.

Theorem 5.5 *Let T_1 and T_2 be two orthogonal transformations in $M(16, \mathbf{C})$ such that*

$$T_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} I_8 & I_8 \\ I_8 & -I_8 \end{pmatrix}, \quad T_2 = S \oplus S, \quad S = \frac{1}{\sqrt{2}}\begin{pmatrix} I_4 & I_4 \\ I_4 & -I_4 \end{pmatrix}. \qquad (5.29)$$

Then it holds that

$$T_2^{-1}T_1^{-1}H_{DC}T_1T_2$$

$$= \begin{pmatrix} h_{12} + h_{21} + V & mI_4 & mI_4 & 0 \\ mI_4 & -h_{12} + h_{21} + V & 0 & mI_4 \\ mI_4 & 0 & h_{12} - h_{21} + V & mI_4 \\ 0 & mI_4 & mI_4 & -h_{12} - h_{21} + V \end{pmatrix}$$

$$(5.30)$$

with

$$V(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{2}k\left(\frac{1}{|\mathbf{y}_2 - \mathbf{y}_1|} + \frac{1}{|\mathbf{y}_2 + \mathbf{y}_1|}\right) + \frac{k_0}{\sqrt{2}|\mathbf{y}_2|}. \tag{5.31}$$

Remark 5.1 *The eigenvalues of the symbol of the operator H_{DC} with $V = 0$ are*

$$0, \quad \sqrt{2|\sigma(D_{\mathbf{y}_1})|^2 + 4m^2}, \quad -\sqrt{2|\sigma(D_{\mathbf{y}_1})|^2 + 4m^2}$$

with multiplicity 8, 4, 4, respectively. Here, $\sigma(D_{\mathbf{y}_1})(\xi) = \xi \in \mathbf{R}^3$ denotes the vector-valued symbol of $D_{\mathbf{y}_1}$.

$$D_{\mathbf{y}_1} u = (2\pi)^{-3} \int_{\mathbf{R}^3 \times \mathbf{R}^3} e^{i(\mathbf{y}_1 - z)\cdot \xi} \xi u(z) dz d\xi \tag{5.32}$$

for $u \in C_0^\infty(\mathbf{R}^3; \ \mathbf{C})$.

6 Proofs of spectral properties of H_{DC}

6.1 Essential self-adjointness

Proof of Theorem 4.1: In view of Theorem 5.3, we can identify H_{DC} with $\tilde{H}_{DC}$. Hereafter we use the same notation H_{DC} instead of $\tilde{H}_{DC}$.

Lemma 6.1 *Let $\varphi(t) \in C^\infty(\mathbf{R}) \cap L^\infty(\mathbf{R})$. Then*

$$[H_{DC}, \varphi(|\mathbf{x}_1 - \mathbf{x}_2|)] = 0. \tag{6.1}$$

Let $\chi \in C_0^\infty(\mathbf{R})$ satisfy that $0 \le \chi \le 1$,

$$\chi(t) = \begin{cases} 1, & t \ge 2, \\ 0, & t \le 1, \end{cases} \tag{6.2}$$

and B_n be a multiplication operator defined by $B_n = \chi(n|\mathbf{x}_1 - \mathbf{x}_2|)$ and

$$V_n = B_n V B_n. \tag{6.3}$$

Lemma 6.2 *$H_{DC,n} = H_{DC,0} + V_n$ is essentially selfadjoint on $[C_0^\infty(\mathbf{R}^3; \ \mathbf{C}^4)]^{\otimes 2} \cap \mathcal{H}_A^2$.*

Lemma 6.3

$$\lim_{n \to \infty} (H^* B_n \psi, \psi - B_n \psi) = 0 \tag{6.4}$$

for any $\psi \in D(H^*)$.

Thanks to Theorem 5.2 of Thaller [10], from Lemma 6.2 and Lemma 6.3, it follows that H_{DC} is also essentially selfadjoint on $[C_0^\infty(\mathbf{R}^3; \ \mathbf{C}^4)]^{\otimes 2} \cap \mathcal{H}_A^2$.

In order to prove Lemma 6.2, it suffices to prove that H_{DC} is essentially self-adjoint in $\mathcal{H}^{\otimes 2}$ because $[C_0^\infty(\mathbf{R}^3; \ \mathbf{C}^4)]^{\otimes 2} \cap \mathcal{H}_A^2$ is an invariant subspace.

We consider an orthogonal transformation T_1 in $M(16, \mathbf{C})$

$$T_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} I_8 & I_8 \\ I_8 & -I_8 \end{pmatrix}. \tag{6.5}$$

Then it holds that

$$T_1^{-1} \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} T_1 = \frac{1}{2} \begin{pmatrix} a+b & a-b \\ a-b & a+b \end{pmatrix}, \tag{6.6}$$

$$T_1^{-1} \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix} T_1 = \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix}, \tag{6.7}$$

so that it follows from Theorem 5.3 that

$$T_1^{-1} H_{DC,n} T_1 = \begin{pmatrix} h_{21} + V_n + m & h_{12} & m & 0 \\ h_{12} & h_{21} + V_n - m & 0 & m \\ m & 0 & -h_{21} + V_n + m & h_{12} \\ 0 & m & h_{12} & -h_{21} + V_n - m \end{pmatrix}. \tag{6.8}$$

Let us consider an orthogonal transformation T_2 in $M(16, \mathbf{C})$

$$T_2 = S \oplus S, \quad S = \frac{1}{\sqrt{2}} \begin{pmatrix} I_4 & I_4 \\ I_4 & -I_4 \end{pmatrix}. \tag{6.9}$$

Then it holds that

$$T_2^{-1} T_1^{-1} H_{DC,n} T_1 T_2$$

$$= \begin{pmatrix} h_{12} + h_{21} + V_n & mI_4 & mI_4 & 0 \\ mI_4 & -h_{12} + h_{21} + V_n & 0 & mI_4 \\ mI_4 & 0 & h_{12} - h_{21} + V_n & mI_4 \\ 0 & mI_4 & mI_4 & -h_{12} - h_{21} + V_n \end{pmatrix}$$

$$= \begin{pmatrix} H_{11} & H_{12} & H_{13} & H_{14} \\ H_{21} & H_{22} & H_{23} & H_{24} \\ H_{31} & H_{32} & H_{33} & H_{34} \\ H_{41} & H_{42} & H_{43} & H_{44} \end{pmatrix} + V_n I_{16}. \tag{6.10}$$

Now we may assume that $m = 0$ because any bounded perturbation does not affect the essential self-adjointness of our operator. Then $H_{DC,1}$ can be reduced to four types of operators H_{jj} ($j = 1, 2, 3, 4$) acting on $L^2(\mathbf{R}^6)^4 = L^2(\mathbf{R}^6)^{2 \times 2}$, where

$$H_{11} = h_{12} + h_{21} = \sqrt{2}^{-1} \left[I_2 \otimes (\vec{\sigma} \cdot \vec{p}_1) + (\vec{\sigma} \cdot \vec{p}_1) \otimes I_2 \right], \tag{6.11}$$

$$H_{22} = -h_{12} + h_{21} = \sqrt{2}^{-1} \left[- I_2 \otimes (\vec{\sigma} \cdot \vec{p}_1) + (\vec{\sigma} \cdot \vec{p}_1) \otimes I_2 \right], \tag{6.12}$$

$$H_{33} = -H_{22}, \quad H_{44} = -H_{11}. \tag{6.13}$$

recall $\vec{p}_1 = -i \nabla_{\mathbf{y}_1}$.

We shall diagonalize H_{jj} by using a unitary transformation. For $\mathbf{y}_1 = (\eta_1, \eta_2, \eta_3)$ define $p_j = -i\partial_{\eta_j}$. Then it holds that

$$\vec{\sigma} \cdot \vec{p} = \begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix}, \tag{6.14}$$

The two by two matrix operator $\vec{\sigma} \cdot \vec{p}$ is formally supersymmetric, so that it can be diagonalized by a unitary transformation (cf. [9]).

Lemma 6.4 *Let*

$$\sigma' = (\sigma_1, \sigma_2), \quad p' = (p_1, p_2), \quad \sigma_3 = \beta_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{6.15}$$

and define a unitary transformation U in $L^2(\mathbf{R}_{\mathbf{y}_1}^3)^2$ by

$$U = \frac{(|p| + p_3)I_2 - \beta_2\sigma' \cdot p'}{\sqrt{(|p| + p_3)^2 + |p'|^2}}, \quad U^{-1} = \frac{(|p| + p_3)I_2 + \beta_2\sigma' \cdot p'}{\sqrt{(|p| + p_3)^2 + |p'|^2}}. \tag{6.16}$$

Then it holds that

$$(\vec{\sigma} \cdot \vec{p})U = U|\vec{p}|\beta_2. \tag{6.17}$$

Remark 6.1 *Each element of U is defined as a Fourier multiplier.*

$$a(D_x)u(x) = (2\pi)^{-3} \iint_{\mathbf{R}^6} e^{i(x-y)\cdot\xi} a(\xi)u(y)dyd\xi, \quad u \in L^2(\mathbf{R}; \ \mathbf{C}). \tag{6.18}$$

Proof: In view of $\vec{\sigma} \cdot \vec{p} = \sigma' \cdot p' + p_3\beta_2$, it holds that

$$(\vec{\sigma} \cdot \vec{p})\{(|p| + p_3)I_2 - \beta_2\sigma' \cdot p'\} = \beta_2|p|^2 + |p|\sigma' \cdot p' + p_3|p|\beta_2$$
$$= \{(|p| + p_3)I - \beta_2\sigma' \cdot p'\}|p|\beta_2, \tag{6.19}$$
$$\{(|p| + p_3)I_2 - \beta_2\sigma' \cdot p'\}\{(|p| + p_3)I_2 - \beta_2\sigma' \cdot p'\}^*$$
$$= \{(|p| + p_3)I_2 - \beta_2\sigma' \cdot p'\}\{(|p| + p_3)I_2 + \beta_2\sigma' \cdot p'\}$$
$$= (|p| + p_3)^2 + |p'|^2. \tag{6.20}$$

Q.E.D.

Proposition 6.5 *Let $T = U \otimes U$ and $\psi = {}^t(\psi_{11}, \psi_{12}, \psi_{21}, \psi_{22}) \in L^2(\mathbf{R}^6; \ \mathbf{C}^4)$. Then, we see that*

$$\sqrt{2}H_{22}T\psi = T\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2|p| & 0 & 0 \\ 0 & 0 & -2|p| & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\psi, \quad \sqrt{2}H_{11}T\psi = T\begin{pmatrix} 2|p| & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2|p| \end{pmatrix}\psi.$$
$$\tag{6.21}$$

Proof: We shall use the following unitary transformations in $L^2(\mathbf{R}^3)^4$.

$$U_1 = U \otimes I_2, \quad U_2 = I_2 \otimes U = U \oplus U. \tag{6.22}$$

Then it follows that

$$\{(\sigma' \cdot p' + p_3\beta_2) \otimes I_2\}U_1 = U_1|p|\beta = U_1\{|p|I_2 \oplus (-|p|I_2)\} \tag{6.23}$$

and

$$\{I_2 \otimes \vec{\sigma} \cdot \vec{p}\}U_2 = (\vec{\sigma} \cdot \vec{p} \oplus \vec{\sigma} \cdot \vec{p})U_2 = U_2(|p|\beta_2 \oplus |p|\beta_2). \tag{6.24}$$

Therefore, we see that

$$\sqrt{2}h_{12}U_2 = U_2 \begin{pmatrix} |p|\beta_2 & 0 \\ 0 & |p|\beta_2 \end{pmatrix} = (I_2 \otimes U)(I_2 \otimes |p|\beta_2), \tag{6.25}$$

$$\sqrt{2}h_{21}U_1 = U_1 \begin{pmatrix} |p|I_2 & 0 \\ 0 & -|p|I_2 \end{pmatrix} = (U \otimes I_2)(|p|\beta_2 \otimes I_2). \tag{6.26}$$

Hence it holds that

$$\sqrt{2}H_{22}T = T\{-I_2 \otimes |p|\beta_2 + |p|\beta_2 \otimes I_2\} \tag{6.27}$$

and

$$\sqrt{2}H_{11}T = T\{I_2 \otimes |p|\beta_2 + |p|\beta_2 \otimes I_2\}. \tag{6.28}$$

Q.E.D.

From this proposition, it follows that $(H_{22} + V_n I_4)\Psi_1 = f_1$ is reduced finally to an equation in $L^2(\mathbf{R}^6; \mathbf{C}^4)$

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \sqrt{2}|p| & 0 & 0 \\ 0 & 0 & -\sqrt{2}|p| & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \psi + \tilde{V}_n\psi = \tilde{f}_1, \tag{6.29}$$

with

$$\tilde{V}_n = T^{-1}V_nT, \quad \tilde{f}_1 = T^{-1}f_1T, \quad T^{-1}\Psi_1 = \psi = {}^t(\psi_{11}, \psi_{12}, \psi_{21}, \psi_{22}). \tag{6.30}$$

Similarly, $(H_{11} + V_n)\Psi_2 = f_2$ is reduced finally to

$$\begin{pmatrix} \sqrt{2}|p| & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{2}|p| \end{pmatrix} \psi + \tilde{V}_n\psi = \tilde{f}_2 \tag{6.31}$$

with $T^{-1}\Psi_2 = \psi$.

Let H be H_{11} or H_{22}, and P and Q are orthogonal projections of $L^2(\mathbf{R}^3)^4$ such that

$$P + Q = Id, \quad PQ = QP = 0 \tag{6.32}$$

and P and Q are invariant with respect to H. We may assume that by suitable choices of P and Q

$$(T^{-1}HT)P = \begin{pmatrix} \sqrt{2}|p| & 0 & 0 & 0 \\ 0 & -\sqrt{2}|p| & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (T^{-1}HT)Q = 0. \tag{6.33}$$

Therefore, each of the equations (6.29) and (6.31) can be represented as follows.

$$H(P,Q) = \begin{pmatrix} K(P) + P\tilde{V}_n P & P\tilde{V}_n Q \\ Q\tilde{V}_n P & Q\tilde{V}_n Q \end{pmatrix} \psi = f, \tag{6.34}$$

where

$$K(p) = \sqrt{2} \begin{pmatrix} |p| & 0 \\ 0 & -|p| \end{pmatrix}. \tag{6.35}$$

Recall

$$T\tilde{V}_n T^{-1} = \chi(n|\mathbf{y_2}|) \left[\frac{\sqrt{2}k}{|\mathbf{y_2} - \mathbf{y_1}|} + \frac{\sqrt{2}k}{|\mathbf{y_2} + \mathbf{y_1}|} + \frac{k_0}{\sqrt{2}|\mathbf{y_2}|} \right] \chi(n|\mathbf{y_2}|)I_2. \tag{6.36}$$

Lemma 6.6 *Suppose that $|k| < 1/4$. Then, $H(P,Q)$ is essentially self-adjoint.*

Proof: It suffices to show that for sufficiently large μ,

$$\overline{H(P,Q) \pm \mu i I_2} = L^2(\mathbf{R}^3;\ \mathbf{C}^4). \tag{6.37}$$

The equation

$$(H(P,Q) \pm i\mu I_2)\ {}^t(u_1, u_2) = {}^t(f_1, f_2). \tag{6.38}$$

is written as

$$(K(p) + W_{11} \pm \mu i I_2)u_1 + W_{12}u_2 = f_1 \tag{6.39}$$

$$W_{21}u_1 + (W_{22} \pm \mu i I_2)u_2 = f_2, \tag{6.40}$$

where

$$W_{12}^* = W_{21}, \quad W_{11}^* = W_{11}, \quad W_{22}^* = W_{22}. \tag{6.41}$$

Since $K(p) + W_{11}$ and W_{22} are essentially self-adjoint if $|k| < 1/2$, we denote their self-adjoint extension by A_1 and A_2, respectively. Then it holds that the closure of

$$(A_j \pm \mu i I_2)(D(A_j)) = L^2(\mathbf{R}^3;\ \mathbf{C}^2) \tag{6.42}$$

and the inverse $(A_j \pm \mu i I_2)^{-1}$ exists for any $j = 1, 2$. From the equation

$$u_1 = (A_1 \pm \mu i I_2)^{-1}(f_1 - W_{12}u_2), \tag{6.43}$$

it follows that the equation (6.40) gives that

$$W_{21}(A_1 \pm \mu i I_2)^{-1}(f_1 - W_{12}u_2) + (A_2 \pm \mu i I_2)u_2 = f_2. \tag{6.44}$$

Hence, we see that

$$\left(- W_{21}(A_1 \pm \mu i I_2)^{-1} W_{12}(A_2 \pm \mu i I_2)^{-1} + I_2 \right)(A_2 \pm \mu i I_2)u_2$$
$$= f_2 - W_{21}(A_1 \pm \mu i I_2)^{-1} f_1. \tag{6.45}$$

Combining Hardy's inequality with a partition of unity, we see that

$$\|W_{21}u\| \le 2|k|\|\sqrt{2}|\vec{p}|u\| + C_1\|u\| \le 2|k|\|K(p)u\| + C_1\|u\| \tag{6.46}$$

and

$$(1 - 2|k|)\|K(p)u\| \le \|A_1 u\| + C_2\|u\| \tag{6.47}$$

for any $u \in C_0^\infty(\mathbf{R}^3; \ \mathbf{C}^2)$. Therefore, it holds that there exists a positive constant C such that

$$\|W_{21}(A_1 \pm \mu i I_2)^{-1}\| \le \frac{2|k|}{1 - 2|k|} + C\mu^{-1}. \tag{6.48}$$

From

$$\|W_{12}(A_2 \pm \mu i I_2)^{-1}\| \le 1 \tag{6.49}$$

it follows that

$$\|W_{21}(A_1 \pm \mu i I_2)^{-1} W_{12}(A_2 \pm \mu i I_2)^{-1}\| < \frac{2|k|}{1 - 2|k|} + \frac{C}{\mu}. \tag{6.50}$$

Hence if the right hand side of the last inequality is strictly less than 1, then $-W_{21}(A_1 \pm \mu i I_2)^{-1} W_{12}(A_2 \pm \mu i I_2)^{-1} + I_2$ is invertible in $\mathcal{L}\big(L^2(\mathbf{R}^3; \ \mathbf{C}^2)\big)$. In view of (6.43) and (6.45), we can show the surjectivity (6.37) if $|k| < 1/4$ and μ is sufficiently large. Q.E.D.

Lemma 6.7 *Suppose that $|k| < 1/4$. Then for any real k_0, $H(P, Q)$ is essentially selfadjoint on $[C_0^\infty(\mathbf{R}^6; \ \mathbf{C}^2)]^{\otimes 2}$.*

Proof: Because of the cutoff function, the scalar potential V_n has singularities which do not coincide. It is known that a real valued multiplication operator V_n is a selfadjoint operator (cf. (5.3) in Page 92 of [12]), so that the unitarily conjugated operator $T^{-1}V_n T$ is also selfadjoint.

On the other hand, as for the remaining operators, we are able to use a technique similar to the one developed by Vogelsang ([11]); see Lemma 6.8, which is stated below. Q.E.D.

Lemma 6.8 *Let $Q \in L_{\text{loc}}^\infty\big(\mathbf{R}^3 \backslash \{0\}\big)^{4 \times 4}$ be an Hermitian matrix with*

$$|Q(\mathbf{y}_1)| \le \mu|\mathbf{y}_1 - b|^{-1}, \ 0 \le \mu < 1/2, \ b \in \mathbf{R}^3 \tag{6.51}$$

Then for all $v \in H^1(\mathbf{R}^3)^4$ we have

$$\||\mathbf{y}_1 - b|^{-1}v\|_{L^2(\mathbf{R}^6)} \le \frac{2}{1 - 2|\mu|}\|(|\vec{p}_1| + Q(\mathbf{y}_1))v\|_{L^2(\mathbf{R}^6)}. \tag{6.52}$$

Proof: Hardy's inequality implies

$$\| \|\mathbf{y}_1 - b\|^{-1} u \| \leq 2\|\vec{p}_1 v\| = 2\| |\vec{p}_1| v \| \leq 2\|(|\vec{p}_1| + Q)v\| + 2\|Qv\|, \tag{6.53}$$

which means

$$(1 - 2|\mu|)\| \|\mathbf{y}_1 - b\|^{-1} u \| \leq 2\|(|\vec{p}_1| + Q)v\|. \tag{6.54}$$

Q.E.D.

Corollary 6.9 *Suppose that $|k| < 1/4$. Then for any real k_0, H_{DC} is essentially selfadjoint on $[C_0^\infty(\mathbf{R}^6)^4]^{\otimes 2}$.*

Proof: It holds that $H_{DC}T = T(H_{DC,0} + M + \widetilde{V}_n)$, where

$$H_{DC,0} = \sqrt{2} \begin{pmatrix} \Lambda_1 & 0 & 0 & 0 \\ 0 & \Lambda_2 & 0 & 0 \\ 0 & 0 & -\Lambda_2 & 0 \\ 0 & 0 & 0 & -\Lambda_1 \end{pmatrix}, \quad M = \begin{pmatrix} 0 & mI_4 & mI_4 & 0 \\ mI_4 & 0 & 0 & mI_4 \\ mI_4 & 0 & 0 & mI_4 \\ 0 & mI_4 & mI_4 & 0 \end{pmatrix} \tag{6.55}$$

with

$$\Lambda_1 = \begin{pmatrix} |p| & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -|p| \end{pmatrix}, \quad \Lambda_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |p| & 0 & 0 \\ 0 & 0 & -|p| & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad p = -i\nabla_{\mathbf{y}_1}. \tag{6.56}$$

From Lemma 6.7, it follows that if $m = 0$, then H_{DC} is essentially selfadjoint. Hence, Kato-Rellich theorem yields that H_{DC} is also essentially selfadjoint. Q.E.D.

The tensor space $\mathcal{H}^{\otimes 2}$ has an orthogonal decomposition as follows.

$$\mathcal{H}^{\otimes 2} = \mathcal{H}_S^2 \oplus \mathcal{H}_A^2, \tag{6.57}$$

where $\mathcal{H}_S^2$ is the symmetric tensor space, and $\mathcal{H}_A^2$ the anti-symmetric tensor space. Let us consider the orthogonal projections P_S and P_A to $\mathcal{H}_S^2$ and $\mathcal{H}_A^2$, respectively. Hence, from Corollary 6.9, it follows that the closure of

$$(H_{DC} \pm i)\big([C_0^\infty(\mathbf{R}^6)^4]^{\otimes 2}\big)$$

is equal to $\mathcal{H}^{\otimes 2}$, so that the closure of

$$(H_{DC} \pm i)\big([C_0^\infty(\mathbf{R}^6)^4]^{\otimes 2} \cap \mathcal{H}_A^2\big) \tag{6.58}$$

is equal to $\mathcal{H}_A^2$. Q.E.D.

Remark 6.2 *Let us denote the symbol of the operator $H_{DC,0}$ by $\sigma(H_{DC,0})$*

$$\sigma(H_{DC,0})(\xi) = \sqrt{2} \begin{pmatrix} \sigma(\Lambda_1) & 0 & 0 & 0 \\ 0 & \sigma(\Lambda_2) & 0 & 0 \\ 0 & 0 & -\sigma(\Lambda_2) & 0 \\ 0 & 0 & 0 & -\sigma(\Lambda_1) \end{pmatrix} \qquad (6.59)$$

$$\sigma(\Lambda_1) = \begin{pmatrix} |\xi| & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -|\xi| \end{pmatrix}, \quad \sigma(\Lambda_2) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & |\xi| & 0 & 0 \\ 0 & 0 & -|\xi| & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \xi \in \mathbf{R}^3. \quad (6.60)$$

The set of eigenvalues of the matrix $\sigma(H_{DC,0}) + M$ consists of

$$0, \quad \sqrt{2|\xi|^2 + 4m^2}, \quad -\sqrt{2|\xi|^2 + 4m^2}$$

with multiplicity 8, 4, 4, *respectively.*

6.2 Essential spectrum

Proof of Theorem 4.2

Consider the operator in $L^2(\mathbf{R}^6)^4$:

$$H_0 = (\vec{\alpha} \cdot \vec{p}_1 + m\beta) \otimes I + I \otimes (\vec{\alpha} \cdot \vec{p}_2 + m\beta) \qquad (6.61)$$

and

$$H_{DC} = H_0 + k/|\mathbf{x}_1| + k/|\mathbf{x}_2| + k_0/|\mathbf{x}_1 - \mathbf{x}_2|. \qquad (6.62)$$

Let $\lambda > m$, $\mu > m$. Let take ξ, $\eta \in \mathbf{R}^3 \backslash \{0\}$ such that

$$|\xi|^2 + m^2 = \lambda^2, \quad |\eta|^2 + m^2 = \mu^2, \quad \xi \cdot \eta = 0. \qquad (6.63)$$

For each $\xi \in \mathbf{R}^4$, let $u, v \in \mathbf{C}^4 \backslash \{0\}$ be normalized eigenvectors to the equations

$$(\alpha \cdot \xi + m\beta)u = \lambda u, \quad |u|_{\mathbf{C}^4} = 1, \qquad (6.64)$$

$$(\alpha \cdot \xi + m\beta)v = -\mu v, \quad |v|_{\mathbf{C}^4} = 1, \qquad (6.65)$$

respectively. Define two functions by

$$u_n(x) = \chi_n(x)e^{ix\cdot\xi}u(\xi), \quad v_n(x) = \chi_n(x)e^{ix\cdot\eta}v(\xi), \qquad (6.66)$$

where $\chi_n \in C_0^\infty(\mathbf{R}^3)$ is a nonnegative function such that

$$\int_{\mathbf{R}^3} |\chi_n(x)|^2 dx = 1, \quad \mathrm{supp}\chi_n \subset \{x \in \mathbf{R}^3 \mid n < |x| < 2n\}. \qquad (6.67)$$

Then it holds that $\{u_n(x)\}$ and $\{v_n(x)\}$ are two sets of singular sequences in $L^2(\mathbf{R}^3)^4$ such that

$$\|u_n\|_{L^2} = \|v_n\|_{L^2} = 1, \quad u_n \rightharpoonup 0, \quad v_n \rightharpoonup 0, \quad weakly, \qquad (6.68)$$

$$[H_0 + m\beta - \lambda]u_n \longrightarrow 0 \quad (n \to \infty), \quad \mathrm{supp}u_n \subset \{x \in \mathbf{R}^3 \mid n < |x| < 2n\} \qquad (6.69)$$

$$[H_0 + m\beta + \mu]v_n \longrightarrow 0 \quad (n \to \infty), \quad \mathrm{supp}v_n \subset \{x \in \mathbf{R}^3 \mid n < |x| < 2n\}. \qquad (6.70)$$

Now we shall construct a singular sequence in $\mathcal{H}_A^2$.

Lemma 6.10

$$w_n := \frac{1}{\sqrt{2}}\{u_{n^2} \otimes v_n - v_n \otimes u_{n^2}\} \in \mathcal{H}_A^2, \tag{6.71}$$

Proof: Let us consider $F = f_1 \otimes \mathbf{i} + f_2 \otimes \mathbf{j}$, $G = g_1 \otimes \mathbf{i} + g_2 \otimes \mathbf{j} \in L^2(\mathbf{R}^3)^4$, where f_j, $g_j \in L^2(\mathbf{R}^3)^2$. Recall the definition of $u \otimes v$:

$$F \otimes G = (f_1 \otimes g_1) \otimes (\mathbf{i} \otimes \mathbf{i}) + (f_1 \otimes g_2) \otimes (\mathbf{i} \otimes \mathbf{j}) + (f_2 \otimes g_1) \otimes (\mathbf{j} \otimes \mathbf{i}) + (f_2 \otimes g_2) \otimes (\mathbf{j} \otimes \mathbf{j}), \tag{6.72}$$

where $f_j \otimes g_k$ $(j, k = 1, 2)$ are defined as

$$f_j \otimes g_k = \begin{pmatrix} u_{1,j} \otimes v_{1,k} \\ u_{1,j} \otimes v_{2,k} \\ u_{2,j} \otimes v_{1,k} \\ u_{2,j} \otimes v_{2,k} \end{pmatrix} = \begin{pmatrix} u_{1,j}(\mathbf{x}_1)v_{1,k}(\mathbf{x}_2) \\ u_{1,j}(\mathbf{x}_1)v_{2,k}(\mathbf{x}_2) \\ u_{2,j}(\mathbf{x}_1)v_{1,k}(\mathbf{x}_2) \\ u_{2,j}(\mathbf{x}_1)v_{2,k}(\mathbf{x}_2) \end{pmatrix}. \tag{6.73}$$

for $f_j = \begin{pmatrix} u_{1,j} \\ u_{2,j} \end{pmatrix}$ and $g_k = \begin{pmatrix} v_{1,k} \\ v_{2,k} \end{pmatrix}$.

It follows that

$$\begin{aligned} F \otimes G - G \otimes F &= (f_1 \otimes g_1 - g_1 \otimes f_1) \otimes (\mathbf{i} \otimes \mathbf{i}) + (f_1 \otimes g_2 - g_1 \otimes f_2) \otimes (\mathbf{i} \otimes \mathbf{j}) \\ &\quad + (f_2 \otimes g_1 - g_2 \otimes f_1) \otimes (\mathbf{j} \otimes \mathbf{i}) + (f_2 \otimes g_2 - g_2 \otimes f_2) \otimes (\mathbf{j} \otimes \mathbf{j}) \\ &\in \mathcal{H}_A^2. \end{aligned} \tag{6.74}$$

Q.E.D.

From Lemma 6.10, it follows that $\{w_n\}$ becomes a singular sequence of $H_{DC} - \lambda + \mu$. In fact, it satisfies that as $n \to \infty$

$$(H_{DC} - (\lambda - \mu))w_n = \frac{k}{|\mathbf{x}_1|}w_n + \frac{k}{|\mathbf{x}_2|}w_n + \frac{k_0}{|\mathbf{x}_1 - \mathbf{x}_2|}w_n \longrightarrow 0, \tag{6.75}$$

$$w_n \rightharpoonup 0, \quad \|w_n\| = 1. \tag{6.76}$$

The last assertion $\|w_n\| = 1$ follows from the fact that the eigenvectors $u(\xi)$, $v(\xi)$ corresponding to the different eigenvalues are orthogonal to each other. Since

$$(m, \infty) + (-\infty, -m) = (-\infty, \infty),$$

we can conclude that $\sigma_{\mathrm{ess}}(H_{DC}) = \mathbf{R}$.　　　　Q.E.D.

6.3　Absence of eigenvalues

Theorem 6.11 *Let* $m > 0$. *Suppose that* $|k| < 1/4$. *Then for any real* k_0, H_{DC} *has no eigenvalues in* $\mathbf{R} \backslash (-2m, 2m)$.

Proof of Theorem 6.11

It suffices to prove that there exist no eigenfunctions in $\mathcal{H}^{\otimes 2}$. We can regard H_{DC} as a sum of three operators on $\mathcal{H}^{\otimes 2}$:

$$H_{DC} = H_1 + V(x) + m\beta_+ + m\beta_-, \qquad (6.77)$$

where H_1 is a symmetric differential system of first order with constant coefficients satisfying

$$i[H_1, x \cdot p] = H_1, \qquad (6.78)$$

V is a scalar homogeneous function of degree -1, and

$$\beta_+ = \begin{pmatrix} I_4 & 0 & 0 & 0 \\ 0 & I_4 & 0 & 0 \\ 0 & 0 & -I_4 & 0 \\ 0 & 0 & 0 & -I_4 \end{pmatrix}, \; \beta_- = \begin{pmatrix} I_4 & 0 & 0 & 0 \\ 0 & -I_4 & 0 & 0 \\ 0 & 0 & I_4 & 0 \\ 0 & 0 & 0 & -I_4 \end{pmatrix}. \qquad (6.79)$$

In view of Theorem 4.1, we can prove our statement by use of a technique of Weidmann ([12] Theorem 10.38) and Kalf [3] because $\lambda - (m\beta_+ + m\beta_-)$ is strictly positive or strict negative if $|\lambda| > 2m$. Q.E.D.

Proof of Theorem 4.3 We first consider the case where $m > 0$. In order to prove the absence of eigenvalues in the whole line $\mathbf{R}$, it suffices to investigate the eigenvalues in $(-2m, 2m)$ of the following operator $H_{\mathbf{y_2}}$ in $L^2(\mathbf{R}^3)^{16}$ with a parameter $\mathbf{y_2}$

$$H_{\mathbf{y_2}} = \begin{pmatrix} H_{11} & mI_4 & mI_4 & 0 \\ mI_4 & H_{22} & 0 & mI_4 \\ mI_4 & 0 & -H_{22} & mI_4 \\ 0 & mI_4 & mI_4 & -H_{11} \end{pmatrix} + T^{-1}V_nT, \qquad (6.80)$$

where

$$H_{11} = T^{-1}(h_{12} + h_{21})T, \quad H_{22} = T^{-1}(-h_{12} + h_{21})T. \qquad (6.81)$$

Since the essential spectrum $H_{\mathbf{y_2}}$ coincides with $(-\infty, -2m] \cup [2m, \infty)$ and $\pm 2m$ are not eigenvalues, the multiplicity of every eigenvalue in $(-2m, 2m)$, if it exists, is finite. Hence it follows from the analytic perturbation theory that the eigenvalues $\lambda_j(\mathbf{y_2})$ are real-analytic in $|\mathbf{y_2}|$. Therefore, if they existed, we would have

$$\lambda_j(\mathbf{y_2}) = \frac{k_0}{|\mathbf{y_2}|} \qquad (6.82)$$

for small $|\mathbf{y_2}|$. This is a contradiction because $|\lambda_j(\mathbf{y_2})| \le 2m$ and $k_0 \ne 0$. When $m = 0$, we can modify the above reasoning to arrive at the conclusion. Q.E.D.

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