

Asymptotics of the scattering phase for the Dirac operator: High energy, semi-classical and non-relativistic limits

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Abstract. In this paper we prove several results for the scattering phase (spectral shift function) related with perturbations of the electromagnetic field for the Dirac operator in the Euclidean space.

Many accurate results are now available for perturbations of the Schrödinger operator, in the high energy regime or in the semi-classical regime. Here we extend these results to the Dirac operator. There are several technical problems to overcome because the Dirac operator is a system, its symbol is a 4×4 matrix, and its continuous spectrum has positive and negative values. We show that we can separate positive and negative energies to prove high energy asymptotic expansion and we construct a semi-classical Foldy–Wouthuysen transformation in the semi-classical case. We also prove an asymptotic expansion for the scattering phase when the speed of light tends to infinity (non-relativistic limit).

1. Introduction

We are interested here in the study of the spectral properties of the Dirac operator on $L^2(\mathbf{R}^3; \mathbf{C}^4)$,

$$H = c \sum_{j=1}^3 \alpha_j (\hbar D_j - A_j(x)) + \beta c^2 + V(x), \quad D_j := -i\partial_{x_j},$$

where $\{\alpha_j\}_{j=1}^3$ and β are the 4×4 -matrices of Dirac satisfying the anti-commutation relations

$$\alpha_j \alpha_k + \alpha_k \alpha_j = 2\delta_{jk} 1_4, \quad 1 \leq j, k \leq 4,$$

($\alpha_4 = \beta$, 1_4 is the 4×4 identity matrix). The vector $A = (A_1, A_2, A_3)$ is the magnetic vector potential and $V = \begin{pmatrix} V_+ 1_2 & 0 \\ 0 & V_- 1_2 \end{pmatrix}$, where V_{\pm} is a scalar potential (1_2 is the

identity matrix on \mathbf{C}^2). The physical constants \hbar (Planck's constant) and c (velocity of light) are parameters.

We assume that the potentials are C^∞ and there exists $\delta > 0$ such that

$$(H_\delta) \quad |\partial_x^\alpha A(x)| + |\partial_x^\alpha V(x)| = O(\langle x \rangle^{-\delta - |\alpha|}) \quad \text{for all } \alpha \in \mathbf{N}^3,$$

where $\langle x \rangle := (1 + |x|^2)^{1/2}$. The operator H is a perturbation of the free Dirac operator,

$$H_0 = c \sum_{j=1}^3 \alpha_j \hbar D_j + c^2 \beta.$$

The spectrum of H_0 is purely absolutely continuous,

$$\sigma(H_0) = \sigma_c(H_0) = \sigma_{ac}(H_0) =]-\infty, -c^2] \cup [c^2, +\infty[,$$

and, for $\delta > 1$ (short range perturbation), we have the following properties [24], [26]:

- (i) the wave-operators for (H, H_0) exist and are complete;
- (ii) the essential spectrum of H is equal to $]-\infty, -c^2] \cup [c^2, +\infty[$;
- (iii) H has no singular spectrum;
- (iv) the discrete spectrum of H is contained in $] -c^2, c^2[$.

According to (i), the scattering operator, S , is defined and unitary. In the spectral representation of H_0 , the operator S becomes an operator-valued function, $S(\lambda)$, on $L^2(S^2; \mathbf{C}^4)$ (S^2 is the unit sphere in \mathbf{R}^3). Moreover, $S(\lambda)$ is unitary and, for $\delta > 3$, $S(\lambda) - \text{Id}$ is a trace class operator on $L^2(S^2; \mathbf{C}^4)$. So, it makes sense to introduce the scattering phase $s(\lambda)$ by the formula

$$(1) \quad s(\lambda) = s_{(H, H_0)}(\lambda) = \frac{i}{2\pi} \log \det(S(\lambda)), \quad s(0) \in [0, 1).$$

According to the Birman-Krein theory [2], $s(\lambda)$ satisfies the Krein formula

$$(2) \quad \text{Tr}(f(H) - f(H_0)) = \int_{\mathbf{R}} s(\lambda) f'(\lambda) d\lambda \quad \text{for all } f \in \mathcal{S}(\mathbf{R}).$$

By the assumption (H_δ) with $\delta > 3$, we have that $s \in C^\infty(]-\infty, -c^2] \cup [c^2, +\infty[)$. This can be proved, as for the Schrödinger operator (see Corollary 5.8 of [20]) by using the stationary representation of $S(\lambda)$ given by E. Balslev and B. Helffer [1].

In this paper, we study three kinds of asymptotics for the scattering phase. First of all, the high energy limit, $|\lambda| \rightarrow \infty$ (c and \hbar being fixed), then the semi-classical limit, $\hbar \searrow 0$ (c is fixed and λ is in a non-trapping compact interval), and at last the non-relativistic limit, $c \rightarrow +\infty$ (\hbar and λ being fixed).

The non-relativistic limit (studied in Section 5) was announced in [5] and proved in the thesis of the first author [4]. Our proof is closely connected with the energy regularity and inspired by [12]. Here we show that the order of regularity (with respect to c^{-1}) is independent of the decrease of the potentials (we need only decrease as $\langle x \rangle^{-\delta}$, $\delta > 3$).

To discuss the high energy regime (in Section 3) and semi-classical regime (in Section 4), we use the close connection between the Dirac operator and Schrödinger type operators in two ways.

For $|\lambda| \rightarrow \infty$, we split positive and negative energies (see formula (7) below), then some known results about local spectral densities for Schrödinger operator [21] give a full asymptotic expansion of $s(\lambda)$ (and their derivatives). In this way, we have a new proof of the Weyl formula established in [7].

For $\hbar \searrow 0$, we exploit the \hbar -decoupling property of the Dirac operator (Proposition 4.2) based on a Foldy–Wouthuysen transformation. Then, we can adapt some classical methods to establish semi-classical estimates of the resolvent and to have short and long time approximations of the propagator. At last, we can prove a semi-classical asymptotic expansion of the derivative $s'(\lambda)$ for λ in a non-trapping energy band.

2. Main results

Theorem 2.1. (High energy asymptotics for $\hbar=1$, $c=1$.) *Let us assume (H_δ) , with $\delta > 3$. Then we have the asymptotic expansions*

(a)

$$\frac{ds}{d\lambda}(\lambda) \asymp (2\pi)^{-3} \sum_{j \geq 1} \gamma_j \lambda^{2-j}, \quad \lambda \rightarrow \pm\infty,$$

with $\gamma_1 = 8\pi \int_{\mathbf{R}^3} (V_+ + V_-)(x) dx$ and

$$\gamma_2 = 4\pi \int_{\mathbf{R}^3} \left(\left(\frac{V_+ - V_-}{2} \right)^2 + (V_+ - V_-) - 2 \left(\frac{V_+ + V_-}{2} \right)^2 \right) (x) dx;$$

(b) if $V=0$, then

$$\frac{ds}{d\lambda}(\lambda) \asymp (2\pi)^{-3} \lambda^{-2} \sum_{j \geq 0} \beta_j \lambda^{-2j}, \quad \lambda \rightarrow \pm\infty,$$

with $\beta_0 = \frac{8}{3}\pi \int_{\mathbf{R}^3} B(x)^2 dx$ where $B = \text{curl } A$ is the magnetic field.

Furthermore, these asymptotics can be differentiated at any order with respect to λ .

We consider now the case $|\lambda| > 1$ fixed and $h \searrow 0$ ($h = \hbar$). To formulate the next result we consider the two eigenvalues λ_{\pm} (of multiplicity 2) of the h -principal-symbol of H which are defined as $\lambda_{\pm}(x, \xi) = \pm \langle \xi - A(x) \rangle + V(x)$ (here, we put $V_+ = V_- = V$).

Classically, we shall say that an energy band $J \subset \mathbf{R}$ is non-trapping for a classical Hamiltonian $\lambda_{\pm}(x, \xi)$ if for every $\mu \in J$, every classical path in

$$\Sigma_{\mu}(\lambda_{\pm}) := \{(x, \xi) \in \mathbf{R}^{2n}; \lambda_{\pm}(x, \xi) = \mu\}$$

escapes to infinity as time goes to plus or minus infinity (see Definition 4.5 for a more precise definition).

Remark 2.2. The value $\lambda \in]-\infty, -1[\cup]1, +\infty[$ is non-trapping for $\lambda_+(x, \xi)$ and $\lambda_-(x, \xi)$ in only two cases:

(1) $\lambda > \nu_+$ is non-trapping for $\lambda_+(x, \xi)$;

(2) $\lambda < \nu_-$ is non-trapping for $\lambda_-(x, \xi)$;

where $\nu_+ = \max(1, \sup V - 1)$ and $\nu_- = \min(-1, \inf V + 1)$.

Indeed, $\lambda \in \mathbf{R}$ being non-trapping for $\lambda_+(x, \xi)$ implies that $\lambda \geq 1$ or $\{\lambda < 1 \text{ and } \Sigma_{\lambda}(\lambda_+) = \emptyset\}$ (that is $\lambda < 1$ and $\lambda < \inf V + 1$) because for $\mu < 1$, $\Sigma_{\mu}(\lambda_+)$ is compact or empty. In the same way, $\lambda \in \mathbf{R}$ being non-trapping for $\lambda_-(x, \xi)$ imply $\lambda \leq -1$ or $\{\lambda > -1 \text{ and } \Sigma_{\lambda}(\lambda_-) = \emptyset\}$ (that is $\lambda > -1$ and $\lambda > \sup V - 1$) because for $\mu > -1$, $\Sigma_{\mu}(\lambda_-)$ is compact or empty.

Theorem 2.3. (Semi-classical asymptotic for $c=1$.) *Let us assume (H_{δ}) , with $\delta > 3$. If J is a compact interval in $]-\infty, -1[\cup]1, +\infty[$ that is non-trapping for $\lambda_+(x, \xi)$ and $\lambda_-(x, \xi)$, then, for h small enough, we have the asymptotic expansion of $(d/d\lambda)s_h(\lambda) := (d/d\lambda)s_{H, H_1}(\lambda)$,*

$$\frac{ds_h}{d\lambda}(\lambda) \asymp (2\pi)^{-3} \sum_{j \geq 0} c_j(\lambda) h^{-3+j}, \quad \text{as } h \searrow 0 \text{ uniformly for } \lambda \in J,$$

where for $\pm\lambda > 1$, we have

$$c_0(\lambda) = \pm \frac{8\pi}{3} \frac{d}{d\lambda} \int_{\mathbf{R}^3} (((\lambda - V(x))^2 - 1)_+^{3/2} - (\lambda^2 - 1)^{3/2}) dx$$

$(x_+ = \max(x, 0) \text{ for } x \in \mathbf{R})$.

Furthermore, this expansion can be differentiated in λ to any order.

Remark 2.4. If $[a, b] \subset]-\infty, -1[\cup]1, +\infty[$ is a compact interval such that a and b are non-trapping energies for λ_{\pm} then Theorem 2.3 gives an asymptotic expansion for $s_h(b) - s_h(a)$, by integrating in λ and using weak asymptotics given by the functional calculus (see Section 4, the proof of Theorem 2.3).

The above theorems hold for fixed $c=1$. Now, we consider the non-relativistic approximation, so c is a variable parameter.

Let us denote by H'_{\pm} (resp. $H'_{0,\pm}$) the operators $H \mp c^2$ (resp. $H_0 \mp c^2$) and by (h_{\pm}, h_0) , the Pauli operators

$$(3) \quad h_{\pm} = \frac{1}{2}(\sigma \cdot (D - A))^2 + V_{\pm} 1_2, \quad h_0 = \frac{1}{2}(\sigma \cdot D)^2 1_2,$$

where $\{\sigma_j\}_{1 \leq j \leq 3}$ are the Pauli 2×2 matrices.

Owing to (H_{δ}) , the scattering phase, $s_{A,V_{\pm}}^{\infty}(\lambda)$, for the pair (h_{\pm}, h_0) , is well defined as a smooth function on $]0, +\infty[$ (see [20], [22]). Let $s^{\pm}(\lambda)$ be the scattering phase for the pair $(H'_{\pm}, H'_{0,\pm})$. We have $s^{\pm}(\lambda) = s_{(H,H_0)}(\lambda \pm c^2)$, and we will show the following theorem.

Theorem 2.5. (Non-relativistic limit for $\hbar=1$.) *Assuming (H_{δ}) , with $\delta > 3$, we have the following results.*

- (i) *The limit $\lim_{c \rightarrow +\infty} \frac{d}{d\lambda} s^{\pm}(\lambda) = \pm \frac{d}{d\lambda} s_{A,V_{\pm}}^{\infty}(\pm\lambda)$ for all $\pm\lambda > 0$.*
- (ii) *There exists a neighbourhood \mathcal{V}_0 of $c^{-1}=0$, such that $s^{\pm}(\lambda)$ is of class C^{∞} with respect to $(c^{-1}, \pm\lambda) \in \mathcal{V}_0 \times]0, +\infty[$.*

In particular, there exists a sequence $\{f_j^{\pm}\}_{j \geq 1}$ of functions in $C^{\infty}(]0, +\infty[)$ such that, for all integers l and N we have

$$\frac{d^l}{d\lambda^l} s^{\pm}(\lambda) = \pm \frac{d^l}{d\lambda^l} s_{A,V_{\pm}}^{\infty}(\pm\lambda) + \sum_{j=1}^N c^{-j} \frac{d^l}{d\lambda^l} f_j^{\pm}(\pm\lambda) + O(c^{-(N+1)}),$$

locally uniformly with respect to $\lambda \in]0, +\infty[$, as $c \rightarrow +\infty$.

- (iii) *If $V=0$, then*

$$s^{\pm}(\lambda) = \pm s_{A,0}^{\infty} \left(\pm\lambda + \frac{\lambda^2}{2c^2} \right) \quad \text{for } \pm\lambda > 0.$$

3. High energies

In this section, we fix $c=\hbar=1$. First of all, we limit our work to the study of the positive energies. The negative case will be deduced from the following proposition.

Proposition 3.1. *Suppose (H_δ) with $\delta > 3$. Let $s_{(A,V)}(\lambda)$ be the scattering phase associated with the Dirac operators*

$$H(e, A, V) = \alpha \cdot (D - eA(x)) + \beta + eV(x), \quad H_0 = \alpha \cdot D + \beta,$$

(e denotes the charge).

We have the symmetry property

$$s_{(A,V)}(\lambda) = -s_{(-A, -\bar{V})}(-\lambda),$$

where $\bar{V} = \begin{pmatrix} V_- 1_2 & 0 \\ 0 & V_+ 1_2 \end{pmatrix}$.

In particular, if $\gamma_j^\pm(A, V)$ are the coefficients of λ^{2-j} in the asymptotic expansion of $(d/d\lambda)s_{(A,V)}(\lambda)$ as $\lambda \rightarrow \pm\infty$, we have

$$\gamma_j^-(A, V) = -\gamma_j^+(-A, -\bar{V}).$$

Proof. Let C be the charge conjugation operator defined by (see Section 1.4.6 of [24])

$$C\psi = i\beta\alpha_2\bar{\psi}.$$

This is a unitary operator on $L^2(\mathbf{R}^3, \mathbf{R}^4)$ satisfying

$$CH(e, A, V)C^{-1} = -H(-e, A, \bar{V}) = -H(e, -A, -\bar{V}).$$

Then we obtain the symmetry property by using the Krein formula (2) and the cyclicity of traces. \square

Now, we study the positive energies.

Formally, $s(\lambda)$ is related to the difference between the spectral projectors of H and H_0 . As in [20], we first prove that $s(\lambda)$ can be computed by using only the spectral projector of H . Let us introduce

$$Q := H^2 - H_0^2, \quad \mathcal{A} := \frac{1}{2}(x \cdot D + D \cdot x).$$

The differential operator Q is of order 1. Its coefficients are matrices, decreasing as fast as A and V (see (H_δ)).

Proposition 3.2. *Suppose (H_δ) with $\delta > 3$. Let $f \in C_0^\infty([-\infty, -1] \cup [1, +\infty])$. We have*

$$\int_{\mathbf{R}} s(\lambda) f'(\lambda) d\lambda = \text{Tr}((Q - \tfrac{1}{2}i[Q, \mathcal{A}]) (H^2 - 1)^{-1} f(H)).$$

Proof. By using the relations

$$2(H_0^2 - I) = i[H_0^2, \mathcal{A}] \quad \text{and} \quad 2(H^2 - I) = i[H^2, \mathcal{A}] + (2Q - i[Q, \mathcal{A}]),$$

and the cyclicity property of traces (see Appendix A of [20]), we obtain

$$\text{Tr}(f(H) - f(H_0)) = \text{Tr}\left((Q - \tfrac{1}{2}i[Q, \mathcal{A}])(H^2 - 1)^{-1}f(H)\right).$$

The Krein formula (2) gives the result. \square

Remark 3.3. Of course the operator $(H^2 - 1)^{-1}$ is not well defined, however for $f \in C_0^\infty(\mathbf{R} \setminus \{-1, 1\})$, we can define $(H^2 - 1)^{-1}f(H)$ as the operator $\varphi(H)$ where $\varphi \in C_0^\infty(\mathbf{R})$ satisfies

$$\varphi(\lambda) = \begin{cases} (\lambda^2 - 1)^{-1}f(\lambda) & \text{for } |\lambda| \neq 1, \\ 0 & \text{for } |\lambda| = 1. \end{cases}$$

To prove Theorem 2.1, we are going to apply a result of D. Robert [21] (Theorem 4.4) concerning asymptotic expansions of local spectral densities, for perturbations of the Laplacian. We will connect $(ds/d\lambda)(\lambda)$ with local spectral densities of $(H^2 - \text{Id})$.

Let us recall the general result we shall use here. Let w be a classical symbol in the symbol class $S_m(\langle x \rangle^{-\delta}, \langle \xi \rangle^\mu)$ defined by

$$\{s \in C^\infty(\mathbf{R}^{2n}, \mathcal{M}_m(\mathbf{C})) : |\partial_x^\alpha \partial_\xi^\beta s(x, \xi)| = O(\langle x \rangle^{-\delta - |\alpha|} \langle \xi \rangle^{\mu - |\beta|})\},$$

where $\mathcal{M}_m(\mathbf{C})$ is the set of $m \times m$ matrices.

Let L the Hamiltonian on $L^2(\mathbf{R}^n, \mathbf{C}^m)$ defined on C_0^∞ by

$$L = -\Delta 1_m + a(x).D + D.a(x) + V(x),$$

where for example $a(x).D = -i \sum_{j=1}^n a_j(x) \partial_{x_j}$. We assume that $a(x) \in C^\infty(\mathbf{R}^n, \mathbf{R}^m)$ and $V(x)$ is a Hermitian matrix, C^∞ on \mathbf{R}^n satisfying (H_δ) with $\delta > n$. Then, for $f \in C_0^\infty(\mathbf{R})$, $w(x, D_x).f(L)$ is of trace class and we can define the local spectral density of L .

Definition 3.4. The distribution $\sigma_w: f \mapsto \text{Tr}(w(x, D_x).f(L))$ is the local spectral density of L , associated with w .

Because the principal symbol of L is scalar, we can easily adapt the proof of Theorem 4.4 in [21], for matrix operators, and we obtain the following theorem.

Theorem 3.5. (D. Robert [21]) *Under the above assumptions, σ_w is C^∞ in $]0, +\infty[$ and we have the full asymptotics*

$$\sigma_w(\lambda) \asymp \lambda^{(n+\mu)/2-1} \left(\sum_{j \geq 0} c_{w,j} \lambda^{-j/2} \right), \quad \lambda \rightarrow +\infty.$$

Furthermore, these asymptotics can be differentiated at any order with respect to λ .

Let us remark that this result also holds for Δ_g , the symmetric Laplace–Beltrami operator associated with an asymptotically flat metric g which is non-trapping.

Let us introduce

$$W := \frac{1}{2} (Q - \frac{1}{2} i [Q, \mathcal{A}]) \quad \text{and} \quad W' = WH.$$

As $Q := H^2 - H_0^2$ and \mathcal{A} are first order differential operators, W is a first order differential operator, and W' is a second order differential operator. Moreover, under the assumption (H_δ) , $Q = q(x, D_x)$ with $q \in S_4(\langle x \rangle^{-\delta}, \langle \xi \rangle)$. Then, $W = w(x, D_x)$ and $W' = w'(x, D_x)$ with

$$w \in S_4(\langle x \rangle^{-\delta}, \langle \xi \rangle), \quad w' \in S_4(\langle x \rangle^{-\delta}, \langle \xi \rangle^2).$$

The operator H^2 is not exactly of L 's type ($\beta^2 = \text{Id}$ occur),

$$H^2 = \Delta 1_4 + (\alpha \cdot DV + V \alpha \cdot D) - (D \cdot A + A \cdot D) - \Sigma \cdot B + (\beta + V - \alpha \cdot A)^2,$$

where $B = \text{curl } A$ and $\Sigma_j = \begin{pmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{pmatrix}$, $(\sigma_j)_{1 \leq j \leq 3}$ being the 2×2 Pauli matrices.

However, $H^2 - \text{Id}$ is of L 's type under the hypothesis (H_δ) with $\delta > 3$ and the local spectral densities σ_W and $\sigma_{W'}$, associated respectively with W and W' , are well defined on $]1, +\infty[$ by

$$(4) \quad \sigma_W: f \in C_0^\infty(]1, +\infty[) \longmapsto \text{Tr}(W f(H^2)) = \text{Tr}(W \tilde{f}(H^2 - \text{Id})),$$

$$(5) \quad \sigma_{W'}: f \in C_0^\infty(]1, +\infty[) \longmapsto \text{Tr}(W' f(H^2)),$$

where $\tilde{f}(\lambda) = f(\lambda + 1)$.

Here $(H^2 - \text{Id})$ is a perturbation of the Laplace operator, thus Theorem 3.5 holds for σ_W and $\sigma_{W'}$. Hence the existence of the asymptotic expansion claimed in Theorem 2.1 will be deduced from the following proposition.

Proposition 3.6. *Let us assume (H_δ) with $\delta > 3$. Then the scattering phase $s(\lambda)$ for (H, H_0) and the local spectral densities $\sigma_W, \sigma_{W'}$ are well defined. In the distribution sense, on $]1, +\infty[$, we have the decomposition*

$$(6) \quad -\frac{ds}{d\lambda}(\lambda) = \frac{2\lambda}{\lambda^2-1}\sigma_W(\lambda^2) + \frac{2}{\lambda^2-1}\sigma_{W'}(\lambda^2).$$

Proof. On $]1, +\infty[$, the distributions $\sigma_W/(\lambda-1)$ and $\sigma_{W'}/(\sqrt{\lambda}(\lambda-1))$ are respectively the mappings

$$\begin{aligned} f \in C_0^\infty(]1, +\infty[) &\longmapsto \text{Tr}(W(H^2-1)^{-1}f(H^2)), \\ f \in C_0^\infty(]1, +\infty[) &\longmapsto \text{Tr}(W'(H^2-1)^{-1}|H|^{-1}f(H^2)). \end{aligned}$$

Then, owing to Proposition 3.2, we want to prove that

$$\begin{aligned} \text{Tr}(2W(H^2-1)^{-1}f(H)) &= \text{Tr}(W(H^2-1)^{-1}f(\sqrt{H^2})) \\ &\quad + \text{Tr}(W'(H^2-1)^{-1}|H|^{-1}f(\sqrt{H^2})) \end{aligned}$$

for all $f \in C_0^\infty(]1, +\infty[)$.

However, this is a consequence of the following equality, true for all f equal to zero on $]-\infty, 0]$ (and for any self-adjoint operator),

$$(7) \quad f(H) = \frac{1}{2}f(|H|) + \frac{1}{2}H|H|^{-1}f(|H|).$$

Hence, we deduce equation (6). \square

Remark 3.7. Of course, as for $(H^2-1)^{-1}$ (see Remark 3.3), $|H|^{-1}$ is not well defined, but for $f \in C_0^\infty(\mathbf{R} \setminus 0)$, we can define $|H|^{-1}f(|H|)$.

Proof of Theorem 2.1. As we saw above, the existence of the asymptotic expansion follows from the equation (6) and from Theorem 3.5 applied to σ_W and $\sigma_{W'}$. This gives an asymptotic of the form

$$\frac{ds}{d\lambda}(\lambda) \asymp (2\pi)^{-3} \sum_{j \geq 0} \gamma_j^+ \lambda^{2-j}, \quad \lambda \rightarrow +\infty.$$

According to Proposition 3.1, we also have an asymptotic as $\lambda \rightarrow -\infty$ with coefficients γ_j^- .

At last, the coefficients are given by the weak asymptotic in [4], [7]. This uses the functional calculus for h -admissible pseudo-differential operators, developed by B. Helffer and D. Robert [14], [19], which is based on the construction of a

parametrix (Seeley's method). In particular, we have $\gamma_0^\pm = 0$ because H^2 and H_0^2 have the same principal symbols. Moreover, by using meromorphic extensions of the zeta relative function for (H^2, H_0^2) and of the eta relative function for (H, H_0) (see [4], [6]) we prove that $\gamma_j^- = \gamma_j^+$.

The case $V=0$ is studied in [7], using some supersymmetry properties of H with only a magnetic potential, we prove (Corollary 6.3 of [7])

$$(8) \quad s(\lambda) = \pm s_\infty \left(\frac{1}{2}(\lambda^2 - 1) \right), \quad \pm \lambda > 1,$$

where s_∞ is the scattering phase for the Pauli operators defined by (3), with $V_+ = 0$. As the asymptotic expansion of s_∞ is known [20], we deduce the asymptotic expansion of s , for $V=0$. \square

Remark 3.8. In this proof, we only use that $(H^2 - I)$ is a perturbation of the Laplacian and the result of D. Robert [21], true in any dimension. Hence, in the same way, we can obtain a high energy asymptotic of the scattering phase for Dirac operators in \mathbf{R}^n , for any n .

Moreover, $s'(\lambda)$ is studied as a particular spectral density of H (see Proposition 3.2). More generally, we can also prove a high energy asymptotic expansion for local spectral densities of Dirac operators.

Remark 3.9. Keeping c (the velocity of light), the formula (8) becomes, for $\lambda > c^2$,

$$s(\lambda) = s_\infty \left(\frac{\lambda^2 - c^4}{2c^2} \right).$$

Then, s_c the scattering phase associated with $(H - c^2, H_0 - c^2)$ satisfies, for $\lambda > 0$,

$$(9) \quad s_c(\lambda) = s_\infty \left(\lambda + \frac{\lambda^2}{2c^2} \right),$$

which is (iii) of Theorem 2.5.

4. Semi-classical limit

In this section we fix $c=1$ and we study the asymptotic of the scattering phase as $\hbar \rightarrow 0$. To prove Theorem 2.3 (in Subsection 4.3), our main tool is \hbar -decoupling (developed in Subsection 4.1).

To simplify, we consider only the case $V_+ = V_- = V$, hence the \hbar -principal symbol of H has two eigenvalues of multiplicity two,

$$\lambda_\pm(x, \xi) = \pm \langle \xi - A(x) \rangle + V(x).$$

Remark 4.1. For $V_+ \neq V_-$ the h -principal symbol of H also has two eigenvalues of multiplicity two, viz. $\lambda_{\pm}(x, \xi) = \pm((1 + \bar{v}(x))^2 + |\xi - A(x)|^2)^{1/2} + v(x)$, with $v = \frac{1}{2}(V_+ + V_-)$ and $\bar{v} = \frac{1}{2}(V_+ - V_-)$. But in this case, when $(1 + \bar{v}(x))$ and $(\xi - A(x))$ vanish together, λ_{\pm} is not differentiable.

4.1. h -decoupling of the Dirac operator

The goal of this section is to prove the following proposition. We will use h -pseudo-differential calculus. To a symbol a and a real $h > 0$, is associated the operator $Op_h^{\omega}(a)$ defined for $u \in \mathcal{S}(\mathbf{R})$ by

$$(Op_h^{\omega}(a)u)(x) = (2\pi)^{-n} \int_{\mathbf{R}^n} \int_{\mathbf{R}^n} e^{i(x-y, \xi)} a\left(\frac{1}{2}(x+y), h\xi\right) u(y) dy d\xi.$$

Let us recall that an operator $A(h)$ is called h -admissible of weight (q, p) if there exists sequences (a_j) of symbols and $R_N(h)$ of bounded operators (on L^2) such that

$$A(h) = \sum_{j=0}^N h^j Op_h^{\omega}(a_j) + h^{N+1} R_N(h),$$

with $R_N(h)$ uniformly bounded for $h \in]0, h_0]$, $h_0 > 0$, and $a_j \in S(\langle x \rangle^p, \langle \xi \rangle^q)$, where

$$S(\langle x \rangle^p, \langle \xi \rangle^q) := \{s \in C^{\infty}(\mathbf{R}^{2n}) : |\partial_x^{\alpha} \partial_{\xi}^{\beta} s(x, \xi)| = O(\langle x \rangle^{p-|\alpha|} \langle \xi \rangle^{q-|\beta|})\}$$

(see the book [19] or [14] for more details).

Proposition 4.2. *Let $H_{A,V}$ be the Dirac operator*

$$H_{A,V} = \alpha \cdot (hD - A(x)) + \beta + V(x)1_4,$$

with A and V satisfying (H_{δ}) .

For all $N \geq 0$, there exists a unitary h -admissible pseudo-differential operator $W_N(h)$ such that

$$W_N^* H_{A,V} W_N = \begin{pmatrix} a_{+,N}(h) & 0 \\ 0 & a_{-,N}(h) \end{pmatrix} + h^{N+1} R_{N+1}(h),$$

where $a_{\pm,N}(h)$ is an h -admissible pseudo-differential operator, of principal symbol $\lambda_{\pm}(x, \xi)1_2$, and $R_{N+1}(h)$ is an h -admissible pseudo-differential operator of order $-(N+1)$.

In particular, for $N=0$ we can choose $a_{\pm,0}(h) = \lambda_{\pm}(x, hD)1_2$.

(W_N^* denotes the adjoint operator of the closed operator W_N .)

Let us mention that a similar result is stated by R. Brummelhuis and J. Nourrigat [3] to study the scattering amplitude. This kind of decoupling is also used by A. Grigis and A. Mohamed (see Lemma 3.4 of [11]) to study the Dirac operator with periodic potentials.

To establish this proposition, we use the following lemma proved in [15] for bounded operators following a method due to M. Taylor.

Lemma 4.3. *Let $M_k(h)$ be a matrix h -admissible pseudo-differential operator,*

$$M_k(h) = \begin{pmatrix} a_+(h) & h^k b^*(h) \\ h^k b(h) & a_-(h) \end{pmatrix}, \quad k \geq 1,$$

where $a_{\pm}(h)$ and $b(h)$ are $m \times m$ matrices of h -admissible pseudo-differential operators satisfying

- (i) $a_{\pm}(h)$ is of weight $(1, 0)$ and $b(h)$ is of weight $(q, 0)$, $q \leq 1$;
- (ii) the principal symbols of $a_{\pm}(h)$ are of scalar type, i.e. there exists $\lambda_{\pm}(x, \xi) \in \mathbf{R}$ such that $\sigma_p(a_{\pm}(h)) = \lambda_{\pm}(x, \xi) 1_m$;

- (iii) there exists $c > 0$ and $C > 0$ such that for all $(x, \xi) \in \mathbf{R}^{2n}$ we have

$$C\langle \xi \rangle \geq \lambda_+(x, \xi) - \lambda_-(x, \xi) \geq c\langle \xi \rangle.$$

(This implies, in particular, that for h sufficiently small, the operator $a_+(h) - a_-(h)$ has an inverse of weight $(-1, 0)$).

Then, there exists a unitary, h -admissible pseudo-differential operator $W(h)$ satisfying

$$W(h)^* M_k(h) W(h) = \begin{pmatrix} a_{+,1}(h) & h^{k+1} b_1^*(h) \\ h^{k+1} b_1(h) & a_{-,1}(h) \end{pmatrix},$$

where $a_{\pm,1}(h)$ is an h -admissible pseudo-differential operator of principal symbol $\lambda_{\pm}(x, \xi) 1_m$ and $b_1(h)$ is an h -admissible pseudo-differential operator of weight $(q-1, 0)$.

Proof of Proposition 4.2. The proof is performed by induction on N , beginning at $N=0$. The Dirac operator without electric potential, $H_{A,0}$, is a particular case of supersymmetric Dirac operators (see Chapter 5 of [24]). For W_0 , we will take the Foldy-Wouthuysen transformation (Section 5.6 of [24]). More precisely, let

$$(10) \quad u(H_0(\xi)) := [2|H_0|(1+|H_0|)]^{-1/2} (H_0\beta + |H_0|)(\xi)$$

the unitary transformation which brings $H_0(\xi) = \alpha \cdot \xi + \beta$ to the diagonal form

$$\beta|H_0(\xi)| = \beta\langle \xi \rangle = \begin{pmatrix} \langle \xi \rangle 1_2 & 0 \\ 0 & -\langle \xi \rangle 1_2 \end{pmatrix}.$$

Let $W_0(h) = u(H_{A,0})$. This is an h -admissible pseudo-differential operator (see functional calculus in [14], [19]) and from the definition of u we get that $W_0(h)$ is unitary and satisfies

$$W_0(h)^* H_{A,0} W_0(h) = \beta |H_{A,0}|,$$

where $|H_{A,0}| = (H_{A,0}^2)^{1/2} = 1_2 \otimes ((\sigma \cdot (hD - A))^2 + 1_2)^{1/2}$.

Using functional calculus and $(\sigma \cdot (hD - A))^2 = (hD - A)^2 1_2 - h\sigma \cdot B$ ($B = \text{curl } A$), it follows that there exists an h -admissible pseudo-differential operator $r_0(h)$, such that

$$W_0(h)^* H_{A,0} W_0(h) = \begin{pmatrix} \langle hD - A \rangle 1_2 + hr_0(h) & 0 \\ 0 & -\langle hD - A \rangle 1_2 - hr_0(h) \end{pmatrix}.$$

For $V \neq 0$ we consequently get that $W_0(h)^* H_{A,V} W_0(h)$ is equal to

$$\begin{pmatrix} (\langle hD - A \rangle + V) 1_2 + hr_0(h) & 0 \\ 0 & -(\langle hD - A \rangle + V) 1_2 - hr_0(h) \end{pmatrix} + hR_1(h),$$

where $R_1(h) = h^{-1}(W_0(h)^* V W_0(h) - V 1_4)$ is an h -admissible pseudo-differential operator of order -1 (we use that V is a scalar potential). Thus, we get the proposition for $N=0$.

We can now start with the induction argument. Let $N \geq 0$ and let us assume the existence of a unitary, h -admissible pseudo-differential operator $W_N(h)$ satisfying

$$W_N(h)^* H_{A,V} W_N(h) = \begin{pmatrix} a_{+,N}(h) & h^{N+1} b_N^*(h) \\ h^{N+1} b_N(h) & a_{-,N}(h) \end{pmatrix},$$

where $a_{\pm,N}(h)$ is an h -admissible pseudo-differential operator of principal symbol $\lambda_{\pm}(x, \xi) 1_2$ and $b_N(h)$ is an h -admissible pseudo-differential operator of order $-(N+1)$. Observing that the principal symbol of $a_{+,N}(h) - a_{-,N}(h)$ is $2\langle \xi - A(x) \rangle 1_2$, we can apply Lemma 4.3. Then, there exists a unitary, h -admissible pseudo-differential operator $W(h)$ satisfying

$$W(h)^* \begin{pmatrix} a_{+,N}(h) & h^{N+1} b_N^*(h) \\ h^{N+1} b_N(h) & a_{-,N}(h) \end{pmatrix} W(h) = \begin{pmatrix} a_{+,N+1}(h) & h^{N+2} b_{N+1}^*(h) \\ h^{N+2} b_{N+1}(h) & a_{-,N+1}(h) \end{pmatrix},$$

where $a_{\pm,N+1}(h)$ is an h -admissible pseudo-differential operator of principal symbol $\lambda_{\pm}(x, \xi) 1_2$ and $b_{N+1}(h)$ is an h -admissible pseudo-differential operator of order $-(N+2)$. The $(N+1)$ th property is satisfied with the unitary operator

$$W_{N+1}(h) = W_N(h) W(h).$$

Thus Proposition 4.2 is proved. \square

Proof of Lemma 4.3. This lemma is proved in [15, Corollary 3.1.2] for bounded operators following a method due to M. Taylor. Here, the principal symbol is not bounded, but it is diagonal.

We get from (iii) that $a_+(h) - a_-(h)$ is invertible, hence we can define

$$J = (a_+ - a_-)^{-1}$$

which has the principal symbol $\sigma_p(J) = (\lambda_+ - \lambda_-)^{-1} 1_m$ of weight $(-1, 0)$.

Let $\widetilde{W}(h)$ be the operator

$$\widetilde{W}(h) = \begin{pmatrix} \text{Id} & -h^k b^* J(h) \\ h^k b J(h) & \text{Id} \end{pmatrix}.$$

We have

$$\widetilde{W}^*(h) \widetilde{W}(h) = \begin{pmatrix} 1_m & h^{k+1} r_1^*(h) \\ h^{k+1} r_1(h) & 1_m \end{pmatrix} + O(h^{2k}),$$

where $r_1(h) = h^{-1}[b, J]$ is an h -admissible pseudo-differential operator of weight $(q-2, 0)$ and

$$(11) \quad \widetilde{W}^*(h) M_k(h) \widetilde{W}(h) = \begin{pmatrix} a_+(h) & h^{k+1} \tilde{b}^*(h) \\ h^{k+1} \tilde{b}(h) & a_-(h) \end{pmatrix} + h^{k+1} R_{k+1}(h),$$

where

$$\tilde{b}(h) = h^{-1}(-Jb a_+ + b + a_- bJ),$$

and $R_{k+1}(h)$ is an h -admissible pseudo-differential operator of weight $(q-1, 0)$. Using (ii) (i.e. that the principal symbol of a_{\pm} commutes with all matrices), we obtain that $\tilde{b}(h)$ is an h -admissible pseudo-differential operator of weight $(q-1, 0)$.

At last, to have a unitary transformation, we put, for sufficiently small h ,

$$W(h) = \widetilde{W}(h) (\widetilde{W}^*(h) \widetilde{W}(h))^{-1/2},$$

which also satisfies the relation (11) because $h^{-k-1}(W(h) - \widetilde{W}(h))$ is an h -admissible pseudo-differential operator of weight $(q-2, 0)$. \square

Corollary 4.4. *Let H be the Dirac operator with A and V satisfying (H_{δ}) with $\delta > 0$.*

For all $N \geq 0$, there exists a unitary h -admissible pseudo-differential operator $W_N(h)$ such that

(i) for all $t \in \mathbf{R}$,

$$W_N^* e^{ith^{-l}H(h)} W_N = \begin{pmatrix} e^{ith^{-l}a_{+,N}(h)} & 0 \\ 0 & e^{ith^{-l}a_{-,N}(h)} \end{pmatrix} + O(|t|h^{N+1-l}), \quad l \in \mathbf{N},$$

uniformly with respect to $(t, h) \in \mathbf{R} \times]0, h_0]$;

(ii) for $f \in \mathcal{S}(\mathbf{R})$,

$$W_N^* f(H) W_N = \begin{pmatrix} f(a_{+,N}(h)) & 0 \\ 0 & f(a_{-,N}(h)) \end{pmatrix} + O(h^{N+1} \|\hat{f}'\|_{L^1(\mathbf{R})}),$$

where $a_{\pm,N}(h)$ is an h -admissible pseudo-differential operator, of principal symbol $\lambda_{\pm}(x, \xi)1_2$.

Proof. According to Proposition 4.2, there is a unitary h -admissible pseudo-differential operator W_N such that, $W_N^* e^{ith^{-l}H(h)} W_N = e^{ith^{-l}\tilde{H}(h)}$ with

$$\tilde{H} = W_N^* H W_N = \begin{pmatrix} a_{+,N} & 0 \\ 0 & a_{-,N} \end{pmatrix} + h^{N+1} R_{N+1},$$

where $R_{N+1}(h)$ is uniformly bounded for $h \in]0, h_0]$, $h_0 > 0$.

Then, (i) is a consequence of the Duhamel formula

$$e^{ith^{-l}\tilde{H}(h)} = e^{ith^{-l}D_N(h)} + ih^{N+1-l} \int_0^t e^{ish^{-l}\tilde{H}(h)} R_{N+1}(h) e^{i(t-s)h^{-l}D_N(h)} ds,$$

where $D_N(h) = \begin{pmatrix} a_{+,N}(h) & 0 \\ 0 & a_{-,N}(h) \end{pmatrix}$.

Part (ii) is a direct consequence of (i) (for $l=0$) using the Fourier transform

$$f(H) = \frac{1}{2\pi} \int_{\mathbf{R}} e^{itH} \hat{f}(t) dt. \quad \square$$

4.2. Semi-classical estimates

We are interested here in quantum propagation estimates controlled in the semi-classical parameter. For that, we introduce an assumption on the corresponding classical systems. For a classical Hamiltonian $\lambda(x, \xi)$ defined in the phase space \mathbf{R}^{2n} , let us consider the flow defined by the Hamiltonian vector field $(\partial_{\xi}\lambda, -\partial_x\lambda)$,

$$\Phi_{\lambda}^t : (x, \xi) \longrightarrow (z(t, x, \xi), \zeta(t, x, \xi)).$$

Definition 4.5. We say that an energy band $J \subset \mathbf{R}$ is non-trapping for $\lambda(x, \xi)$ if for every $R > 0$ there exists $T_R \geq 0$ such that

$$|z(t, x, \xi)| > R \quad \text{for } \lambda(x, \xi) \in J, \quad |t| > T_R, |x| < R.$$

In the following, we consider the two eigenvalues λ_{\pm} (of multiplicity 2) of the h -principal-symbol of H which are defined as $\lambda_{\pm}(x, \xi) = \pm \langle \xi - A(x) \rangle + V(x)$.

Assuming (H_{δ}) with $\delta > 1$, for $\mu \in]-\infty, -1[\cup]1, +\infty[$, the following limit exists in the uniform operator topology of $L^2(\mathbf{R}^3, \mathbf{C}^4)$, uniformly on compact sets:

$$\langle x \rangle^{-s} (H - \mu \pm i0)^{-1} \langle x \rangle^{-s} = \lim_{\varepsilon \rightarrow 0^+} \langle x \rangle^{-s} (H - \mu \pm i\varepsilon)^{-1} \langle x \rangle^{-s}$$

for every real $s > \frac{1}{2}$ (see [1], [12], [26]), and for every $s > \frac{1}{2} + k$, it is of class C^k with

$$\frac{d^k}{d\mu^k} [\langle x \rangle^{-s} (H - \mu \pm i0)^{-1} \langle x \rangle^{-s}] = k! \langle x \rangle^{-s} (H - \mu \pm i0)^{-k-1} \langle x \rangle^{-s}.$$

Under the non-trapping assumption, we also have the following result.

Proposition 4.6. *Assume (H_{δ}) with $\delta > 0$ and that $J \subset]-\infty, -1[\cup]1, +\infty[$ is a non-trapping compact interval for $\lambda_{\pm}(x, \xi)$. Then, for every $s > k - \frac{1}{2}$,*

$$\| \langle x \rangle^{-s} (H - \mu \pm i0)^{-k} \langle x \rangle^{-s} \| = O(h^{-k}), \quad \text{as } h \searrow 0 \text{ uniformly for } \mu \in J.$$

This estimate is established by S. Cerbahi [8] (for $A=0$ and $V \in C_0^{\infty}(\mathbf{R}^3)$) and by T. Jecko [17] (for $A=0$ and assuming (H_{δ}) for V). As in [8] and [17], our proof is based on Mourre's commutator method (see [18], or [16] for the semi-classical case) and a construction of global escape function given by Gerard–Martinez [10].

According to Remark 2.2, for λ_0 non-trapping for λ_+ and λ_- , only one of the two surfaces $\Sigma_{\lambda_0}(\lambda_+)$, $\Sigma_{\lambda_0}(\lambda_-)$ is non-empty. Then it is sufficient to construct escape functions $g_{\pm}(x, \xi)$ of $\lambda_{\pm}(x, \xi)$.

Lemma 4.7. *Assume (H_{δ}) with $\delta > 0$. Then, for any energy level $\pm\lambda_0 > 1$, non-trapping for λ_{\pm} , there exists g_{\pm} in the symbol class $S_1(\langle x \rangle^1, \langle \xi \rangle^1)$, $\varepsilon > 0$ and $C_0 > 0$ such that*

$$\{\lambda_{\pm}, g_{\pm}\} \geq C_0$$

on $\lambda_{\pm}^{-1}([\lambda_0 - \varepsilon, \lambda_0 + \varepsilon]) := \bigcup_{\mu \in]\lambda_0 - \varepsilon, \lambda_0 + \varepsilon[} \Sigma_{\mu}(\lambda_{\pm})$, where $\{a, b\} := \partial_{\xi} a \partial_x b - \partial_x a \partial_{\xi} b$ is the Poisson bracket.

Proof of Lemma 4.7. We construct an escape function $g_+(A, V)$ for $\lambda_+(A, V)$, then the function $g_- = -g_+(A, -V)$ will be an escape function for λ_- , because $\lambda_-(A, V) = -\lambda_+(A, -V)$.

Let $(x, \xi) \in \lambda_+^{-1}([\lambda_0 - \varepsilon, \lambda_0 + \varepsilon])$,

$$\{\lambda_+, x \cdot \xi\}(x, \xi) = \frac{\xi - A(x)}{\langle \xi - A(x) \rangle} \cdot \xi - x \cdot \left(\nabla_x V - \frac{\nabla_x(\xi - A(x))^2}{2\langle \xi - A(x) \rangle} \right).$$

Then, owing to (H_δ) , for $\lambda_0 > 1$, there exists $R > 0$ such that, for $\varepsilon > 0$ small enough,

$$\{\lambda_+, x \cdot \xi\}(x, \xi) \geq \frac{1}{2}(\lambda_0 - 1) \quad \text{for } |x| > R.$$

Let $\Psi \in C_0^\infty(\{x \in \mathbf{R}^3 : |x| \leq 2\})$ such that $\Psi(x) = 1$ for $|x| \leq 1$ and $0 \leq \Psi \leq 1$. Let us denote $\Psi_R(x) = \Psi(x/R)$ and

$$\tilde{g}_+(x, \xi) = - \int_0^{+\infty} \Psi_R(z_+(t, x, \xi)) dt$$

where $z_+(t, x, \xi)$ is the first component of the flow defined by λ_+ . The non-trapping condition implies that \tilde{g}_+ is bounded and of class C^∞ on $\lambda_+^{-1}([\lambda_0 - \varepsilon, \lambda_0 + \varepsilon])$, and $\{\lambda_+, \tilde{g}_+\}(x, \xi) = \Psi_R(x)$.

Then, we introduce

$$g_+(x, \xi) := C_+ \Psi_{MR}(x) \tilde{g}_+(x, \xi) + x \cdot \xi.$$

The function g_+ is of class C^∞ on $\lambda_+^{-1}([\lambda_0 - \varepsilon, \lambda_0 + \varepsilon])$, belongs to $S_1(\langle x \rangle^1, \langle \xi \rangle^1)$ and satisfies

$$\{\lambda_+, g_+\} = C_+ \Psi_R + \{\lambda_+, x \cdot \xi\} + C_+ \tilde{g}_+ \{\lambda_+, \Psi_{MR}(x)\}.$$

Moreover, by the definition of R and Ψ_R , we have

$$\{\lambda_+, x \cdot \xi\}(1 - \Psi_R) \geq \frac{1}{2}(\lambda_0 - 1)(1 - \Psi_R),$$

hence, for $C_+ > 0$ large enough,

$$C_+ \Psi_R + \{\lambda_+, x \cdot \xi\} \geq \frac{1}{2}(\lambda_0 - 1).$$

Here we have used that $\{\lambda_+, x \cdot \xi\}$ is bounded on $\lambda_+^{-1}([\lambda_0 - \varepsilon, \lambda_0 + \varepsilon]) \cap \{|x| \leq 2R\}$.

Next, we choose a large $M > 1$ such that

$$|C_+ \tilde{g}_+ \{\lambda_+, \Psi_{MR}(x)\}| \leq \frac{1}{4}(\lambda_0 - 1),$$

and we obtain that for such C_+ and M we have

$$\{\lambda_+, g_+\} \geq \frac{1}{4}(\lambda_0 - 1)$$

on $\lambda_+^{-1}(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon]$. This proves the lemma with $C_0 = \frac{1}{4}(\lambda_0 - 1)$. \square

Proof of Proposition 4.6. We consider the case $\lambda_0 > 1$, the same proof works for $\lambda_0 < -1$ (replacing ‘+’ by ‘-’ and $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ by $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$).

Let

$$G_+(x, hD) = W_1(h) \begin{pmatrix} g_+(x, hD)1_2 & 0 \\ 0 & 0 \end{pmatrix} W_1^*(h),$$

where $W_1(h)$ is defined in Proposition 4.2 (for $N=1$) and $g_+(x, hD) = Op_h^\omega(g_+)$, g_+ being the escape function of Lemma 4.7.

Using functional calculus [14], [19], we easily prove that G_+ is a conjugate operator of H (in the sense of Mourre) and that H is k -smooth with respect to G_+ . The main property is the so-called Mourre estimate

$$(12) \quad \chi(H)[H, G_+]\chi(H) \geq Ch\chi^2(H)$$

uniformly for small h and for $\chi \in C_0^\infty(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon]$ such that $\chi(\lambda_0) = 1$.

According to the definition of $W_1(h)$ (see Proposition 4.2), and to Corollary 4.4, we have

$$\chi(H)[H, G_+]\chi(H) = W_1(h) \begin{pmatrix} C_+(x, hD) & 0 \\ 0 & 0 \end{pmatrix} W_1^*(h) + O(h^2),$$

where

$$C_+(x, hD) = \chi(a_{+,1}(x, hD))[a_{+,1}(x, hD), g_+(x, hD)1_2]\chi(a_{+,1}(x, hD))$$

which, by the construction of g_+ , is bounded from below by $Ch\chi(a_{+,1}(x, hD))^2$.

Let us recall that

$$\chi(H) = W_1(h) \begin{pmatrix} \chi(a_{+,1}(x, hD)) & 0 \\ 0 & \chi(a_{-,1}(x, hD)) \end{pmatrix} W_1^*(h) + O(h^2),$$

with $\chi(a_{-,1}(x, hD)) = O(h^\infty)$, because $\lambda_0 > 1$ non-trapping implies that $\lambda_-^{-1}(\lambda_0) := \Sigma_{\lambda_0}(\lambda_-) = \emptyset$, i.e. for small ε and for any $k \in \mathbf{N}$, $\chi^{(k)}(\lambda_-(x, \xi)) = 0$.

This gives the Mourre inequality (12). Then using Mourre’s results [18], we have Proposition 4.6 for $\mu \in [\lambda_0 - \varepsilon, \lambda_0 + \varepsilon]$, and at last, using compactness of J we deduce the Mourre estimate uniformly for $\mu \in J$. \square

The following crude estimate will be used later.

Corollary 4.8. *Assume (H_δ) with $\delta > 3$ and that $J \subset]-\infty, -1[\cup]1, +\infty[$ is a non-trapping compact interval for $\lambda_\pm(x, \xi)$. Then*

$$\left| \frac{d}{d\lambda} s_h(\lambda) \right| + \left| \frac{d^2}{d\lambda^2} s_h(\lambda) \right| = O(h^{-6}), \quad \text{as } h \searrow 0 \text{ uniformly for } \lambda \in J.$$

Proof. It follows from the definition of $s(\lambda)$, (1), that

$$\frac{d}{d\lambda} s_h(\lambda) = -\frac{1}{2i\pi} \operatorname{Tr} \left(\frac{dS_h}{d\lambda} S_h(\lambda)^* \right),$$

where $S_h(\lambda)$ is the scattering matrix for the pair $(H(h), H_0(h))$. Then, as in Corollary 5.8 of [20], the above corollary is a consequence of trace norm estimates for $S_h(\lambda) - \operatorname{Id}$ deduced from Proposition 4.6 and from the stationary representation of $S_h(\lambda)$ [1]. \square

4.3. Proof of Theorem 2.3

Keeping h fixed in the proof of Proposition 3.2, we obtain that $(d/d\lambda)s_h$ is the distribution

$$f \longmapsto \operatorname{Tr}(W(h)(H^2 - 1)^{-1} f(H)) \quad \text{for all } f \in C_0^\infty(]-\infty, -1[\cup]1, +\infty[),$$

where $W(h) = (Q - \frac{1}{2}i[Q, \mathcal{A}])(h)$ with $Q(h) \doteq H^2 - H_0^2$ and $\mathcal{A}(h) = \frac{1}{2}(x \cdot hD + hD \cdot x)$. That is, in the distribution sense, on $]-\infty, -1[\cup]1, +\infty[$, we have

$$\frac{d}{d\lambda} s_h = \operatorname{Tr} \left(W(h)(H^2 - 1)^{-1} \frac{dE_h}{d\lambda} \right)$$

(E_h is the spectral projector associated with H).

For $I \subset]-\infty, -1[\cup]1, +\infty[$ non-trapping for λ_\pm and J a compact subset of I , let us introduce

$$\tau_r(h, \lambda) = \frac{1}{2\pi h} \int_{\mathbf{R}} e^{-ith^{-1}\lambda} \operatorname{Tr}(W(h)(H^2 - 1)^{-1} g(H) e^{ith^{-1}H}) \theta(r^{-1}t) dt,$$

where $g \in C_0^\infty(I)$ such that $g(\lambda) = 1$ for $\lambda \in J$ and $\theta \in C_0^\infty(]-2, 2[)$ such that $\theta(t) = 1$ for $|t| \leq 1$, $0 \leq \theta \leq 1$.

Lemma 4.9. *Under the hypothesis of Theorem 2.3, for all $M \in \mathbf{N}$, we have*

- (i) $\frac{d}{d\lambda} s_h(\lambda) - \tau_{(h^{-M})}(h, \lambda) = O(h^{M-6});$
- (ii) *for fixed $T > 0$, $\tau_{(h^{-M})}(h, \lambda) - \tau_T(h, \lambda) = O(h^\infty)$ as $h \searrow 0$ uniformly for $\lambda \in J$.*

Proof. To prove (i), we use a classical method of smoothing by convolution. Indeed, we have

$$\tau_{(h^{-M})}(h, \lambda) = \left(g \frac{d}{d\lambda} s_h * \hat{\theta}_M \right)(\lambda),$$

where $\theta_M(t) = \theta(h^M t)$. Using that $\int \hat{\theta}_M(\lambda) d\lambda = \theta_M(0) = 1$, (i) follows from Corollary 4.8 (see step (4) in the proof of Theorem 0.1 of [23]).

The proof of (ii) is based on the h -decoupling of the Dirac operator (Subsection 4.1) and on some known results concerning the scalar case.

For $r = h^{-M}$ or $r = T$, Corollary 4.4 gives

$$\tau_r(h, \lambda) = \tau_r^{+,N}(h, \lambda) + \tau_r^{-,N}(h, \lambda) + R_r^N(h, \lambda),$$

where

$$\begin{aligned} \tau_r^{\pm,N}(h, \lambda) &= \frac{1}{2\pi h} \int_{\mathbf{R}} e^{-ith^{-1}\lambda} \text{Tr}\{W_N^* W W_N p_{\pm} \otimes [(a_{\pm,N}^2 - 1)^{-1} g(a_{\pm,N}) e^{ith^{-1}a_{\pm,N}}]\} \theta(r^{-1}t) dt, \end{aligned}$$

where $p_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $p_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ and for an operator a on $L^2(\mathbf{R}^3, \mathbf{C}^2)$,

$$p_+ \otimes a = \begin{pmatrix} a & 0 \\ 0 & 0 \end{pmatrix}, \quad p_- \otimes a = \begin{pmatrix} 0 & 0 \\ 0 & a \end{pmatrix}$$

are operators on $L^2(\mathbf{R}^3, \mathbf{C}^4)$, and

$$R_r^N(h, \lambda) = \frac{1}{2\pi h} \int_{\mathbf{R}} e^{-ith^{-1}\lambda} O(|t|h^N) \theta(r^{-1}t) dt.$$

Because the support of $\theta(h^M t) - \theta(T^{-1}t)$ is a subset of $\{t: T < |t| \leq h^{-M}\}$, we have

$$(13) \quad R_{(h^{-M})}^N(h, \lambda) - R_T^N(h, \lambda) = O(h^{N-M-1}).$$

At last, following the proof of Lemmas 3.2 and 3.3 of [23], we get

$$\tau_{(h^{-M})}^{\pm,N}(h, \lambda) - \tau_T^{\pm,N}(h, \lambda) = O(h^\infty)$$

under the non-trapping condition. The methods used in [23] (or in [13]) work in the same way, because the principal symbol of $a_{\pm,N}$ is of scalar type $(=\lambda_{\pm}(x, \xi)1_2)$. \square

Then, asymptotic expansion of $(d/d\lambda)s_h(\lambda)$ is a consequence of the following lemma.

Lemma 4.10. *Under the hypothesis of Theorem 2.3, there exists $T>0$ such that for h small enough, $\tau_T(h, \lambda)$ has an asymptotic expansion in h ,*

$$\tau_T(h, \lambda) \asymp (2\pi)^{-3} \sum_{j \geq 1} c_j(\lambda) h^{-3+j}, \quad \text{as } h \searrow 0 \text{ uniformly for } \lambda \in J.$$

Proof. We can prove this lemma in two different ways: using h -decoupling and studying short time parametrix for $e^{ith^{-1}a_{\pm, N}}$ (as in [13]), or using directly short time parametrix construction for $e^{ith^{-1}H}$ developed by K. Yajima in [25].

In the same standard way, as in [23] (proof of Lemma 3.1) (or for example in [9], [13]), short time parametrix construction for the propagator gives an asymptotic expansion of $\tau_T(h, \lambda)$. \square

Proof of Theorem 2.3. The existence of the asymptotic expansion is given by Lemmas 4.9 and 4.10. For computation of $c_0(\lambda)$, we use weak asymptotic which is a direct consequence of functional calculus on pseudo-differential operators, as settled in [14], [19]. We have

$$\int s_h(\lambda) f'(\lambda) d\lambda = \text{Tr}(f(H) - f(H_0)) = h^{-3} \sum_{j \geq 0} \gamma_j(f) h^j$$

with

$$(14) \quad \gamma_0(f) = (2\pi)^{-3} \int_{\mathbf{R}^6} \text{tr}\{f(\alpha \cdot (\xi - A(x)) + \beta + V(x)1_4) - f(\alpha \cdot \xi + \beta)\} d\xi dx$$

(tr is the trace of the matrix).

The unitary transformation $u(H(x, \xi))$ (defined by (10)) brings $H(x, \xi) := \alpha \cdot (\xi - A(x)) + \beta + V(x)1_4$ to $\begin{pmatrix} \lambda_+ 1_2 & 0 \\ 0 & \lambda_- 1_2 \end{pmatrix}$. Then, the integrand term in (14) is equal to

$$2(f(\lambda_+) + f(\lambda_-) - f(\langle \xi \rangle) - f(-\langle \xi \rangle)).$$

This gives

$$c_0(\lambda) = 2 \frac{d}{d\lambda} \int_{\mathbf{R}^3} \left(\int_{\lambda_+(x, \xi) \leq \lambda} d\xi - \int_{\langle \xi \rangle \leq \lambda} d\xi \right) - \left(\int_{\lambda_-(x, \xi) \geq \lambda} d\xi - \int_{-\langle \xi \rangle \geq \lambda} d\xi \right) dx.$$

Putting $\zeta = \xi - A(x)$ and $\zeta = r\omega$ ($\omega \in S^2$), we have

$$\int_{\pm \lambda_{\pm}(x, \xi) \leq \pm \lambda} d\xi = \int_{\langle \zeta \rangle \pm V(x) \leq \pm \lambda} d\xi = \frac{4\pi}{3} \int_{\mathbf{R}^3} ((\lambda - V(x))^2 - 1)_+^{3/2} dx$$

for $\pm\lambda > \nu_{\pm}$ defined in Remark 2.2. Thus, we obtain $c_0(\lambda)$ as claimed in Theorem 2.3. \square

Remark 4.11. In the same way, known methods can be easily adapted to apply Tauberian theorems like in [22], to get a Weyl type formula when λ_+ have trapped trajectories. More precisely, if $I \subset]-\infty, -1[\cup]1, +\infty[$ is such that λ_+ and λ_- have no critical values in I , then we can prove the Weyl formula

$$s_h(\lambda) = (2\pi)^{-3} C_0(\lambda) h^{-3} + O(h^{-2}), \quad \text{as } h \searrow 0,$$

uniformly for λ in each compact subset of J , where

$$C_0(\lambda) = \int_{\mathbf{R}^3} \left(\int_{\lambda_+(x, \xi) \leq \lambda} d\xi - \int_{\langle \xi \rangle \leq \lambda} d\xi \right) - \left(\int_{\lambda_-(x, \xi) \geq \lambda} d\xi - \int_{-\langle \xi \rangle \geq \lambda} d\xi \right) dx.$$

5. Non-relativistic limit

In this section, we introduce again the parameter c (keeping $\hbar=1$) and we will study the behaviour as $c \rightarrow +\infty$ of the scattering phase, $s^{\pm}(\lambda)$, related to the operators $(H'_{\pm}, H'_{0, \pm})$, where

$$H'_{\pm} := H \mp c^2, \quad H'_{0, \pm} := H_0 \mp c^2.$$

The operators H'_+ (resp. H'_-) and $H'_{0,+}$ (resp. $H'_{0,-}$) have the same essential spectrum

$$\sigma_e(H'_+) = \sigma_e(H'_{0,+}) =]-\infty, -2c^2] \cup [0, +\infty[,$$

of which the negative part “tends” to $-\infty$, as $c \rightarrow +\infty$, and

$$\sigma_e(H'_-) = \sigma_e(H'_{0,-}) =]-\infty, 0] \cup [2c^2, +\infty[,$$

of which the positive part “tends” to $+\infty$, as $c \rightarrow +\infty$.

In the following, we study only $s^+(\lambda)$ (the same proof works for $s^-(\lambda)$) and to simplify the notation, we drop the sign ‘+’. Thus, we write H' (resp. H'_0) for H'_+ (resp. $H'_{0,+}$), and for $s^+(\lambda)$ we write $s_{\times}(\lambda)$, where

$$\varkappa := \frac{1}{c}$$

tends to 0^+ , as $c \rightarrow +\infty$.

The operators acting in $L^2(\mathbf{R}^3; \mathbf{C}^2)$ (resp. $\mathbf{C}^2 \otimes L^2(\mathbf{R}^3; \mathbf{C}^2)$) will be denoted, in general, by small (resp. capital) letters. Let us introduce some matrices, $I = 1_2 \otimes 1_2$ the identity on $\mathbf{C}^2 \otimes \mathbf{C}^2 \simeq \mathbf{C}^4$ and the matrices on \mathbf{C}^2 ,

$$\begin{aligned} \sigma_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \nu = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \\ \mu &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \eta = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \bar{\eta} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \end{aligned}$$

These matrices satisfy

$$(15) \quad \begin{aligned} \nu \sigma_1 &= \bar{\eta}, \quad \sigma_1 \nu = \eta, \\ \mu \sigma_1 &= \eta, \quad \sigma_1 \mu = \bar{\eta}. \end{aligned}$$

So, the Dirac operators, H and H_0 , can be defined in the Hilbert space

$$\mathcal{H} := \mathbf{C}^2 \otimes L^2(\mathbf{R}^3; \mathbf{C}^2)$$

by

$$(16) \quad H = H_{\varkappa} = \frac{1}{\varkappa^2} (\sigma_3 \otimes 1_2 + \varkappa \sigma_1 \otimes \sigma \cdot (D - A) + \varkappa^2 \nu \otimes V_+ + \varkappa^2 \mu \otimes V_-),$$

$$(17) \quad H_0 = H_{0, \varkappa} = \frac{1}{\varkappa^2} (\sigma_3 \otimes 1_2 + \varkappa \sigma_1 \otimes \sigma \cdot D).$$

In this section, our goal is to compare $s_{\varkappa}(\lambda)$ with $s_{\infty}(\lambda)$, the scattering phase for (h_+, h_0) (see (3)), as $\varkappa \rightarrow 0^+$ (for λ fixed). We will give a Taylor series expansion, in \varkappa , of s_{\varkappa} (and also for its derivatives with respect to $\lambda > 0$). It will be a consequence of the C^∞ -regularity of s_{\varkappa} with respect to (\varkappa, λ) near $\varkappa = 0$.

For that, we study the smoothness of

$$T_{\varkappa}(\lambda) := \text{Id} - S_{\varkappa}(\lambda),$$

where $S_{\varkappa}(\lambda)$ is the scattering matrix for (H', H'_0) which is related to $s_{\varkappa}(\lambda)$ by the relation

$$\frac{d}{d\lambda} s_{\varkappa}(\lambda) = \frac{i}{2\pi} \text{tr} \left(\frac{dS_{\varkappa}}{d\lambda}(\lambda) S_{\varkappa}^*(\lambda) \right).$$

Introduce \varkappa and substitute (H, H_0) for (H', H'_0) in the proof of Theorem 4.2 of [1]. Then for A and V satisfying (H_δ) with $\delta > 1$, we obtain

$$T_{\varkappa}(\lambda) = 2i\pi T_{0, \varkappa}(\lambda) \left(V_{\varkappa} - V_{\varkappa} R_{\varkappa} \left(\lambda + \frac{1}{\varkappa^2} + i0 \right) V_{\varkappa} \right) T_{0, \varkappa}^*(\lambda),$$

with

$$V_{\varkappa} = V - \frac{1}{\varkappa} \alpha \cdot A, \quad R_{\varkappa} \left(\lambda + \frac{1}{\varkappa^2} + i0 \right) = \left(H_{\varkappa} - \lambda - \frac{1}{\varkappa^2} - i0 \right)^{-1},$$

and $T_{0,\varkappa}$ is the trace operator for $H_{0,\varkappa} - (1/\varkappa^2)$,

$$T_{0,\varkappa}(\lambda) = \left(\frac{1}{2} \varrho \right)^{1/2} \gamma_0(\varrho) \mathcal{F} \mathcal{P}_{+,\varkappa}, \quad \varrho = \left(\lambda + \frac{1}{2} \lambda^2 \varkappa^2 \right)^{1/2},$$

where \mathcal{F} is the Fourier transform on $\mathbf{C}^2 \otimes L^2(\mathbf{R}^3, \mathbf{C}^2)$, $\gamma_0(\varrho)$ is the trace operator for the free Schrödinger operator, $(\gamma_0(\varrho)f)(\omega) = f(\varrho\omega)$. The operator $\mathcal{P}_{+,\varkappa}$ is defined by

$$\mathcal{P}_{+,\varkappa} = \frac{1}{\sqrt{2}} q(\varkappa^2 \lambda, \varkappa D) P_+ G_{\varkappa}, \quad q(\varkappa^2 \lambda, \varkappa D) = ((1 + \varkappa^2 D^2)^{1/2} + \varkappa^2 \lambda + 1)^{1/2},$$

where G_{\varkappa} is the Foldy-Wouthuysen transformation,

$$(18) \quad G_{\varkappa} = (2(1 + \varkappa^2 D^2)^{1/2} + (1 + (1 + \varkappa^2 D^2)^{1/2}))^{-1/2} (1_2 \otimes (1 + (1 + \varkappa^2 D^2)^{1/2}) + \varkappa(\bar{\eta} \otimes \sigma \cdot D - \eta \otimes \sigma \cdot D)),$$

and $P_+ := \nu \otimes 1_2$.

Let us introduce the dilation group $\mathcal{U}(\varrho)$, $\mathcal{U}(\varrho)f(x) := \varrho^{3/2} f(\varrho x)$.

Lemma 5.1. *For $\lambda > 0$ and $\varrho = (\lambda + \frac{1}{2} \lambda^2 \varkappa^2)^{1/2}$ we have*

$$T_{0,\varkappa}(\lambda) = \frac{\varrho^{-1}}{\sqrt{2}} \gamma_0(1) \mathcal{F} \mathcal{P}_{+,\varkappa}(\varrho) \mathcal{U}(\varrho^{-1}), \quad T_{0,\varkappa}^*(\lambda) = \frac{\varrho^{-1}}{\sqrt{2}} \mathcal{U}(\varrho) \mathcal{P}_{+,\varkappa}^*(\varrho) \mathcal{F}^* \gamma_0(1)^*,$$

where $\mathcal{P}_{+,\varkappa}(\varrho)$ and its adjoint are operators of the form

$$\begin{aligned} \mathcal{P}_{+,\varkappa}(\varrho) &= \nu \otimes p_{\varkappa}(\varrho) + \varkappa \bar{\eta} \otimes q_{\varkappa}(\varrho), \\ \mathcal{P}_{+,\varkappa}^*(\varrho) &= \nu \otimes p_{\varkappa}(\varrho) + \varkappa \eta \otimes q_{\varkappa}(\varrho); \end{aligned}$$

$p_{\varkappa}(\varrho)$ and $q_{\varkappa}(\varrho)$ are operators on $L^2(\mathbf{R}^3, \mathbf{C}^2)$, and they are C^∞ with respect to $(\varkappa, \varrho) \in \mathbf{R} \times]0, +\infty[$ in $\mathcal{L}(H^{t,s}, H^{t-1/2,s})$ for all t and s reals.

The space $H^{t,s}$ is the weighted Sobolev space $\{f : \|\langle x \rangle^s f\|_{H^t} < \infty\}$.

Proof. Owing to $\gamma_0(\varrho) = \varrho^{-3/2} \gamma_0(1) \mathcal{U}(\varrho)$ and $\mathcal{U}(\varrho) \mathcal{F} = \mathcal{F} \mathcal{U}(\varrho^{-1})$, we deduce that $T_{0,\varkappa}(\lambda)$ is of the claimed form, with

$$\mathcal{P}_{+,\varkappa}(\varrho) = \mathcal{U}(\varrho^{-1}) \mathcal{P}_{+,\varkappa} \mathcal{U}(\varrho) = \frac{1}{\sqrt{2}} q(\varkappa^2 \lambda, \varkappa \varrho D) P_+ G_{\varkappa \varrho}.$$

Now by using $\nu \bar{\eta} = \bar{\eta}$ and $\nu \eta = 0$ (resp. $\bar{\eta} \nu = 0$ and $\eta \nu = \eta$) we obtain that $P_+ G_{\varkappa \varrho}$ (resp. $G_{\varkappa \varrho}^* P_+$) has no term with η (resp. $\bar{\eta}$). Thus, $\mathcal{P}_{+,\varkappa}(\varrho)$ and $\mathcal{P}_{+,\varkappa}^*(\varrho)$ are of the claimed form.

From the smoothness of the symbol of $q(\varkappa^2 \lambda, \varkappa \varrho D) P_+ G_{\varkappa \varrho}$, in $S(\langle \xi \rangle^{1/2})$, with respect to (\varkappa, ϱ) , we deduce the result. \square

Lemma 5.2. *Let H_\varkappa and $H_{0,\varkappa}$ be the Dirac operators defined by (16) and (17) such that the potentials A and V satisfy the hypothesis (H_δ) with $\delta > 1$. For $\lambda > 0$ and $\varrho > 0$, let*

$$R_\varkappa\left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0\right) := \mathcal{U}(\varrho^{-1})R_\varkappa\left(\lambda + \frac{1}{\varkappa^2} + i0\right)\mathcal{U}(\varrho),$$

$$R_\varkappa\left(\lambda + \frac{1}{\varkappa^2} + i0\right) = \left(H_\varkappa - \lambda - \frac{1}{\varkappa^2} - i0\right)^{-1}.$$

Then, there exists a neighbourhood \mathcal{V}_0 of $\varkappa=0$, and $s > \frac{1}{2}$, such that the map

$$(\varkappa, \varrho, \lambda) \longmapsto R_\varkappa\left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0\right)$$

is C^∞ from $\mathcal{V}_0 \times]0, +\infty[\times]0, +\infty[$ to $\mathcal{L}(L^{2,s}, L^{2,-s})$.

Moreover, there exist some operators r_0, r_1, \bar{r}_1 in $\mathcal{L}(L^{2,s}, L^{2,-s})$ such that

$$(19) \quad R_\varkappa(\varrho^{-1}) = \nu \otimes r_0(\varrho) + \varkappa(\bar{\eta} \otimes \bar{r}_1(\varrho) + \eta \otimes r_1(\varrho)) + O(\varkappa^2).$$

Proof. A straightforward calculation gives

$$R_\varkappa(\varrho^{-1}) := R_\varkappa(\varrho^{-1}, \lambda + 1/\varkappa^2 + i0)$$

$$= \left(\frac{1}{\varkappa} \mathcal{D}_A(\varrho) + \frac{1}{\varkappa^2} \beta + V(\varrho^{-1}) - \lambda - \frac{1}{\varkappa^2} - i0 \right)^{-1},$$

where $\mathcal{D}_A(\varrho) = \mathcal{U}(\varrho^{-1})\alpha \cdot (D - A)\mathcal{U}(\varrho) = \varrho\alpha \cdot (D - \varrho^{-1}A(\varrho^{-1}))$, $V(\varrho^{-1}) = \mathcal{U}(\varrho^{-1})V\mathcal{U}(\varrho)$ is the multiplication operator by $V(\varrho^{-1}x)$, and $A(\varrho^{-1}) = \mathcal{U}(\varrho^{-1})A\mathcal{U}(\varrho)$ is the multiplication operator by $A(\varrho^{-1}x)$.

For $s > \frac{1}{2}$, we have, in $\mathcal{L}(L^{2,s}, L^{2,-s})$,

$$(20) \quad R_\varkappa\left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0\right) = R_{A,\varkappa}\left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0\right)$$

$$\times \left(1 + V(\varrho^{-1})R_{A,\varkappa}\left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0\right) \right)^{-1},$$

where

$$R_{A,\varkappa}\left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0\right) = \left(\frac{1}{\varkappa} \mathcal{D}_A(\varrho) + \frac{1}{\varkappa^2} \beta - \lambda - \frac{1}{\varkappa^2} - i0 \right)^{-1}.$$

According to properties of the Dirac matrices, we obtain

$$R_{A,\varkappa}\left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0\right) = (\varkappa \mathcal{D}_A(\varrho) + \beta + 1 + \varkappa^2 \lambda) \frac{1}{2\varrho^2} K_{A,\varrho}(1 + i0),$$

where

$$K_{A,\varrho}(1+i0) = \left(\frac{1}{2}(\varrho^{-1}\mathcal{D}_A(\varrho))^2 - 1 - i0\right)^{-1}.$$

Let us put $\mathcal{A}(\varrho) = (\varrho^{-2}\mathcal{D}_A^2(\varrho) - \frac{1}{2}D^2)$, then

$$K_{A,\varrho}(1+i0) = \left(\frac{1}{2}D^2 - 1 - i0\right)^{-1} (1 + \mathcal{A}(\varrho) \left(\frac{1}{2}D^2 - 1 - i0\right)^{-1})^{-1}.$$

Moreover for A and V satisfying (H_δ) with $\delta > 1$, there exists $s > \frac{1}{2}$ such that the maps

$$\varrho \mapsto V(\varrho^{-1}), \quad \varrho \mapsto A(\varrho^{-1}), \quad \varrho \mapsto \mathcal{A}(\varrho)$$

are C^∞ in $\mathcal{L}(L^{2,-s}, L^{2,s})$, $\mathcal{L}(L^{2,-s}, (L^{2,s})^3)$ and $\mathcal{L}(H^{1,-s}, L^{2,s})$, resp. Hence from the previous equations, we deduce the existence of a neighbourhood \mathcal{V}_0 of $\varkappa=0$, and $s > \frac{1}{2}$, such that the map

$$(\varkappa, \varrho, \lambda) \mapsto R_\varkappa \left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0 \right)$$

is C^∞ from $\mathcal{V}_0 \times]0, +\infty[$ to $\mathcal{L}(L^{2,s}, L^{2,-s})$.

Now, to obtain (19) we prove that the limit of $R_\varkappa(\varrho^{-1}, \lambda + 1/\varkappa^2 + i0)$, as \varkappa tends to 0, belongs to $\nu \otimes \mathcal{L}(L^{2,s}, L^{2,-s})$, and its first derivative, with respect to \varkappa , at $\varkappa=0$, belongs to $\bar{\eta} \otimes \mathcal{L}(L^{2,s}, L^{2,-s}) \oplus \eta \otimes \mathcal{L}(L^{2,s}, L^{2,-s})$ for $s > \frac{1}{2}$.

We let

$$\begin{aligned} T_0(\varrho) &= \frac{1}{2}(1+\beta)K_{A,\varrho}(1+i0), \\ T_1(\varrho) &= \frac{1}{2}\varrho^{-2}\mathcal{D}_A(\varrho)K_{A,\varrho}(1+i0), \\ T_2(\varrho) &= \frac{1}{2}\varrho^{-2}\lambda K_{A,\varrho}(1+i0). \end{aligned}$$

We have

$$\begin{aligned} R_\varkappa \left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0 \right) &= (T_0(\varrho) + \varkappa T_1(\varrho) + \varkappa^2 T_2(\varrho)) \\ &\quad \times (1 + V(\varrho^{-1})(T_0(\varrho) + \varkappa T_1(\varrho) + \varkappa^2 T_2(\varrho)))^{-1}. \end{aligned}$$

Then, the limit as \varkappa tends to 0 of $R_\varkappa(\varrho^{-1}, \lambda + 1/\varkappa^2 + i0)$ is

$$(21) \quad T_0(\varrho)(1 + V(\varrho^{-1})T_0(\varrho))^{-1},$$

and its first derivative, with respect to \varkappa , at $\varkappa=0$, is

$$(22) \quad \begin{aligned} &T_1(\varrho)(1 + V(\varrho^{-1})T_0(\varrho))^{-1} \\ &\quad - T_0(\varrho)(1 + V(\varrho^{-1})T_0(\varrho))^{-1}V(\varrho^{-1})T_1(\varrho)(1 + V(\varrho^{-1})T_0(\varrho))^{-1}. \end{aligned}$$

Let us study the matrix representation of these terms. As $\alpha = \eta \otimes \sigma + \bar{\eta} \otimes \sigma$ and owing to

$$\eta \bar{\eta} = \mu, \quad \bar{\eta} \eta = \nu, \quad \eta^2 = \bar{\eta}^2 = 0,$$

we deduce that $\mathcal{D}_A(\varrho)$ is of the type $\eta \otimes d_A(\varrho) + \bar{\eta} \otimes d_A(\varrho)$ and also that $\mathcal{D}_A^2(\varrho) = \nu \otimes d_A^2(\varrho) + \mu \otimes d_A^2(\varrho)$. Then $K_{A,\varrho}(1+i0) \in \nu \otimes \mathcal{L}(L^{2,s}, L^{2,-s}) \oplus \mu \otimes \mathcal{L}(L^{2,s}, L^{2,-s})$ and as $\frac{1}{2}(1+\beta) = \nu \otimes 1_2$, $T_0(\varrho) \in \nu \otimes \mathcal{L}(L^{2,s}, L^{2,-s})$. Lastly, by assumption, $V(\varrho^{-1})$ belongs to $\nu \otimes \mathcal{L}(L^{2,-s}, L^{2,s}) \oplus \mu \otimes \mathcal{L}(L^{2,-s}, L^{2,s})$, thus, the limit as \varkappa tends to 0, given by (21), belongs to $\nu \otimes \mathcal{L}(L^{2,s}, L^{2,-s})$.

The matrix representation of $\mathcal{D}_A(\varrho)$, $K_{A,\varrho}(1+i0)$, and the equations

$$(23) \quad \eta \nu = \eta, \quad \bar{\eta} \mu = \bar{\eta}, \quad \eta \mu = \bar{\eta} \nu = 0,$$

give that $T_1(\varrho), T_1(\varrho)(1+V(\varrho^{-1})T_0(\varrho))^{-1} \in \eta \otimes \mathcal{L}(L^{2,s}, L^{2,-s}) \oplus \bar{\eta} \otimes \mathcal{L}(L^{2,s}, L^{2,-s})$. In the same way, using the transposition of the relations (23), we obtain that (22) are in $\eta \otimes \mathcal{L}(L^{2,s}, L^{2,-s}) \oplus \bar{\eta} \otimes \mathcal{L}(L^{2,s}, L^{2,-s})$. \square

Before expressing the main theorem of this section, let us give some relations, resulting from the properties of ν , μ , η and $\bar{\eta}$.

Lemma 5.3. *Let \mathcal{P} , \mathcal{P}^* , V and R be matrices on $\mathbf{C}^2 \otimes \mathbf{C}^2$, of the types*

$$\begin{aligned} \mathcal{P} &= \nu \otimes p + \varkappa \bar{\eta} \otimes q, & V &= \nu \otimes V_+ + \mu \otimes V_- + \frac{1}{\varkappa}(\eta \otimes A + \bar{\eta} \otimes \bar{A}), \\ \mathcal{P}^* &= \nu \otimes p + \varkappa \eta \otimes q, & R &= \nu \otimes r + \varkappa(\eta \otimes r_1 + \bar{\eta} \otimes \bar{r}_1) + \varkappa^2 R_2, \end{aligned}$$

ν , μ , η and $\bar{\eta}$ being the matrices defined at the beginning of this section.

Then, $\mathcal{P}V\mathcal{P}^*$ and $\mathcal{P}VRV\mathcal{P}^*$ are polynomials with respect to \varkappa . In particular the singularity of V vanishes.

Theorem 5.4. *Let H_\varkappa and $H_{0,\varkappa}$ be the Dirac operators defined by (16) and (17) such that the potentials A and V satisfy (H_δ) with $\delta > 1$. Let $T_\varkappa := \text{Id} - S_\varkappa(\lambda)$, with $S_\varkappa(\lambda)$ being the scattering matrix associated with $(H_\varkappa - 1/\varkappa^2, H_{0,\varkappa} - 1/\varkappa^2)$.*

If $\delta > 1 + 2/p$, $p \geq 1$, then $T_\varkappa(\lambda)$ is a Schatten class operator, i.e. $T_\varkappa(\lambda)$ is in $\sigma_p(\mathbf{C}^2 \otimes L^2(S^2, \mathbf{C}^2))$. In particular, if $\delta > 3$, $T_\varkappa(\lambda)$ is a trace class operator; if $\delta > 2$, $T_\varkappa(\lambda)$ is a Hilbert–Schmidt class operator.

Moreover, there exists a neighbourhood \mathcal{V}_0 of $\varkappa = 0$ such that the map

$$(\varkappa, \lambda) \longmapsto T_\varkappa(\lambda)$$

is C^∞ from $\mathcal{V}_0 \times]0, +\infty[$ to $\sigma_p(\mathbf{C}^2 \otimes L^2(S^2, \mathbf{C}^2))$.

Proof. Our starting point is the formula

$$T_{\varkappa}(\lambda) = 2i\pi \frac{\varrho^{-2}}{2} \gamma_0(1) \mathcal{F} \mathcal{P}_{+,\varkappa}(\varrho) \\ \times \left(V_{\varkappa}(\varrho^{-1}) - V_{\varkappa}(\varrho^{-1}) R_{\varkappa} \left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0 \right) V_{\varkappa}(\varrho^{-1}) \right) \mathcal{P}_{+,\varkappa}^*(\varrho) \mathcal{F}^* \gamma_0(1)^*,$$

where ϱ is the smoothness function (with respect to (λ, \varkappa) , $\lambda > 0$) $\varrho = (\lambda + \frac{1}{2} \lambda^2 \varkappa^2)^{1/2}$.

Let us recall that $\gamma_0(1) \mathcal{F} \langle x \rangle^{-s} \langle D_x \rangle^m$ is a Schatten class $\sigma_{p/2}(L^2(\mathbf{R}^3), L^2(S^2))$ operator for any $m \in \mathbf{R}$ and for $s > 1/p + \frac{1}{2}$ (see Lemma 5.7 of [20]). Then we are going to prove that there exists $s > 1/p + \frac{1}{2}$ and m_1, m_2 in \mathbf{R} such that the map

$$(24) \quad (\varkappa, \varrho) \mapsto \mathcal{P}_{+,\varkappa}(\varrho) \left(V_{\varkappa}(\varrho^{-1}) - V_{\varkappa}(\varrho^{-1}) R_{\varkappa} \left(\varrho^{-1}, \lambda + \frac{1}{\varkappa^2} + i0 \right) V_{\varkappa}(\varrho^{-1}) \right) \mathcal{P}_{+,\varkappa}^*(\varrho)$$

is C^∞ from $\mathcal{V}_0 \times]0, +\infty[$ to $\mathcal{L}(H^{m_1, -s}, H^{m_2, s})$ where \mathcal{V}_0 is a neighbourhood of $\varkappa = 0$.

Under the assumption (H_δ) , with $\delta > 1 + 2/p$, according to the previous lemmas, the main problem is to make the singularity of $V_{\varkappa}(\varrho^{-1})$, at $\varkappa = 0$,

$$V_{\varkappa}(\varrho^{-1}) = V(\varrho^{-1}) - \frac{1}{\varkappa} A(\varrho^{-1})$$

vanish. But, according to Lemmas 5.1 and 5.2, we can apply Lemma 5.3 to $V = V_{\varkappa}(\varrho^{-1})$, $\mathcal{P} = \mathcal{P}_{+,\varkappa}(\varrho)$, $\mathcal{P}^* = \mathcal{P}_{+,\varkappa}^*(\varrho)$ and $R = R_{\varkappa}(\varrho^{-1}, \lambda + 1/\varkappa^2 + i0)$.

Thus, we obtain the smoothness of the map (24) from $\mathcal{V}_0 \times]0, +\infty[$ to $\mathcal{L}(H^{m_1, -s}, H^{m_2, s})$. This ends the proof of Theorem 5.4. \square

Remark 5.5. This smoothness result is better than the result we could get from (2) of Theorem 4.2 in [12]. In [12], the order of the regularity of the scattering amplitude (the integral kernel of $T_{\varkappa}(\lambda)$) is connected to the decrease of the potentials. Here, we need only a fixed decrease, of the order $\langle x \rangle^{-\delta}$ (for an arbitrary fixed $\delta > 3$), to obtain C^∞ -smoothness of $T_{\varkappa}(\lambda)$.

Proof of Theorem 2.5. Owing to the formula

$$\frac{ds_{\varkappa}}{d\lambda}(\lambda) = \frac{i}{2\pi} \operatorname{tr} \left(\frac{dS_{\varkappa}}{d\lambda}(\lambda) S_{\varkappa}^*(\lambda) \right),$$

and to Theorem 5.4, we obtain the smoothness of $s_{\varkappa}(\lambda)$ claimed in (b).

To prove the convergence to $s_\infty(\lambda)$, we will establish it in the weak sense, which means that for all $\varphi \in C_0^\infty([0, +\infty[)$,

$$\lim_{\varkappa \rightarrow 0} \int_0^{+\infty} s_{\varkappa}(\lambda) \varphi'(\lambda) d\lambda = \int_0^{+\infty} s_\infty(\lambda) \varphi'(\lambda) d\lambda.$$

It will be a consequence of the following proposition, using the Krein formula (2).

At last, the case $V=0$ is discussed in Remark 3.9. \square

Proposition 5.6. *Let H_\varkappa and $H_{0,\varkappa}$ be the Dirac operators defined by (16) and (17) such that the potentials A and V satisfy the hypothesis (H_δ) with $\delta > 3$.*

For all $\varphi \in C_0^\infty([0, +\infty[)$, in the trace class, we have

$$\lim_{\varkappa \rightarrow 0} \left(\varphi \left(H_\varkappa - \frac{I}{\varkappa^2} \right) - \varphi \left(H_{0,\varkappa} - \frac{I}{\varkappa^2} \right) \right) = \nu \otimes (\varphi(h_+) - \varphi(h_0)),$$

where h_+ and h_0 are the Pauli operators defined by (3).

Proof. Our starting formula, owing to (7), is

$$(25) \quad \varphi \left(H_\varkappa - \frac{I}{\varkappa^2} \right) = \frac{1}{2} \varphi_1(\varkappa, H_\infty(\varkappa)) + \frac{1}{2} \varkappa^2 H_\varkappa \varphi_2(\varkappa, H_\infty(\varkappa)),$$

where, for $\lambda > -1/2\varkappa^2$ and for $\varkappa \neq 0$,

$$\begin{aligned} \varphi_1(\varkappa, \lambda) &= \varphi \left(\frac{(1+2\varkappa^2\lambda)^{1/2} - 1}{\varkappa^2} \right), \\ \varphi_2(\varkappa, \lambda) &= (1+2\varkappa^2\lambda)^{-1/2} \varphi_1(\varkappa, \lambda) \end{aligned}$$

and

$$(26) \quad H_\infty(\varkappa) := \frac{1}{2\varkappa^2} (\varkappa^4 H_\varkappa^2 - I).$$

On $\mathbf{C}^2 \otimes L^2(\mathbf{R}^3, \mathbf{C}^2)$ we have

$$(27) \quad H_\infty(\varkappa) = \nu \otimes h + \mu \otimes h^- + \varkappa \mathcal{D}_{A,V} + \frac{1}{2} \varkappa^2 V^2,$$

where

$$h^- := \frac{(\sigma \cdot (D - A))^2}{2m} - V_- \quad \text{and} \quad \mathcal{D}_{A,V} = \alpha \cdot (D - A)V + V\alpha \cdot (D - A).$$

First of all, let us remark that the convergence property is formally obvious (in the space of bounded operators). Indeed, as \varkappa tends to 0, $\varphi_1(\varkappa, \lambda)$ and $\varphi_2(\varkappa, \lambda)$ tend to $\varphi(\lambda)$ and $H_\infty(\varkappa)$ tends to $\nu \otimes h + \mu \otimes h^-$. Then, formally, for $j=1, 2$, we have

$$\varphi_j(\varkappa, H_\infty(\varkappa)) \rightarrow \nu \otimes \varphi(h) + \mu \otimes \varphi(h^-).$$

Thus, owing to (25) and (16), we have, as $\varkappa \rightarrow 0$,

$$\varphi \left(H_\varkappa - \frac{I}{\varkappa^2} \right) \rightarrow \left[\frac{1}{2} (1_2 + \sigma_3) \otimes 1_2 \right] \cdot [\nu \otimes \varphi(h) + \mu \otimes \varphi(h^-)].$$

Moreover $\frac{1}{2}(1_2 + \sigma_3) = \nu$, then we deduce that formally

$$\varphi\left(H_{\varkappa} - \frac{I}{\varkappa^2}\right) \rightarrow \nu \otimes \varphi(h).$$

This formal approach can be justified using functional calculus. For $j=1, 2$, we have

$$(28) \quad \varphi_j(\varkappa, H_{\infty}(\varkappa)) = \frac{1}{2i\pi} \int_{\varrho-i\infty}^{\varrho+i\infty} \mathcal{M}[\varphi_j(\varkappa, \cdot)](s) \frac{i}{2\pi} \int_{\Gamma_s} z^{-s} (H_{\infty}(\varkappa) - z)^{-1} dz ds,$$

where Γ_s is a path in \mathbf{C} (which does not contain the semi-bounded spectrum of $H_{\infty}(\varkappa)$) and $\mathcal{M}[\varphi_j(\varkappa, \cdot)](s)$ is the Mellin transform of φ_j ,

$$\mathcal{M}[\varphi_j(\varkappa, \cdot)](s) = \int_0^{\infty} t^{s-1} \varphi_j(\varkappa, t) dt.$$

After the change of variable $\varkappa^2 t' = (1 + 2\varkappa^2 t)^{1/2} - 1$ we have

$$\begin{aligned} \mathcal{M}[\varphi_1(\varkappa, \cdot)](s) &= \int_0^{\infty} (1 + \varkappa^2 t) \left(t + \frac{1}{2}\varkappa^2 t^2\right)^{s-1} \varphi(t) dt, \\ \mathcal{M}[\varphi_2(\varkappa, \cdot)](s) &= \int_0^{\infty} \left(t + \frac{1}{2}\varkappa^2 t^2\right)^{s-1} \varphi(t) dt, \end{aligned}$$

which tends to $\mathcal{M}[\varphi](s)$ as \varkappa tends to 0.

As $H_{\infty}(\varkappa)$ is a polynomial with respect to \varkappa , then $(H_{\infty}(\varkappa) - z)^{-1}$ is smooth with respect to \varkappa and tends to $(H_{\infty}(0) - z)^{-1}$. Thus we have easily the convergence of $\varphi(H_{\varkappa} - I/\varkappa^2)$ to $\nu \otimes \varphi(h_+)$ in the space of bounded operators.

To obtain the convergence of $\varphi(H_{\varkappa} - I/\varkappa^2) - \varphi(H_{0,\varkappa} - I/\varkappa^2)$ in the trace norm, we construct a parametrix for $(H_{\infty}(\varkappa) - z)^{-1}$, and the functional calculus by the Mellin transform gives the expression

$$\begin{aligned} \varphi_j(\varkappa, H_{\infty}(\varkappa)) &= \sum_{k=0}^N Op^{\omega}(b_{\varphi_j,k}^{\varkappa}) + \frac{1}{2i\pi} \int_{\varrho-i\infty}^{\varrho+i\infty} \mathcal{M}[\varphi_j(\varkappa, \cdot)](s) \\ &\quad \times \frac{i}{2\pi} \int_{\Gamma_s} z^{-s} Op^{\omega}(\delta_{N+1,z}^{\varkappa})(H_{\infty}(\varkappa) - z)^{-1} dz ds, \end{aligned}$$

with $Op^{\omega}(b_{\varphi_j,k}^{\varkappa})$ and $Op^{\omega}(\delta_{N+1,z}^{\varkappa})$ in a trace class for N large enough. Because $H_{\infty}(\varkappa)$ is a polynomial with respect to \varkappa , we deduce that $\delta_{N+1,z}^{\varkappa}$ is also a polynomial, and the control with respect to small \varkappa , is not difficult. Thus, we have proved Proposition 5.6 (see Part 4 of [4] for more details). \square

Remark 5.7. As remarked by the referee, it would be nice to prove multiparameter asymptotics in the three parameters (h, λ, c) . This problem seems difficult. However, we can get partial results when one of the parameters is fixed.

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