EIGENVALUE ESTIMATES IN THE SEMI-CLASSICAL LIMIT FOR PAULI AND DIRAC OPERATORS WITH A MAGNETIC FIELD

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ABSTRACT. Leading order semi-classical asymptotics are given for the distribution of the eigenvalues of Dirac and Pauli operators describing an electron in an electro-magnetic field. Minimal conditions are assumed on the electric and magnetic potentials to ensure the existence of only a finite number of eigenvalues outside the essential spectra. The method used is based on coherent state analysis.

1. INTRODUCTION

The Dirac operator with a magnetic vector potential $k\mathbf{a}$ is given by

$$T_V(\mathbf{a}) := \alpha \cdot (D - k\mathbf{a}) + \beta + V, \qquad D := \frac{\hbar}{i}\nabla$$

where $\alpha := (\alpha_1, \alpha_2, \alpha_3)$ and $k = k(\hbar)$. Here $\mathbf{a} := (a_1, a_2, a_3)$ and the functions a_ν, $\nu = 1, 2, 3$, and V are assumed to be real-valued. The Dirac matrices are given by

$$\alpha_\nu = \begin{pmatrix} 0 & \sigma_\nu \\ \sigma_\nu & 0 \end{pmatrix}, \ \nu = 1, 2, 3, \qquad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix},$$

where I_2 is the 2×2 identity matrix and $\sigma := (\sigma_1, \sigma_2, \sigma_3)$ in which the Pauli matrices are

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We will occasionally use the notation $\mathcal{D}_{\mathbf{a}} := \alpha \cdot (D - k\mathbf{a}(\cdot))$.

Usually $k(\hbar)$ is taken to be 1, but we wish to allow for the dependence upon Planck's constant $\hbar$ in order to account in part for strong magnetic fields; e.g., see related work of Yngvason [24], Lieb and Solovej [17], and Lieb, Loss, and Solovej [16]. Throughout this paper we will assume that $k(\hbar) = O(\hbar^{-t})$ for some $t \in [0, 1)$, which includes the case of $k = 1$ when $t = 0$; work is in progress on the cases $t \geq 1$.

Note that

$$[\alpha \cdot (D - k\mathbf{a})]^2 = (D - k\mathbf{a})^2 - \hbar k \Sigma \cdot \mathbf{B}$$

where $\Sigma := (\Sigma_1, \Sigma_2, \Sigma_3)$,

$$\Sigma_\nu := \begin{pmatrix} \sigma_\nu & 0 \\ 0 & \sigma_\nu \end{pmatrix}, \nu = 1, 2, 3,$$

and $\mathbf{B} := \nabla \times \mathbf{a}$ is the magnetic field. There is gauge invariance, the magnetic field being unchanged if $\mathbf{a}$ is replaced by $\mathbf{a}' := \mathbf{a} + \nabla\phi$ for any $\phi \in C^2(\mathbb{R}^3)$, and with $T_V(\mathbf{a})$ and $T_V(\mathbf{a}')$ unitarily equivalent via the unitary map $U\psi = e^{ik\hbar^{-1}\phi}\psi$. Setting $V = 0$ and squaring we obtain the expression

$$T_0(\mathbf{a})^2 = \begin{pmatrix} H(\mathbf{a}) + 1 & 0 \\ 0 & H(\mathbf{a}) + 1 \end{pmatrix}, \qquad H(\mathbf{a}) := [\sigma \cdot (D - k\mathbf{a})]^2 = (D - k\mathbf{a})^2 - \hbar k \sigma \cdot \mathbf{B},$$

$H(\mathbf{a})$ being the Pauli operator in $L^2(\mathbb{R}^3)^2$.

Date: August 14, 2000.

The first author (WDE) gratefully acknowledges the hospitality and support of the Department of Mathematics, UAB, where much of this work was done, and also the European Union for support under the TMR grant FMRX-CT 96-0001. The second author (RTL) wishes to express gratitude to the British Engineering and Physical Sciences Research Council for support to participate in the Gregynog Workshop, University of Wales, Gregynog Hall, in July, 1996, where some of this work was done and to the School of Mathematics, University of Wales, Cardiff, for their kind hospitality during that same period.

The problem of interest here is to estimate the $\mathrm{tr}[\chi_{(-\infty,0)}(T_V(\mathbf{a})^2-1-\Phi)]$ in the semiclassical limit for a real-valued function Φ. That is, as Planck's constant $\hbar \to 0$ what is the number $N(T_V(\mathbf{a})^2-1-\Phi)$ of negative eigenvalues of $T_V(\mathbf{a})^2-1-\Phi$? Important special cases are given by

(a) $V=0$, $\Phi=-W$, which would give the $\mathrm{tr}[\chi_{(-\infty,0)}(H(\mathbf{a})+W)]$, i.e., the number of eigenvalues below 0 of the Pauli operator with a potential W; and

(b) $\Phi=0$, which would give

$$\mathrm{tr}[\chi_{(-\infty,0)}(T_V(\mathbf{a})^2-1))]=\mathrm{tr}[\chi_{(-1,1)}(T_V(\mathbf{a}))].$$

Under appropriate conditions on V and $\mathbf{a}$, the interval $(-1,1)$ is a gap in the essential spectrum of $T_V(\mathbf{a})$, and hence the above trace coincides with the number of eigenvalues in this gap.

Our basic tools are the methods of coherent states used previously in the work of Berezin [4], Li and Yau [13], Lieb [14], and Thirring [22]. This paper follows closely earlier work of Evans, Lewis, Siedentop, and Solovej [7].

Throughout this paper $(\cdot,\cdot)$ and $\|\cdot\|$ are used to denote the usual inner product and norm in $L^2(\mathbb{R}^3)^4$; the norms of $L^p(\mathbb{R}^3)$ and $L^p(\mathbb{R}^3)^4$ are both denoted by $\|\cdot\|_p$, the precise meaning being clear from the context. In $\mathbb{C}^4$, the Euclidean inner-product and norm are denoted by $<\cdot,\cdot>$ and $|\cdot|$ respectively. We adopt the convention that inner-products are linear in the second argument and conjugate-linear in the first argument.

2. Essential Self-Adjointness and the Essential Spectrum

We refer to the papers of Avron, Herbst, and Simon [1], [2], and [3], (see also Solnyshkin [21], and Sobolev [20]) for an analysis of the significance of introducing magnetic potentials in Schrödinger operators, and important differences for the Pauli operator.

In this section we define and analyze the operators $T_V(\mathbf{a})$ and $T_V(\mathbf{a})^2-1-\Phi$. We shall assume throughout that $a_\nu(x)$, $\nu=1,2,3$, are real-valued elements of $L^2_{loc}(\mathbb{R}^3)$. For the potential V to be considered the operator $T'_V(\mathbf{a}):=[\alpha\cdot(D-k\mathbf{a})+\beta+V]|_{C_0^\infty(\mathbb{R}^3)^4}$ will be symmetric and therefore closable. The operator $T_V(\mathbf{a})$ will denote the closure of $T'_V(\mathbf{a})$.

Define

$$\mathcal{H}^1_{\mathbf{a}}\equiv\mathcal{H}^1_{\mathbf{a}}(\mathbb{R}^3):=\{u:u,(D_\nu-ka_\nu)u\in L^2(\mathbb{R}^3)^4,\nu=1,2,3\}$$

for $D_\nu:=\frac{\hbar}{i}\partial_\nu$, in which $D_\nu u$ is taken in the distributional sense, with norm

$$\|u\|_{\mathcal{H}^1_{\mathbf{a}}}:=(\|u\|^2+\sum_{\nu=1}^{3}\|(D_\nu-ka_\nu)u\|^2)^{\frac{1}{2}}.$$

Since $\mathbf{a}\in L^2_{loc}(\mathbb{R}^3)^3$, it follows that $C_0^\infty(\mathbb{R}^3)^4$ is dense in $\mathcal{H}^1_{\mathbf{a}}$ (see Kato [8], Simon [19], and Leinfelder and Simader [12]), and from the proof of the diamagnetic inequality we have that

$$|D_\nu(|u|)|\le|(D_\nu-ka_\nu)u|,\qquad \nu=1,2,3, \tag{1}$$

holds for almost every $x\in\mathbb{R}^3$ and $u\in\mathcal{H}^1_{\mathbf{a}}$ (see Lieb and Loss [15], p.179). As a consequence we have that $u\mapsto|u|$ maps $\mathcal{H}^1_{\mathbf{a}}$ continuously into the Sobolev space $H^1(\mathbb{R}^3)$ which implies the existence of a continuous embedding

$$\mathcal{H}^1_{\mathbf{a}}\hookrightarrow L^s(\mathbb{R}^3)^4,\qquad s\in[2,6], \tag{2}$$

(see Edmunds and Evans [6], Theorem 3.7). For the ball B_N centered at the origin with radius N, it follows from Rellich's embedding theorem that the embedding

$$\mathcal{H}^1_{\mathbf{a}}\hookrightarrow L^2(B_N)^4 \tag{3}$$

is compact.

Lemma 1. *If $a_\nu\in L^2_{loc}(\mathbb{R}^3)$, $\nu=1,2,3$, and $|\mathbf{B}|\in L^{\frac{3}{2}}(\mathbb{R}^3)$, then the domain of $T_0(\mathbf{a})$ is given by*

$$\mathcal{D}(T_0(\mathbf{a}))=\{u\in L^2(\mathbb{R}^3)^4:u\in\mathcal{H}^1_{\mathbf{a}}\}.$$

Proof. For $\phi \in C_0^\infty(\mathbb{R}^3)^4$, we have that

$$\begin{aligned} \|T_0(\mathbf{a})\phi\|^2 = & \ ([\alpha \cdot (D - k\mathbf{a})]^2\phi, \phi) + \|\phi\|^2 \\ = & \ \|(D - k\mathbf{a})\phi\|^2 - \hbar k(\Sigma \cdot \mathbf{B}\phi, \phi) + \|\phi\|^2. \end{aligned}$$

Since $|\mathbf{B}| \in L^{\frac{3}{2}}(\mathbb{R}^3)$, then there are functions b_1 and b_2 such that $|\mathbf{B}| = b_1 + b_2$ with $\|b_1\|_{\frac{3}{2}} < \epsilon$ and $\|b_2\|_\infty < K_\epsilon$ for a given $\epsilon > 0$ and some $K_\epsilon > 0$. In this case we have for any $\phi \in C_0^\infty(\mathbb{R}^3)^4$

$$\begin{aligned} |(\Sigma \cdot \mathbf{B}\phi, \phi)| \leq & \ (|\mathbf{B}|\phi, \phi) \\ = & \ (b_1\phi, \phi) + (b_2\phi, \phi) \\ \leq & \ \|b_1\|_{\frac{3}{2}}\|\phi\|_6^2 + K_\epsilon\|\phi\|^2 \\ \lesssim & \ \left[\epsilon\|\phi\|^2_{\mathcal{H}^1_{\mathbf{a}}} + K_\epsilon\|\phi\|^2\right] \end{aligned} \tag{4}$$

by (2).[1] Therefore, there are positive constants C_1 and C_2 such that

$$C_1\|\phi\|^2_{\mathcal{H}^1_{\mathbf{a}}} \leq \left[\|T_0(\mathbf{a})\phi\|^2 + \|\phi\|^2\right] \leq C_2\|\phi\|^2_{\mathcal{H}^1_{\mathbf{a}}}, \qquad \phi \in C_0^\infty(\mathbb{R}^3)^4, \tag{5}$$

i.e., the graph norm of $T_0(\mathbf{a})$ and $\|\cdot\|_{\mathcal{H}^1_{\mathbf{a}}}$ are equivalent on $C_0^\infty(\mathbb{R}^3)^4$, which is dense in $\mathcal{H}^1_{\mathbf{a}}$ and $\mathcal{D}(T_0(\mathbf{a}))$. Hence, $\mathcal{D}(T_0(\mathbf{a})) = \mathcal{H}^1_{\mathbf{a}}$.

□

Theorem 1. *Let $a_\nu \in L^2_{loc}(\mathbb{R}^3)$, $\nu = 1, 2, 3$, $|\mathbf{B}| \in L^{\frac{3}{2}}(\mathbb{R}^3)$, and either*

(i) *for some*[2] $\eta > 0$, $M > 0$, *and* $\rho_0 > 0$

$$|\mathbf{a}(x) - \mathbf{a}(q)| \leq M|x - q|^\eta \qquad \text{whenever} \quad |x - q| \leq \rho < \rho_0, \tag{6}$$

or

(ii) $|\mathbf{a}| \in L^\infty(\mathbb{R}^3)$.

Then $T_0'(\mathbf{a})$ is essentially self-adjoint.

Proof. [3] In view of Lemma 1 it is sufficient to prove that $\mathcal{D}(T_0(\mathbf{a})^*) \subseteq \mathcal{H}^1_{\mathbf{a}}$. Let $u \in \mathcal{D}(T_0(\mathbf{a})^*)$ and $v := T_0(\mathbf{a})^*u$. For each $N > 0$ choose $\chi_N \in C_0^\infty(\mathbb{R}^3)$ such that

$$\chi_N(x) = \chi_N(|x|) = \begin{cases} 1, & |x| \leq N \\ 0, & |x| > N + 1 \end{cases}$$

and $|\chi_N'(t)| \leq 1$ for all $t \in [0, \infty)$. Let $J_\epsilon f := j_\epsilon * f$ denote the Friedrichs mollifier with $j_\epsilon \in C_0^\infty(\mathbb{R}^3)$, and set

$$u_\epsilon := J_\epsilon(\chi_N u), \qquad v_\epsilon := J_\epsilon(\chi_N v).$$

For any $\phi \in C_0^\infty(\mathbb{R}^3)^4$,

$$\begin{aligned} (\phi, v_\epsilon) = & \ \textstyle\int_{\mathbb{R}^3} < \chi_N J_\epsilon\phi, v > dx \\ = & \ (\chi_N J_\epsilon\phi, T_0(\mathbf{a})^*u) \\ = & \ (T_0(\mathbf{a})(\chi_N J_\epsilon\phi), u) \\ = & \ \big(\chi_N T_0(\mathbf{a})(J_\epsilon\phi) + (\alpha \cdot D\chi_N)J_\epsilon\phi, u\big) \end{aligned} \tag{7}$$

in which

$$\begin{aligned} T_0(\mathbf{a})(J_\epsilon\phi)(x) = & \ \textstyle\int_{\mathbb{R}^3} j_\epsilon(x - y)\big(\alpha \cdot (D - k\mathbf{a}(y)) + \beta\big)\phi(y)dy \\ & + \textstyle\int_{\mathbb{R}^3} j_\epsilon(x - y)[\alpha \cdot (\mathbf{a}(x) - \mathbf{a}(y))]\phi(y)dy \\ = & \ J_\epsilon\big[T_0(\mathbf{a})\phi\big](x) + J_\epsilon\big[\alpha \cdot (\mathbf{a}(x) - \mathbf{a}(\cdot))\phi(\cdot)\big](x). \end{aligned}$$

Hence,

$$\begin{aligned} (\phi, v_\epsilon) = & \ (T_0(\mathbf{a})\phi, J_\epsilon[\chi_N u]) + \textstyle\int_{\mathbb{R}^3} < \phi(y), \int_{\mathbb{R}^3} j_\epsilon(y - x)[\alpha \cdot (\mathbf{a}(x) - \mathbf{a}(y))]\chi_N(x)u(x)dx > dy \\ & + (\phi, J_\epsilon[(\alpha \cdot D\chi_N)u]) \end{aligned}$$

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[1] The symbol " $\lesssim$ " should be interpreted as "less than or equal to a positive constant times".

[2] That is, the magnetic vector potential $\mathbf{a}$ is locally, uniformly Hölder continuous with exponent η. Note that if condition (6) holds for $\eta > 1$ then $\mathbf{B} \equiv 0$. We will assume that $\eta \in [0, 1]$ throughout this paper.

[3] This proof is based on the proof of Proposition 1 of Schmidt [18]. We are grateful to Dr. Schmidt for telling us of this result.

for all $\phi \in C_0^\infty(\mathbb{R}^3)^4$. Since $T_0(\mathbf{a})^*$ is an extension of $T_0(\mathbf{a})$, then we may conclude from the last identity that

$$v_\epsilon(x) = T_0(\mathbf{a})u_\epsilon(x) + J_\epsilon[\alpha\cdot(\mathbf{a}(\cdot)-\mathbf{a}(x))(\chi_N u)(\cdot)](x) + J_\epsilon[(\alpha\cdot D\chi_N)u](x). \tag{8}$$

If (i) is assumed, we have

$$|J_\epsilon[\alpha\cdot(\mathbf{a}(\cdot)-\mathbf{a}(x))(\chi_N u)(\cdot)](x)| \lesssim \epsilon^\eta J_\epsilon(|\chi_N u|)(x) \tag{9}$$

by (6). It follows from (5) and (8) that[4] for $\epsilon > 0$ and $\delta > 0$

(10)
$$\begin{aligned} \|u_\epsilon - u_\delta\|^2_{\mathcal{H}^1_{\mathbf{a}}} \approx\ & \|T_0(\mathbf{a})u_\epsilon - T_0(\mathbf{a})u_\delta\|^2 \\ \lesssim\ & \big\{\|v_\epsilon - v_\delta\|^2 + \|J_\epsilon[\alpha\cdot(\mathbf{a}(\cdot)-\mathbf{a}(x))(\chi_N u)(\cdot)] - J_\delta[\alpha\cdot(\mathbf{a}(\cdot)-\mathbf{a}(x))(\chi_N u)(\cdot)]\|^2 \\ & + \|J_\epsilon[(\alpha\cdot D\chi_N)u] - J_\delta[(\alpha\cdot D\chi_N)u]\|^2\big\}. \end{aligned}$$

Since $v, (\alpha\cdot D\chi_N)u \in L^2(\mathbb{R}^3)^4$ then the first and third term on the right side of the inequality in (10) approach zero as $\epsilon, \delta \to 0$. Also, for $\eta > 0$ in (6),

$$\|J_\epsilon[\alpha\cdot(\mathbf{a}(\cdot)-\mathbf{a}(x))(\chi_N u)(\cdot)]\| \lesssim \epsilon^\eta \|J_\epsilon(|\chi_N u|)\| \to 0$$

as $\epsilon \to 0$, and similarly as $\delta \to 0$. However, if $\eta = 0$ this is still the case since $|\mathbf{a}(y)-\mathbf{a}(x)|$ would be bounded. In conclusion, as $\epsilon, \delta \to 0$, $\|u_\epsilon - u_\delta\|_{\mathcal{H}^1_{\mathbf{a}}} \to 0$ and hence $(D_\nu - ka_\nu)u_\epsilon \to U_\nu$, $\nu = 1, 2, 3$, for some $U_\nu \in L^2(\mathbb{R}^3)^4$. Thus for $\nu = 1, 2, 3$, and $\psi \in C_0^\infty(B_N)^4$

$$\begin{aligned} (U_\nu, \psi) =\ & \lim_{\epsilon\to 0}((D_\nu - ka_\nu)u_\epsilon, \psi) = \lim_{\epsilon\to 0}(u_\epsilon, (D_\nu - ka_\nu)\psi) \\ =\ & (\chi_N u, (D_\nu - ka_\nu)\psi) = (u, (D_\nu - ka_\nu)\psi) = ((D_\nu - ka_\nu)u, \psi) \end{aligned}$$

which implies that $U_\nu = (D_\nu - ka_\nu)u$ in B_N. However, by the analysis associated with (10) we have that

$$\|(D - k\mathbf{a})u_\epsilon\|^2 \le \|u_\epsilon\|^2_{\mathcal{H}^1_{\mathbf{a}}} \lesssim \big[\|v_\epsilon\|^2 + \|J_\epsilon(|u|)\|^2\big].$$

By letting $\epsilon \to 0$ we conclude that

$$\|(D - k\mathbf{a})u\|^2_{L^2(B_N)^4} \lesssim \big[\|v\|^2 + \|u\|^2\big].$$

Since N is arbitrary, then this implies that $u \in \mathcal{H}^1_{\mathbf{a}}$, i.e., $\mathcal{D}(T_0(\mathbf{a})^* \subseteq \mathcal{H}^1_{\mathbf{a}}$.

If (ii) is satisfied, we proceed as follows to replace (9). Setting $v_{j,N} = \alpha_j \chi_N u$, $j = 1, 2, 3$, we have

$$J_\epsilon[(a_j(\cdot) - a_j(x))v_{j,N}(\cdot)](x) = J_\epsilon[a_j v_{j,N}](x) - (a_j v_{j,N})(x) + a_j(x)\{[J_\epsilon v_{j,N}](x) - v_{j,N}(x)\}.$$

Since $a_j \in L^\infty(\mathbb{R}^3)$ and $v_{j,N} \in L^2(\mathbb{R}^3)^4$, it follows that

$$\|J_\epsilon[(a_j(\cdot) - a_j(x))v_{j,N}(\cdot)]\| \to 0 \qquad \text{as } \epsilon \to 0.$$

The rest of the proof follows as before. ☐

Corollary 1. *Let the hypothesis of Theorem 1 hold and assume that $V \in L^3(\mathbb{R}^3)$. Then $T'_V(\mathbf{a})$ is essentially self-adjoint and $T_V(\mathbf{a})$ has domain $\mathcal{H}^1_{\mathbf{a}}$.*

Proof. It follows as in (4) that V has $T'_0(\mathbf{a})$-bound zero. Since $T'_0(\mathbf{a})$ is essentially self-adjoint, then $T'_V(\mathbf{a})$ is essentially self-adjoint and $\mathcal{D}(T_V(\mathbf{a})) = \mathcal{D}(T_0(\mathbf{a})) = \mathcal{H}^1_{\mathbf{a}}$.[5] ☐

Theorem 2. *If the hypothesis of Corollary 1 holds, then*[6]

(i) $\sigma_e(T_V(\mathbf{a})) = \sigma_e(T_0(\mathbf{a}))$;
(ii) $\sigma_e(T_0(\mathbf{a})) \subseteq \sigma(T_0(\mathbf{a})) \subseteq \mathbb{R}\setminus(-1, 1)$; *and*
(iii) $\sigma_e(T_0(\mathbf{a})) = \{\lambda : \lambda^2 - 1 \in \sigma_e((D - k\mathbf{a})^2)\}$.

[4] Here, the symbol $\approx$ denotes norm equivalence.
[5] See Kato [9], Theorems IV.1.1 and V.4.4.
[6] In the usual manner the symbols $\sigma(T)$ and $\sigma_e(T)$ denote the spectrum and the essential spectrum, respectively, of the operator T.

Proof. First we claim that V is $T_0(\mathbf{a})$-compact which will imply (i). To show this it will suffice to show that $V(T_0(\mathbf{a})+i)^{-1}$ is compact. Assume that $\{\phi_m\}$ is a bounded sequence in $L^2(\mathbb{R}^3)^4$. We need to show that $\{V(T_0(\mathbf{a})+i)^{-1}\phi_m\}$ has a convergent subsequence, i.e., that it is precompact in $L^2(\mathbb{R}^3)^4$. Set $\psi_m=(T_0(\mathbf{a})+i)^{-1}\phi_m$. Then $\{\psi_m\}$ is bounded in $\mathcal{H}^1_{\mathbf{a}}$ since

$$\|\phi_m\|^2=\|T_0(\mathbf{a})\psi_m\|^2+\|\psi_m\|^2\geq C_1^{-1}\|\psi_m\|^2_{\mathcal{H}^1_{\mathbf{a}}}$$

by (5). Consequently, it follows from (2) that

$$\int_\Omega |V\psi_m|^2dx\leq\Big[\int_\Omega |V|^3dx\Big]^{\frac{2}{3}}\|\psi_m\|_6^2\lesssim\Big[\int_\Omega |V|^3dx\Big]^{\frac{2}{3}}$$

for any $\Omega\subseteq\mathbb{R}^3$ which implies that for any $\epsilon>0$ there exists an $N>0$ such that for all m

$$\int_{\mathbb{R}^3\setminus B_N}|V\psi_m|^2dx<\epsilon. \tag{11}$$

By (3), $\{\psi_m\}$ is precompact in $L^2(B_N)^4$. For arbitrary $\delta>0$ we may set $V=V_1+V_2$ for which $\|V_1\|_3<\delta$ and $\|V_2\|_\infty<K_\delta$ for some $K_\delta>0$. Then

$$\begin{aligned}\int_{B_N}V^2|\psi_m-\psi_n|^2dx\leq\ & \|V_1\|_3^2\|\psi_m-\psi_n\|_6^2+\|V_2\|^2_\infty\|\psi_m-\psi_n\|^2_{L^2(B_N)^4}\\ \lesssim\ & \big[\delta^2\|\psi_m-\psi_n\|^2_{\mathcal{H}^1_{\mathbf{a}}}+K_\delta^2\|\psi_m-\psi_n\|^2_{L^2(B_N)^4}\big]\\ \lesssim\ & \big[\delta^2+K_\delta^2\|\psi_m-\psi_n\|^2_{L^2(B_N)^4}\big]\end{aligned}$$

by (2). Since $\{\psi_m\}$ is precompact in $L^2(B_N)^4$, then (for a subsequence)

$$\lim_{m,n\to\infty}\|V(\psi_m-\psi_n)\|^2_{L^2(B_N)^4}\lesssim\delta^2. \tag{12}$$

Since δ and ϵ are arbitrary, it now follows from (11) that $\{V(T_0(\mathbf{a})+i)^{-1}\phi_m\}$ is precompact in $L^2(\mathbb{R}^3)^4$ which implies that (i) holds.

Part (ii) follows from the fact that

$$\|T_0(\mathbf{a})\phi\|^2=\|\alpha\cdot(D-k\mathbf{a})\phi\|^2+\|\phi\|^2.$$

The self-adjoint operator $T_0(\mathbf{a})^2$ is that associated with the sesquilinear form

$$(T_0(\mathbf{a})\phi,T_0(\mathbf{a})\psi)=(\phi,\psi)_{\mathcal{H}^1_{\mathbf{a}}}-\hbar k(\Sigma\cdot\mathbf{B}\phi,\psi),\qquad \phi,\psi\in\mathcal{H}^1_{\mathbf{a}}.$$

The continuous embedding $E:\mathcal{H}^1_{\mathbf{a}}\hookrightarrow L^2(\mathbb{R}^3)^4$ has norm $\|E\|\leq1$ and dense range. The adjoint map E^* is a linear injection of $L^2(\mathbb{R}^3)^4$ into the adjoint space $(\mathcal{H}^1_{\mathbf{a}})^*$, the conjugate linear functionals on $\mathcal{H}^1_{\mathbf{a}}$: for $\phi\in\mathcal{H}^1_{\mathbf{a}}$, $x\in L^2(\mathbb{R}^3)^4$, we have

$$(E\phi,x)=(\phi,E^*x)_{\mathcal{H}^1_{\mathbf{a}}}.$$

Thus we have the triplet

$$\mathcal{H}^1_{\mathbf{a}}\overset{E}{\hookrightarrow}L^2(\mathbb{R}^3)^4\overset{E^*}{\hookrightarrow}(\mathcal{H}^1_{\mathbf{a}})^*$$

(see [6], §IV.4). For $\phi,\psi\in\mathcal{H}^1_{\mathbf{a}}$ set

$$\mathfrak{a}_0[\phi,\psi]:=(\phi,\psi)_{\mathcal{H}^1_{\mathbf{a}}},\qquad \mathfrak{p}[\phi,\psi]:=(\Sigma\cdot\mathbf{B}\phi,\psi).$$

By (4) $\mathfrak{p}$ has $\mathfrak{a}_0$-bound zero, and

$$|\mathfrak{p}[\phi,\psi]|\leq\||\mathbf{B}|^{\frac{1}{2}}\phi\|\||\mathbf{B}|^{\frac{1}{2}}\psi\|\lesssim\|\phi\|_{\mathcal{H}^1_{\mathbf{a}}}\|\psi\|_{\mathcal{H}^1_{\mathbf{a}}}$$

which shows that $\mathfrak{p}$ is a bounded sesquilinear form on $\mathcal{H}^1_{\mathbf{a}}\times\mathcal{H}^1_{\mathbf{a}}$ where $\mathcal{H}^1_{\mathbf{a}}$ is the form domain of $(D-k\mathbf{a})^2$. Thus there is bounded linear map $\hat{P}:\mathcal{H}^1_{\mathbf{a}}\to{\mathcal{H}^1_{\mathbf{a}}}^*$ such that for $\phi,\psi\in\mathcal{H}^1_{\mathbf{a}}$

$$\mathfrak{p}[\psi,\phi]=<\psi,\hat{P}\phi>$$

where $<\cdot,\cdot>$ denotes the duality bracket in this context. We now invoke Theorem IV.4.2(vi) in [6] from which it follows that $T_0(\mathbf{a})^2$ and $A:=(D-k\mathbf{a})^2+1$, the self-adjoint operator associated with $\mathfrak{a}_0$, have the same essential spectrum if for a nonzero real number z, $\hat{P}(A-izI)^{-1}$ is a compact mapping from $L^2(\mathbb{R}^3)^4$ to $(\mathcal{H}^1_{\mathbf{a}})^*$. Let $\{\phi_m\}$ be a bounded sequence in $L^2(\mathbb{R}^3)^4$ and set $\psi_m=$

$(A-izI)^{-1}\phi_m \in \mathcal{D}(A) \subset \mathcal{H}^1_{\mathbf{a}}$. Then $|z|\|\psi_m\| \le \|\phi_m\|$ which implies that $\|\psi_m\|^2_{\mathcal{H}^1_{\mathbf{a}}} = (A\psi_m, \psi_m)$ is bounded, i.e., $\{\psi_m\}$ is bounded in $\mathcal{H}^1_{\mathbf{a}}$. Therefore for $\phi \in \mathcal{H}^1_{\mathbf{a}}$,

$$\begin{aligned} |<\phi, \hat{P}(\psi_m - \psi_n)>| = & \ |\mathfrak{p}[\phi, \psi_m - \psi_n]| \\ \le & \ \int_{\mathbb{R}^3} |\mathbf{B}||\psi_m - \psi_n||\phi| dx \\ \le & \ \||\mathbf{B}|^{\frac{1}{2}}(\psi_m - \psi_n)\|\||\mathbf{B}|^{\frac{1}{2}}\phi\| \\ \lesssim & \ \||\mathbf{B}|^{\frac{1}{2}}(\psi_m - \psi_n)\|\|\phi\|_{\mathcal{H}^1_{\mathbf{a}}} \end{aligned}$$

as in (4). As in the analysis leading to (11) and (12), given $\epsilon > 0$ there are positive numbers M, N such that

$$\||\mathbf{B}|^{\frac{1}{2}}(\psi_m - \psi_n)\|^2_{L^2(\mathbb{R}^3 \setminus B_N)} \le \||\mathbf{B}|\|_{\frac{3}{2}} \|\psi_m - \psi_n\|^2_{\mathcal{H}^1_{\mathbf{a}}} < \epsilon$$

and

$$\||\mathbf{B}|^{\frac{1}{2}}(\psi_m - \psi_n)\|^2_{L^2(B_N)} < \epsilon, \qquad m, n > M.$$

Hence

$$\|\hat{P}(\psi_m - \psi_n)\|_{(\mathcal{H}^1_{\mathbf{a}})^*} = \sup\{<\phi, \hat{P}(\psi_m - \psi_n)>: \phi \in \mathcal{H}^1_{\mathbf{a}}, \|\phi\|_{\mathcal{H}^1_{\mathbf{a}}} = 1\} \to 0 \qquad \text{as } m, n \to \infty,$$

which implies that $\{\hat{P}\psi_m\}$ is precompact in ${\mathcal{H}^1_{\mathbf{a}}}^*$. This completes the proof.

□

If $V \in L^3(\mathbb{R}^3)$ and we assume the hypothesis of Theorem 1, then $T_V(\mathbf{a})^2$, the square of the operator given in Corollary 1, is also that associated with the quadratic form $(T_V(\mathbf{a})\phi, T_V(\mathbf{a})\phi)$, $\phi \in \mathcal{H}^1_{\mathbf{a}}$, i.e., it has form domain $\mathcal{H}^1_{\mathbf{a}}$. Moreover, we know by Theorem 2 (i) and (iii) that $\sigma_e(T_V(\mathbf{a})) = \sigma_e(T_0(\mathbf{a})) = \mathbb{R} \setminus (-1, 1)$ by a comparison to the essential spectrum of $(D - k\mathbf{a})^2$ if either

$$\mathbf{a} \in C^\infty(\mathbb{R}^3)^3 \qquad \text{and } |\mathbf{B}(x)| \to 0 \qquad \text{as } |x| \to \infty,$$

cf. Cycon et al [5], Theorem 6.1, p. 117; or

$$\mathbf{a} \in L^2_{loc}(\mathbb{R}^3)^3 \qquad \text{and } |\mathbf{B}| \in L^2(\mathbb{R}^3),$$

cf. Leinfelder [11], Theorem 2.5.

3. The Main Theorems

We will assume that the magnetic vector potential $\mathbf{a}$ and the magnetic field $\mathbf{B}$ satisfy at least one of the following two conditions:

(13)
(i) $|\mathbf{B}| \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^4(\mathbb{R}^3)$, $\mathbf{a}$ satisfies (6) with $\eta = 1$, and $k(\hbar) = O(\hbar^{-t})$ for some $t \in [0, 1)$,
(ii) $|\mathbf{B}| \in L^{\frac{3}{2}}(\mathbb{R}^3)$, $|\mathbf{a}| \in L^3(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, and $k(\hbar) = O(\hbar^{-t})$ for some $t \in [0, 1)$.

Let ψ_ν, $\nu = 1, 2, \dots$, be the eigenfunctions of $T_V(\mathbf{a})^2 - 1 + W$ corresponding to negative eigenvalues, and denote the sum of the density of these states by $n(x) := \sum_{\nu=1}^\infty |\psi_\nu(x)|^2$.

Theorem 3. *Let $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, $\nabla V \in L^\infty(\mathbb{R}^3)$, $Z, W \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^4(\mathbb{R}^3)$, and assume that (13)(i) holds. Then, as $\hbar \to 0$*

$$\begin{aligned} &\int_{\mathbb{R}^3} Z(x) n(x) dx = \\ &\quad \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^6} Z(q) \operatorname{tr} \chi_{(-\infty,0)} \left[p^2 + V(q)^2 + W(q) + 2V(q)(\alpha \cdot p + \beta)\right] dp dq + o(\tfrac{1}{\hbar^3}) \end{aligned}$$

Theorem 4. *Assume that $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$, $W \in L^{\frac{3}{2}}(\mathbb{R}^3)$, and either (13)(i) or (ii) holds. Then, as $\hbar \to 0$*

$$\begin{aligned} &N(T_V(\mathbf{a})^2 - 1 + W) = \\ &\quad \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^6} \operatorname{tr} \chi_{(-\infty,0)} \left[p^2 + V(q)^2 + W(q) + 2V(q)(\alpha \cdot p + \beta)\right] dp dq + o(\hbar^{-3}). \end{aligned}$$

Corollary 2. *If either (13)(i) or (ii) holds, then the number of eigenvalues in the spectral gap* $(-1,1)$ *of the Dirac operator* $T_V(\mathbf{a})$ *with a potential* $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$ *is given by*

$$\begin{aligned} N(T_V(\mathbf{a})^2 - 1) = & \ \tfrac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^6} \operatorname{tr} \chi_{(-\infty,0)} \left[p^2 + V(q)^2 + 2V(q)(\alpha \cdot p + \beta)\right] dpdq + o(\hbar^{-3}) \\ = & \ \tfrac{2}{(2\pi\hbar)^3} \int_{\{(p,q): p^2 + |V|^2 \le 2|V|\sqrt{p^2+1}\}} dpdq + o(\hbar^{-3}) \end{aligned}$$

as $\hbar \to 0$.

Proof. Since the number of eigenvalues of $T_V(\mathbf{a})$ in $(-1,1)$ is the number of negative eigenvalues of $T_V(\mathbf{a})^2 - 1$, then the proof follows since the only negative eigenvalue of the matrix $p^2 + V(q)^2 + 2V(q)(\alpha \cdot p + \beta)$ is $[p^2 + V(q)^2 - 2|V(q)|\sqrt{p^2+1}]_-$ which is of multiplicity 2. ☐

Corollary 3. *If either (13)(i) or (ii) holds, then the number of negative eigenvalues of the Pauli operator* $H(\mathbf{a}) + W$ *with a potential* $W \in L^{\frac{3}{2}}(\mathbb{R}^3)$ *is given by*

$$N(H(\mathbf{a}) + W)) = \frac{1}{2(2\pi\hbar)^3} \int_{\{(p,q): p^2 + W(q) \le 0\}} dpdq + o(\hbar^{-3})$$

as $\hbar \to 0$.

4. Proof of Theorem 3

The proof of Theorem 3 will follow from upper and lower bounds for $-\operatorname{tr}(T_V(\mathbf{a})^2 - 1 - \Phi)_-$. A useful fact in obtaining these bounds is the following: for a self-adjoint operator S that is bounded below[7]

$$-\operatorname{tr}(S_-) = \inf\{\operatorname{tr}(Sd) : Sd \in \mathfrak{S}_1, d \text{ self-adjoint}, 0 \le d \le 1\} \tag{14}$$

where $\mathfrak{S}_1$ denotes the trace class operators.[8] In general both sides could be infinite. Note that a minimizer for the right side of (14) is given by $d := \chi_{(-\infty,0)}(S)$.

In order to be assured that the number of negative eigenvalues $N(T_V(\mathbf{a})^2 - 1 - \Phi)$ is finite we give an estimate which follows from the Cwikel-Lieb-Rosenblum inequality for Schrödinger operators.

Lemma 2. *If* $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$, $|\mathbf{B}| \in L^{\frac{3}{2}}(\mathbb{R}^3)$, *and* $\Phi \in L^{\frac{3}{2}}(\mathbb{R}^3)$ *then*

$$\operatorname{tr}\left[\chi_{(-\infty,0)}(T_V(\mathbf{a})^2 - 1 - \Phi)\right] \le K_{CLR} \frac{2^{\frac{5}{2}}}{\hbar^3} \int_{\mathbb{R}^3} [2|V| + V^2 + \Phi + \frac{1}{2}k\hbar|\mathbf{B}|]_+^{\frac{3}{2}} dx \tag{15}$$

where K_{CLR} *is the best constant in the Cwikel-Lieb-Rosenblum inequality.*[9]

Proof. For $\phi \in C_0^\infty(\mathbb{R}^3)^4$

$$\begin{aligned} (\phi, [T_V(\mathbf{a})^2 - 1]\phi) = & \ \|T_V(\mathbf{a})\phi\|^2 - \|\phi\|^2 \\ = & \ \|\alpha \cdot (D - k\mathbf{a})\phi\|^2 + 2\Re\mathfrak{e}(\alpha \cdot (D - k\mathbf{a})\phi, V\phi) + (\phi, [2V\beta + V^2]\phi) \\ \ge & \ (1-\epsilon)\|\alpha \cdot (D - k\mathbf{a})\phi\|^2 + (\phi, [-2|V| + (1 - \tfrac{1}{\epsilon})V^2]\phi). \end{aligned}$$

Choose $\epsilon = \frac{1}{2}$ and recall that $[\alpha \cdot (D - k\mathbf{a})]^2 = (D - k\mathbf{a})^2 - \hbar k \Sigma \cdot \mathbf{B}$ to see that

$$\begin{aligned} (\phi, [T_V(\mathbf{a})^2 - 1]\phi) \ge & \ \tfrac{1}{2}(\phi, (D - k\mathbf{a})^2\phi) - \tfrac{k\hbar}{2}(\phi, \Sigma \cdot \mathbf{B}\phi) - (\phi, [2|V| + V^2]\phi) \\ \ge & \ \tfrac{\hbar^2}{2}(\phi, (\tfrac{1}{i}\nabla - \tfrac{k}{\hbar}\mathbf{a})^2\phi) - \tfrac{k\hbar}{2}(\phi, |\mathbf{B}|\phi) - (\phi, [2|V| + V^2]\phi) \\ \ge & \ \tfrac{\hbar^2}{2}(\phi, -\Delta\phi) - (\phi, [\tfrac{k\hbar}{2}|\mathbf{B}| + 2|V| + V^2]\phi) \end{aligned}$$

by the diamagnetic inequality. The result then follows from the Cwikel-Lieb-Rosenblum inequality. ☐

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[7] See, e.g., Weinstein and Stenger [23].

[8] By S_- we mean the negative part of S given by $-\chi_{(-\infty,0)}(S)S$ in which $\chi_{(-\infty,0)}(S)$ is defined using the spectral representation of S.

[9] For more details we refer the reader to Chapter XI, §5, of [6].

4.1. **A lower bound for** $-\operatorname{tr}(T_V(\mathbf{a})^2-1-\Phi)_-$**.** Our methods here require that we approximate $T_V(\mathbf{a})^2-1-\Phi$ with an operator $\mathcal{A}$ having a coherent state symbol. The form for $\mathcal{A}$ is suggested by the sesquilinear form $\mathfrak{h}$ of $T_V(\mathbf{a})^2-1-\Phi$: with $\mathcal{D}_{\mathbf{a}} := \alpha\cdot(D-k\mathbf{a}(x))$ we have that $T_V(\mathbf{a}) = \mathcal{D}_{\mathbf{a}}+\beta+V$ and

$$\begin{aligned}\mathfrak{h}[\phi,\psi] :=\ & (T_V(\mathbf{a})\phi, T_V(\mathbf{a})\psi) - (\phi,(1+\Phi)\psi)\\ =\ & (\phi,((D-k\mathbf{a})^2-\hbar k\Sigma\cdot\mathbf{B})\psi) + (\mathcal{D}_{\mathbf{a}}\phi, V\psi) + (V\phi,\mathcal{D}_{\mathbf{a}}\psi)\\ & +2(\phi, V\beta\psi) + (\phi,(V^2-\Phi)\psi)\end{aligned} \tag{16}$$

for all $\phi,\psi \in C_0^\infty(\mathbb{R}^3)^4$, which is the form corresponding to $T_V(\mathbf{a})^2-1-\Phi$.

To define $\mathcal{A}$ we first define a 4×4 matrix-valued function $U_\delta(p,q)$ for $(p,q)\in\mathbb{R}^3\times\mathbb{R}^3$, $\delta\in[0,1)$:

(17)
$$U_\delta(p,q) := (1-\delta)\{(p-k\mathbf{a}(q))^2-\hbar k\Sigma\cdot\mathbf{B}(q)\} + V(q)^2-\Phi(q)+2V(q)\{\alpha\cdot(p-k\mathbf{a}(q))+\beta\}$$

with eigenvectors $\mathfrak{u}_\mu$, $\mu=1,2,3,4$, which are orthonormal in $\mathbb{C}^4$, and corresponding eigenvalues u_μ. For much of our discussion below we will suppress the δ-dependence of U_δ and simply write U for the matrix in (17).

Let $g\in C_0^\infty(\mathbb{R}^3)$ be a real-valued, spherically symmetric function with support in the unit ball and $L^2(\mathbb{R}^3)$-norm equal to one. For $\rho>0$ let $g_\rho(x) := \rho^{-\frac{3}{2}}g(x/\rho)$. Then a normalized coherent state[10] is defined by

$$F_\gamma^U(x) := e^{ip\cdot x/\hbar}g_\rho(x-q)\mathfrak{u}_\mu(p,q), \qquad x\in\mathbb{R}^3 \tag{18}$$

in which $\gamma := (\mu,p,q)$, $\mu=1,2,3,4$, is a point in phase space $\Gamma := \{1,2,3,4\}\times\mathbb{R}^3\times\mathbb{R}^3$.

• By $d\!\!\!{}^{-}\Omega$ we denote the following measure on Γ

$$d\!\!\!{}^{-}\Omega(\gamma) := \frac{1}{(2\pi\hbar)^3}d\Omega(\gamma) := \frac{1}{(2\pi\hbar)^3}\sum_{\mu=1}^4 dpdq,$$

i.e., it is a product of counting measure in the first factor, the variable μ, and Lebesgue measure in the last six factors of Γ.

• We have for any $\psi,\phi\in L^2(\mathbb{R}^3)^4$ and any set of coherent states F_γ, in particular the ones defined in (18) and (22),

$$(\psi,\phi) = \int_\Gamma d\!\!\!{}^{-}\Omega(\gamma)(\psi,F_\gamma)(F_\gamma,\phi),$$

i.e., coherent states are complete.

• For a function l taking its values in the interval $[a,b]$, $\gamma\in\{1,2,3,4\}\times\mathbb{R}^3\times\mathbb{R}^3$, and the coherent states defined in (18), the expression

$$(\psi,L\phi) := \int_\Gamma d\!\!\!{}^{-}\Omega(\gamma)\ l(\gamma)(\psi,F_\gamma^U)(F_\gamma^U,\phi) \tag{19}$$

defines a bounded self-adjoint operator on $L^2(\mathbb{R}^3)^4$, with coherent state symbol $l(\gamma)$, which satisfies $a\le L\le b$ and

$$\begin{aligned}\operatorname{tr} L =\ & \textstyle\int_\Gamma d\!\!\!{}^{-}\Omega(\gamma)\ l(\gamma)(F_\gamma^U,F_\gamma^U)\\ =\ & (2\pi\hbar)^{-3}\textstyle\sum_{\mu=1}^4\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} l(\gamma)|u_\mu(p,q)|^2dpdq.\end{aligned}$$

The operator $\mathcal{A}$ which we seek will be defined via its association with the sesquilinear form

$$\begin{aligned}\mathfrak{t}[\phi,\psi] :=\ & \tfrac{1}{(2\pi\hbar)^3}\textstyle\sum_{\mu=1}^4\int_{\mathbb{R}^6}(\phi,F_\gamma^U)(F_\gamma^U,\psi)u_\mu(p,q)dpdq\\ =\ & \textstyle\int_\Gamma d\!\!\!{}^{-}\Omega(\gamma)(\phi,F_\gamma^U)(F_\gamma^U,\psi)u(\gamma),\end{aligned}$$

[10] "Coherent state" is the name originally reserved for a wave function of the state of a linear oscillator which minimizes the uncertainty relation (see Landau and Lifshitz [10], p.71) the form of which is similar to the "coherent state" given here. More recently the term has been used in a broader sense.

for $\phi,\psi \in C_0^\infty(\mathbb{R}^3)^4$ where $u(\gamma) = u_\mu(p,q)$. In order to describe $\mathcal{A}$ it is helpful to adopt the following notation: for a function $f \in L^1_{loc}(\mathbb{R}^3)$

$$\begin{aligned} < f >_\rho (x) &:= f * g_\rho^2 = \textstyle\int_{\mathbb{R}^3} f(q) g_\rho(x-q)^2 dq, \\ \mathfrak{d}_\rho f &:= f - < f >_\rho, \\ \mathbf{A}(x,q) &:= \mathbf{a}(x) - \mathbf{a}(q) \ \text{ with } \ A_j(x,q) := a_j(x) - a_j(q), \ \text{and} \\ < \mathbf{A} V >_\rho (x) &:= \textstyle\int \mathbf{A}(x,q) V(q) g_\rho(x-q)^2 dq. \end{aligned}$$

Lemma 3. *For $\phi,\psi \in C_0^\infty(\mathbb{R}^3)^4$ we have the identity*

$$\begin{aligned} \mathfrak{t}[\phi,\psi] = \ & (1-\delta)\big[(\phi, ((D-k\mathbf{a})^2 - \hbar k\Sigma\cdot < \mathbf{B} >_\rho)\psi) + (\phi,\psi)\|Dg_\rho\|^2 + (\phi, k^2 < \mathbf{A}^2 >_\rho \psi) \\ & + k \textstyle\sum_{\nu=1}^3 \big\{((D_\nu - k a_\nu)\phi, < A_\nu >_\rho \psi) + (< A_\nu >_\rho \phi, (D_\nu - k a_\nu)\psi)\big\}\big] \\ & + (\phi, < V^2 - \Phi >_\rho \psi) + (\mathcal{D}_{\mathbf{a}}\phi, < V >_\rho \psi) + (< V >_\rho \phi, \mathcal{D}_{\mathbf{a}}\psi) + 2(\phi, < V >_\rho \beta\psi) \\ & + 2(\phi, k\alpha\cdot < \mathbf{A} V >_\rho \psi). \end{aligned}$$

Proof. By recalling the spectral representation of the matrix U in terms of its eigenvalues u_μ and eigenvectors $\mathfrak{u}_\mu$, $\mu = 1,2,3,4$, we have that

$$\begin{aligned} \mathfrak{t}[\phi,\psi] &= (2\pi\hbar)^{-3} \textstyle\int dpdq \int dxdy e^{ip\cdot(x-y)/\hbar} < \phi(x), U(p,q)\psi(y) > g_\rho(x-q) g_\rho(y-q) \\ &= (1-\delta)(I_1 - I_2) + I_3 + I_4 + I_5, \end{aligned}$$

say, corresponding to the different terms in $U(p,q)$ given in (17). A calculation yields that

$$(2\pi\hbar)^3 I_1 :=$$
$$\sum_{j=1}^3 \int dpdq \int dxdy e^{ip\cdot(x-y)/\hbar} < (D_j^x - k a_j(q))(g_\rho(x-q)\phi(x)), (D_j^y - k a_j(q))(g_\rho(y-q)\psi(y)) >$$

implying that

$$I_1 = \sum_{j=1}^3 \int dqdx < (D_j - k a_j(q))(g_\rho(x-q)\phi(x)), (D_j - k a_j(q))(g_\rho(x-q)\psi(x)) >$$

on using the fact that

$$\Psi(x) = \frac{1}{(2\pi\hbar)^3} \int dp \int dy e^{ip\cdot(x-y)/\hbar} \Psi(y).$$

Then further calculations show that

$$\begin{aligned} I_1 = \ & (\phi, (D-k\mathbf{a})^2\psi) + \textstyle\sum_{j=1}^3 \big\{((D_j - k a_j)\phi, k < A_j >_\rho \psi) + (k < A_j >_\rho \phi, (D_j - k a_j)\psi)\big\} \\ & + (\phi,\psi)\|Dg_\rho\|^2 + (\phi, k^2 < \mathbf{A}^2 >_\rho \psi) \end{aligned}$$

where $< A_j >_\rho (x) = \int (a_j(x) - a_j(q)) g_\rho(x-q)^2 dq$.

The next term becomes

$$\begin{aligned} I_2 &= \tfrac{1}{(2\pi\hbar)^3} \textstyle\int dpdqdxdy e^{ip\cdot(x-y)/\hbar} < \phi(x), \hbar k\Sigma\cdot B(q)\psi(y) > g_\rho(x-q) g_\rho(y-q) \\ &= \hbar \textstyle\int dqdx < \phi(x), k\Sigma\cdot B(q)\psi(x) > g_\rho^2(x-q) \\ &= (\phi, \hbar k\Sigma\cdot < B >_\rho \psi), \end{aligned}$$

and

$$\begin{aligned} I_3 &= (2\pi\hbar)^{-3} \textstyle\int dpdq \int dxdy e^{ip\cdot(x-y)/\hbar} < \phi(x), (V^2(q) - \Phi(q))\psi(y) > g_\rho(x-q) g_\rho(y-q) \\ &= (\phi, < V^2 - \Phi >_\rho \psi). \end{aligned}$$

For I_4 we have

$$\begin{aligned} & \tfrac{1}{2}(2\pi\hbar)^3 I_4 \\ & := \textstyle\int dpdq \int dxdy e^{ip\cdot(x-y)/\hbar} < \phi(x), V(q)\alpha\cdot(p - k\mathbf{a}(q))\psi(y) > g_\rho(x-q) g_\rho(y-q) \\ & = \textstyle\sum_{j=1}^3 \int dpdq \int dxdy e^{ip\cdot(x-y)/\hbar} < \phi(x), \alpha_j(D_j^y - k a_j(q))[g_\rho(y-q)\psi(y)] > V(q) g_\rho(x-q) \end{aligned}$$

which implies that

$$\begin{aligned} & \tfrac{1}{2} I_4 = (\phi, < V >_\rho \mathcal{D}_{\mathbf{a}}\psi) + \textstyle\sum_{j=1}^3 \int dqdx < \phi(x), k A_j(x,q)\alpha_j\psi(x) > V(q) g_\rho(x-q)^2 \\ & + \tfrac{1}{2} \textstyle\sum_{j=1}^3 \int dqdx < \phi(x), \alpha_j(D_j g_\rho(x-q)^2) V(q)\psi(x) > \\ & = (< V >_\rho \phi, \mathcal{D}_{\mathbf{a}}\psi) + (\phi, k\alpha\cdot < \mathbf{A} V >_\rho \psi) + \tfrac{1}{2} \textstyle\sum_{j=1}^3 \int dqdx < \phi, \alpha_j\psi > (D_j g_\rho(x-q)^2) V(q). \end{aligned}$$

Alternatively we have that

$$\frac{1}{2}I_4 = (\mathcal{D}_{\mathbf{a}}\phi, < V >_\rho \psi) + (k\alpha\cdot < \mathbf{A}V >_\rho \phi, \psi) - \frac{1}{2}\sum_{j=1}^{3}\int dqdx < \alpha_j\phi, \psi > (D_j g_\rho(x-q)^2)V(q).$$

Adding the last two expressions gives the identity

$$I_4 = (\mathcal{D}_{\mathbf{a}}\phi, < V >_\rho \psi) + (< V >_\rho \phi, \mathcal{D}_{\mathbf{a}}\psi) + 2(\phi, k\alpha\cdot < \mathbf{A}V >_\rho \psi).$$

Finally, it is easy to see that

$$\begin{aligned} I_5 := & \quad (2\pi\hbar)^{-3}\int dpdq \int dxdy e^{ip\cdot(x-y)/\hbar} < \phi(x), 2V(q)\beta\psi(y) > g_\rho(x-q)g_\rho(y-q) \\ = & \quad 2(\phi, < V >_\rho \beta\psi). \end{aligned}$$

The result follows by combining these expressions as

$$\mathfrak{t}[\phi,\psi] = (1-\delta)(I_1 - I_2) + I_3 + I_4 + I_5.$$

$\square$

The operator $\mathcal{A}$ described by $(\phi, \mathcal{A}\psi) = \mathfrak{t}[\phi,\psi]$ via Lemma 3 can be written as

$$\begin{aligned} &\mathcal{A} = \\ &(1-\delta)\{{\mathcal{D}_{\mathbf{a}}}^2 + \hbar k\Sigma\cdot\mathfrak{d}_\rho\mathbf{B} + 2k < \mathbf{A} >_\rho \cdot(D - k\mathbf{a}) + k(D\cdot < \mathbf{A} >_\rho) + k^2 < \mathbf{A}^2 >_\rho + \hbar^2\|\nabla g_\rho\|^2\} \\ &+2 < V >_\rho (\mathcal{D}_{\mathbf{a}} + \beta) + [(\alpha\cdot D) < V >_\rho] + 2k\alpha\cdot < \mathbf{A}V >_\rho + < V^2 - \Phi >_\rho . \end{aligned}$$

Now we consider the difference of these two operators: $R := [T_V(\mathbf{a})^2 - 1 - \Phi] - \mathcal{A}$ as given by

$$(\phi, R\psi) := \mathfrak{h}[\phi,\psi] - \mathfrak{t}[\phi,\psi], \qquad \phi,\psi \in C_0^\infty(\mathbb{R}^3)^4, \tag{20}$$

for $\mathfrak{h}$ given in (16) and $\mathfrak{t}$ described in Lemma 3.

The lower bound for $-\operatorname{tr}(T_V(\mathbf{a})^2 - 1 - \Phi)_-$ which we seek is given by the next lemma.

Lemma 4. *Let $V \in L^{\frac{3}{2}}(\mathbb{R}^3)\cap L^\infty(\mathbb{R}^3)$, $\nabla V \in L^\infty(\mathbb{R}^3)$, $|\mathbf{B}| \in L^{\frac{3}{2}}(\mathbb{R}^3)\cap L^3(\mathbb{R}^3)$, and $\Phi \in L^{\frac{3}{2}}(\mathbb{R}^3)\cap L^4(\mathbb{R}^3)$. Assume that (6) holds with $\eta = 1$. Then*

$$-\operatorname{tr}(T_V(\mathbf{a})^2 - 1 - \Phi)_- \geq -\frac{1}{(2\pi\hbar)^3}\int u(\gamma)_- d\Omega(\gamma) + \operatorname{tr}[Rd_{min}]$$

where $d_{min} := \chi_{(-\infty,0)}(T_V(\mathbf{a})^2 - 1 - \Phi)$.

Proof. According to Lemma 2, d_{min} is in trace class $\mathfrak{S}_1$ provided $V \in L^{\frac{3}{2}}(\mathbb{R}^3)\cap L^3(\mathbb{R}^3)$, $|\mathbf{B}| \in L^{\frac{3}{2}}(\mathbb{R}^3)$, and $\Phi \in L^{\frac{3}{2}}(\mathbb{R}^3)$. By the proof of Lemma 2, we have that

$$T_V(\mathbf{a})^2 - 1 - \Phi \geq \frac{1}{2}{\mathcal{D}_{\mathbf{a}}}^2 - (2|V| + V^2 + \Phi).$$

As a consequence it follows from Theorem 2 of Lieb, Loss, and Solovej [16] that $(T_V(\mathbf{a})^2 - 1 - \Phi)_-$ is in $\mathfrak{S}_1$ provided $(2|V| + V^2 + \Phi) \in L^{\frac{5}{2}}(\mathbb{R}^3)\cap L^4(\mathbb{R}^3)$ and $|\mathbf{B}| \in L^2(\mathbb{R}^3)$.

Since $V \in L^2(\mathbb{R}^3)$ and $\Phi \in L^{\frac{3}{2}}(\mathbb{R}^3)$, then $< V >_\rho$ and $< V^2 - \Phi >_\rho$, and their derivatives are smooth functions decaying at ∞. Since (6) holds with $\eta = 1$, then $< \mathbf{A}V >_\rho$, $< \mathbf{A} >_\rho$, $< \mathbf{A}^2 >_\rho$, and $D\cdot < \mathbf{A} >_\rho = \sum_{\nu=1}^3[\partial_\nu a_\nu(x) - < \partial_\nu a_\nu >_\rho]$ are bounded. As a consequence it follows that $\mathcal{A}$ is the sum of $(1-\delta)(D - k\mathbf{a})^2$ and a perturbation of relative bound 0. In particular, $\mathcal{A}$ has domain $\mathcal{D}((D - k\mathbf{a})^2)$.

The operator $d_{min} := \chi_{(-\infty,0)}(T_V(\mathbf{a})^2 - 1 - \Phi)$ is a finite rank operator with range in $\mathcal{D}(T_V(\mathbf{a})^2 - 1 - \Phi) = \mathcal{D}(T_V(\mathbf{a})^2)$. Thus, if $\psi \in \mathcal{R}(d_{min})$,

$$\psi \in \mathcal{H}^1_{\mathbf{a}}, \qquad T_V(\mathbf{a})\psi \in \mathcal{H}^1_{\mathbf{a}},$$

on using Corollary 1. Thus, for $\nu = 1, 2, 3$,

$$(D_\nu - ka_\nu)(\alpha\cdot(D - k\mathbf{a}) + \beta + V)\psi = (D_\nu - ka_\nu)T_V(\mathbf{a})\psi \in L^2(\mathbb{R}^3)^4.$$

Since $\psi \in \mathcal{H}^1_{\mathbf{a}}$ and $V, \nabla V \in L^\infty(\mathbb{R}^3)$, then $(D_\nu - ka_\nu)(\beta + V)\psi \in L^2(\mathbb{R}^3)^4$. Hence, we have

$$[(D - k\mathbf{a})^2 - k\Sigma\cdot\mathbf{B}]\psi = [\alpha\cdot(D - k\mathbf{a})]^2\psi \in L^2(\mathbb{R}^3)^4.$$

It follows from (2) that $|\mathbf{B}|\psi \in L^2(\mathbb{R}^3)^4$ which implies that $(D-k\mathbf{a})^2\psi \in L^2(\mathbb{R}^3)^4$. Therefore $\psi \in \mathcal{D}((D-k\mathbf{a})^2) = \mathcal{D}(\mathcal{A})$.

We now know that $\mathcal{A}d_{min}$ is defined and is of finite rank, i.e., $\mathcal{A}d_{min} \in \mathfrak{S}_1$. Thus[11]

$$(21)\qquad \begin{aligned} -\operatorname{tr}(T_V(\mathbf{a})^2 - 1 - \Phi)_- &= \operatorname{tr}[(\mathcal{A}+R)d_{min}] \\ &= \operatorname{tr}[\mathcal{A}d_{min}] + \operatorname{tr}[Rd_{min}] \\ &\geq \inf\{\operatorname{tr}[\mathcal{A}d] : d \text{ self-adjoint}, 0 \leq d \leq 1, \mathcal{A}d \in \mathfrak{S}_1\} + \operatorname{tr}[Rd_{min}] \\ &= -\operatorname{tr}[\mathcal{A}_-] + \operatorname{tr}[Rd_{min}]. \end{aligned}$$

If $\{\phi_\nu\}_\nu$ is any orthonormal basis of the negative spectral subspace of $\mathcal{A}$, then

$$\begin{aligned} -\operatorname{tr}(\mathcal{A}_-) := &\sum_\nu(\phi_\nu, \mathcal{A}\phi_\nu) = \sum_\nu \mathfrak{t}[\phi_\nu,\phi_\nu] = \sum_\nu \int_\Gamma d\!\!\!/\Omega(\gamma)(\phi_\nu, F_\gamma^U)(F_\gamma^U,\phi_\nu)u(\gamma) \\ \geq &-\int_\Gamma d\!\!\!/\Omega(\gamma)u(\gamma)_- \sum_\nu |(\phi, F_\gamma^U)|^2 \geq -\int_\Gamma u(\gamma)_- d\!\!\!/\Omega(\gamma) \end{aligned}$$

by the Bessel inequality. Substituting this inequality into (21) completes the proof. □

Now we work towards an estimate for $\operatorname{tr}[Rd_{min}]$.

Lemma 5. *Let $(\phi, R\psi)$ be given by (20). Then for all positive δ and θ sufficiently small and*

$$\begin{aligned} R_1 := &\tfrac{\delta}{2}\big\{\mathcal{D}_\mathbf{a}{}^2 - \tfrac{2}{\delta^2\theta}[\mathfrak{d}_\rho(V)]^2 - \tfrac{4}{\delta}|\mathfrak{d}_\rho(V)| + \tfrac{2}{\delta}\mathfrak{d}_\rho(V^2-\Phi)_- - \tfrac{4k}{\delta}\textstyle\sum_j |< A_jV >_\rho| \\ &- \tfrac{2\hbar k}{\delta}|\mathfrak{d}_\rho\mathbf{B}| - 2\theta\hbar k|\mathbf{B}| - \tfrac{2k^2}{\delta^2\theta}|< \mathbf{A}^2 >_\rho|\big\} \end{aligned}$$

we have that

$$R \geq R_1 - \hbar^2\|\nabla g_\rho\|^2$$

in the form sense. If (6) holds and $\rho < \rho_0$, then $R_1 \geq R_2 - \frac{k^2M^2\rho^{2\eta}}{\delta\theta}$ for

$$\begin{aligned} R_2 := &\tfrac{\delta}{2}\big\{\mathcal{D}_\mathbf{a}{}^2 - \tfrac{2}{\delta^2\theta}[\mathfrak{d}_\rho(V)]^2 - \tfrac{4}{\delta}|\mathfrak{d}_\rho(V)| + \tfrac{2}{\delta}[\mathfrak{d}_\rho(V^2-\Phi)]_- - \tfrac{12kM\rho^\eta}{\delta} < |V| >_\rho \\ &- \tfrac{2\hbar k}{\delta}|\mathfrak{d}_\rho\mathbf{B}| - 2\theta\hbar k|\mathbf{B}|\big\}. \end{aligned}$$

Proof. For all $\phi \in C_0^\infty(\mathbb{R}^3)^4$ we have the equality

$$\begin{aligned} (\phi, R\phi) = &(\phi,[T_V(\mathbf{a})^2 - 1 - \Phi]\phi) - (\phi,\mathcal{A}\phi) \\ = &(\phi,\mathcal{D}_\mathbf{a}{}^2\phi) + 2\Re e(\phi, V(\mathcal{D}_\mathbf{a}+\beta)\phi) + (\phi,(V^2-\Phi)\phi) \\ &-\big\{(1-\delta)\{(\phi,\mathcal{D}_\mathbf{a}{}^2\phi) + \hbar(\phi, k\Sigma\cdot\partial_\rho\mathbf{B}\phi)\} \\ &+(\phi, < V^2-\Phi >_\rho \phi) + 2\mathfrak{Re}(\phi, < V >_\rho (\mathcal{D}_\mathbf{a}+\beta)\phi) + 2(\phi, k\alpha\cdot < \mathbf{A}V >_\rho \phi) \\ &+(1-\delta)\big[2k\mathfrak{Re}(\phi, < \mathbf{A} >_\rho \cdot(D-k\mathbf{a})\phi) \\ &+\hbar^2\|\nabla g_\rho\|^2\|\phi\|^2 + (\phi, k^2 < \mathbf{A}^2 >_\rho \phi)\big]\big\} \\ = &\delta(\phi,\mathcal{D}_\mathbf{a}{}^2\phi) + 2\Re e(\phi,\mathfrak{d}_\rho(V)(\mathcal{D}_\mathbf{a}+\beta)\phi) + (\phi,\mathfrak{d}_\rho(V^2-\Phi)\phi) - 2(\phi, k\alpha\cdot < \mathbf{A}V >_\rho \phi) \\ &-(1-\delta)\big[\hbar(\phi, k\Sigma\cdot\mathfrak{d}_\rho\mathbf{B}\phi) + 2k\mathfrak{Re}(\phi, < \mathbf{A} >_\rho \cdot(D-k\mathbf{a})\phi) \\ &+\hbar^2\|\nabla g_\rho\|^2\|\phi\|^2 + (\phi, k^2 < \mathbf{A}^2 >_\rho \phi)\big] \\ \geq &\delta(1-\theta)(\phi,\mathcal{D}_\mathbf{a}{}^2\phi) - \tfrac{1}{\delta\theta}(\phi,[\mathfrak{d}_\rho(V)]^2\phi) - 2(\phi,|\mathfrak{d}_\rho(V)|\phi) \\ &+(\phi,\mathfrak{d}_\rho(V^2-\Phi)\phi) - 2(\phi, k\alpha\cdot < \mathbf{A}V >_\rho \phi) \\ &-(1-\delta)\big[\hbar(\phi, k\Sigma\cdot\mathfrak{d}_\rho\mathbf{B}\phi) + 2k\mathfrak{Re}(\phi, < \mathbf{A} >_\rho \cdot(D-k\mathbf{a})\phi) \\ &+\hbar^2\|\nabla g_\rho\|^2\|\phi\|^2 + (\phi, k^2 < \mathbf{A}^2 >_\rho \phi)\big]. \end{aligned}$$

Using the fact that

$$\begin{aligned} 2k\Re e(\phi, < \mathbf{A} >_\rho \cdot(D-k\mathbf{a})\phi) &\leq 2k\textstyle\sum_{j=1}^3 \| < A_j >_\rho \phi\|\|(D_j - ka_j)\phi\| \\ &\leq 2\big[\textstyle\sum_{j=1}^3 \|k < A_j >_\rho \phi\|^2\big]^{\frac12}\big[\textstyle\sum_{j=1}^3\|(D_j-ka_j)\phi\|^2\big]^{\frac12} \\ &= 2(\phi, k^2 < \mathbf{A} >_\rho^2 \phi)^{\frac12}(\phi,(D-k\mathbf{a})^2\phi)^{\frac12} \\ &\leq \tfrac{\delta\theta}{1-\delta}(\phi,(D-k\mathbf{a})^2\phi) + \tfrac{1-\delta}{\delta\theta}(\phi, k^2 < \mathbf{A} >_\rho^2 \phi) \\ &= \tfrac{\delta\theta}{1-\delta}[(\phi,\mathcal{D}_\mathbf{a}{}^2\phi) + (\phi,\hbar k\Sigma\cdot\mathbf{B}\phi)] + \tfrac{1-\delta}{\delta\theta}(\phi, k^2 < \mathbf{A} >_\rho^2 \phi) \end{aligned}$$

[11] Note that $T_V(\mathbf{a})^2 - 1 - \Phi$, $\mathcal{A}$, and R have the same form domains and that $T_V(\mathbf{a})^2 - 1 - \Phi$ is the form sum $\mathcal{A} + R$. It follows that $\mathcal{R}(d_{min}) \subset \mathcal{D}(R)$ and hence, $(\mathcal{A}+R)d_{min} = \mathcal{A}d_{min} + Rd_{min}$.

and since $< \mathbf{A}^2 >_\rho \geq < \mathbf{A} >_\rho^2$, we have that

$$\begin{aligned}(\phi, R\phi) \geq \; & \delta(1-2\theta)(\phi, \mathcal{D}_{\mathbf{a}}{}^2\phi) - \tfrac{1}{\delta\theta}(\phi, [\mathfrak{d}_\rho(V)]^2\phi) - 2(\phi, |\mathfrak{d}_\rho(V)|\phi) \\ & +(\phi, \mathfrak{d}_\rho(V^2-\Phi)\phi) - 2(\phi, k\textstyle\sum_j | < A_j V >_\rho |\phi) \\ & -(1-\delta)\big[\hbar(\phi, k\Sigma\cdot\mathfrak{d}_\rho\mathbf{B}\phi) + \tfrac{\delta\theta}{1-\delta}(\phi, \hbar k\Sigma\cdot\mathbf{B}\phi) + \tfrac{1-\delta}{\delta\theta}(\phi, k^2 < \mathbf{A}^2 >_\rho \phi) \\ & +\hbar^2\|\nabla g_\rho\|^2\|\phi\|^2 + (\phi, k^2 < \mathbf{A}^2 >_\rho \phi)\big].\end{aligned}$$

Assuming that $\theta \leq \frac{1}{4}$ we have that

$$R \geq R_1 - \hbar^2\|\nabla g_\rho\|^2.$$

The last statement in the lemma follows from the fact that

$$< \mathbf{A}^2 >_\rho = \int_{\mathbb{R}^3} |\mathbf{a}(x) - \mathbf{a}(q)|^2 g_\rho(x-q)^2 dq \leq M^2\rho^{2\eta}$$

and

$$| < A_j V >_\rho | \leq M\rho^\eta < |V| >_\rho .$$

$\square$

Lemma 6. *Define*

$$\hbar^2\mathcal{U}_{\delta,\hbar,\theta}(x) := \tfrac{1}{\delta^2\theta}[\mathfrak{d}_\rho(V)]^2 + \tfrac{1}{\delta}|\mathfrak{d}_\rho(V)| + \tfrac{1}{\delta}[\mathfrak{d}_\rho(V^2-\Phi)]_- + \tfrac{\hbar k}{\delta}|\mathfrak{d}_\rho\mathbf{B}| + \hbar k\theta|\mathbf{B}| + \tfrac{k\rho^\eta}{\delta} < |V| >_\rho$$

and suppose that (6) holds with $\rho < \rho_0$, $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^8(\mathbb{R}^3)$, and $|\mathbf{B}|, \Phi \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^4(\mathbb{R}^3)$. Then

$$\mathrm{tr}[Rd_{min}] \geq -K\left[\delta\hbar^2\left\{\textstyle\int \mathcal{U}^{\frac{5}{2}}_{\delta,\hbar,\theta}(x)dx + \left(\frac{k}{\hbar}\right)^{\frac{3}{2}}\left(\int \mathbf{B}^2(x)dx\right)^{\frac{3}{4}}\left(\int \mathcal{U}^4_{\delta,\hbar,\theta}(x)dx\right)^{\frac{1}{4}}\right\} + \tfrac{1}{\hbar\rho^2} + \tfrac{k^2\rho^{2\eta}}{\hbar^3\delta\theta}\right]$$

for some constant $K > 0$.

Proof. Since for some $C > 0$

$$R_2 \geq \frac{\delta\hbar^2}{2}\left\{\left(\alpha\cdot(\frac{1}{i}\nabla - \frac{k}{\hbar}\mathbf{a})\right)^2 - C\mathcal{U}_{\delta,\hbar,\theta}\right\},$$

it follows from Theorem 2 of Lieb, Loss, and Solovej [16] that there are positive constants C_1 and C_2 such that

$$\mathrm{tr}[R_2]_- \leq \delta\hbar^2\left\{C_1\int \mathcal{U}^{\frac{5}{2}}_{\delta,\hbar,\theta}(x)dx + C_2\frac{k^{\frac{3}{2}}}{\hbar^{\frac{3}{2}}}\left(\int \mathbf{B}^2(x)dx\right)^{\frac{3}{4}}\left(\int \mathcal{U}^4_{\delta,\hbar,\theta}(x)dx\right)^{\frac{1}{4}}\right\}$$

which is finite by the hypothesis. Since $\mathrm{tr}(d_{min}) = O(\hbar^{-3})$ by Lemma 2 then the conclusion follows from Lemma 5 and (14). $\square$

4.2. **An upper bound for $-\mathrm{tr}(T_V(\mathbf{a})^2 - 1 - \Phi)_-$.** The main idea here is to use (14) with a good approximating d in order to produce an upper bound for the operator $T_V(\mathbf{a})^2 - 1 - \Phi$. (For a similar treatment see Lieb [14], p.621.)

Let $O(p,q)$, $p, q \in \mathbb{R}^3$, be a 4×4 matrix with eigenvectors $\mathfrak{o}_\mu$, $\mu = 1,2,3,4$, orthonormal in $\mathbb{C}^4$. Define the normalized coherent state

(22) $$F^O_\gamma(x) := e^{ip\cdot x/\hbar} g_\rho(x-q)\mathfrak{o}_\mu(p,q)$$

(cf. $F^U_\gamma(x)$ above). For $\mu = 1,2,3,4$, let $M_\mu(p,q)$ be a function defined on $\mathbb{R}^6$ which takes values only in $(0,1)$ and has support with finite volume in $\mathbb{R}^6$. The approximating d will be defined as L was in (19) in which $l(\gamma)$ is replaced by $M(\gamma)$, i.e.,

(23) $$(\psi, d\phi) := \int_\Gamma d\!\!\!{}^{-}\Omega(\gamma)\ M(\gamma)(\psi, F^O_\gamma)(F^O_\gamma, \phi).$$

With respect to (14) we note that $d : L^2(\mathbb{R}^3)^4 \to L^2(\mathbb{R}^3)^4$ is trace class, self-adjoint, and $0 \le d \le 1$. Let S be a self-adjoint operator that is bounded below and densely defined in $L^2(\mathbb{R}^3)^4$ whose domain contains the range of d. If $\{e_k(x)\}$ is an orthonormal basis for $L^2(\mathbb{R}^3)^4$ then

$$\begin{aligned}\operatorname{tr}[Sd] = &\ \tfrac{1}{(2\pi\hbar)^3}\textstyle\sum_{\mu=1}^4 \int_{\mathbb{R}^6} M_\mu(p,q)\sum_k (e_k, SF_\gamma^O)(F_\gamma^O, e_k)dpdq \\ = &\ \tfrac{1}{(2\pi\hbar)^3}\textstyle\int_{\mathbb{R}^6} d\Omega(\gamma) M(\gamma)(F_\gamma^O, SF_\gamma^O).\end{aligned} \tag{24}$$

In the next lemma we use these ideas to give an upper bound for $-\operatorname{tr}(T_V(\mathbf{a})^2 - 1 - \Phi)_-$. For the best upper and lower bounds we need the matrices $U_\delta(p,q)$ (given in (17)) and $O(p,q)$ to be equal asymptotically as $\delta \to 0$, $\rho \to 0$. The choice for $O(p,q)$ is given by[12]

$$\begin{aligned} O(p,q) := &\ < U_0(p,x) >_\rho (q) \\ = &\ < (p - k\mathbf{a})^2 >_\rho (q) - \hbar k \Sigma\cdot < \mathbf{B} >_\rho (q) \\ &+ 2 < V\{\alpha\cdot(p-k\mathbf{a}) + \beta\} >_\rho (q) + < V^2 - \Phi >_\rho (q).\end{aligned} \tag{25}$$

Lemma 7. *Let $\mathfrak{o}_\mu$ denote the eigenvectors of $O(p,q)$ defined in (25), which are orthonormal in $\mathbb{C}^4$, with corresponding eigenvalues o_μ for $\mu = 1,2,3,4$, and set $o(\gamma) = o_\mu(p,q)$, Let d be given by (23) with F_γ^O defined by (22) and $M(\gamma) := \chi_{\{\gamma : o(\gamma) < 0\}}$. Then we have the inequality*

$$-\operatorname{tr}(T_V(\mathbf{a})^2 - 1 - \Phi)_- \le \operatorname{tr}(T_V(\mathbf{a})^2 - 1 - \Phi)d = \int_{o(\gamma)<0} [o(\gamma) + \hbar^2\|\nabla g_\rho\|^2]\, d\!\!{}^-\Omega(\gamma). \tag{26}$$

Proof. The inequality in (26) follows from (14). By (24) we have that

$$\operatorname{tr}(T_V(\mathbf{a})^2 - 1 - \Phi)d = \int_{\mathbb{R}^6} d\!\!{}^-\Omega(\gamma) M(\gamma)(F_\gamma^O, (T_V(\mathbf{a})^2 - 1 - \Phi)F_\gamma^O).$$

The expression in the integrand above reduces as follows:

$$(F_\gamma^O, (T_V(\mathbf{a})^2 - 1 - \Phi)F_\gamma^O) = \|\mathcal{D}_\mathbf{a} F_\gamma^O\|^2 + 2\mathfrak{Re}(\mathcal{D}_\mathbf{a}F_\gamma^O, VF_\gamma^O) + (F_\gamma^O, (2V\beta + V^2 - \Phi)F_\gamma^O). \tag{27}$$

Recall that the Dirac matrices satisfy $\alpha_\nu\alpha_\mu + \alpha_\mu\alpha_\nu = 2\delta_{\mu\nu}I_4$ for $\mu,\nu = 1,2,3$, and that the Pauli matrices satisfy $\sigma_1\sigma_2 = i\sigma_3$, $\sigma_2\sigma_3 = i\sigma_1$, and $\sigma_3\sigma_1 = i\sigma_2$. Using these identities calculations show that the first term of the right-hand side of (27) can be written

$$\begin{aligned}\|\mathcal{D}_\mathbf{a}F_\gamma^O\|^2 = &\ (F_\gamma^O, (\alpha\cdot(p-k\mathbf{a}))^2 F_\gamma^O) - \hbar k \mathfrak{Re}(F_\gamma^O, (\Sigma\cdot\mathbf{B})F_\gamma^O) + \hbar^2\|\nabla g_\rho\|^2 \\ = &\ < \mathfrak{o}_\mu(p,q), (< (p-k\mathbf{a})^2 >_\rho - \hbar k\Sigma\cdot < \mathbf{B} >_\rho)\mathfrak{o}_\mu(p,q) > + \hbar^2\|\nabla g_\rho\|^2.\end{aligned} \tag{28}$$

The second term in (27) is given by

$$2\mathfrak{Re}(\mathcal{D}_\mathbf{a}F_\gamma^O, VF_\gamma^O) = < \mathfrak{o}_\mu(p,q), 2\alpha\cdot < (p-k\mathbf{a})V >_\rho \mathfrak{o}_\mu(p,q) > .$$

The last term in (27) reduces as

$$(F_\gamma^O, (2V\beta + V^2 - \Phi)F_\gamma^O) = < \mathfrak{o}_\mu(p,q), [2 < V >_\rho \beta + < V^2 - \Phi >_\rho]\mathfrak{o}_\mu(p,q) > .$$

Then (26) follows from the fact that

$$(F_\gamma^O, (T_V(\mathbf{a})^2 - 1 - \Phi)F_\gamma^O) = < \mathfrak{o}_\mu(p,q), O(p,q)\mathfrak{o}_\mu(p,q) > + \hbar^2\|\nabla g_\rho\|^2. \tag{29}$$

□

The eigenvalues $o(\gamma)$ and $u(\gamma)$ are computed in the Appendix. We will need to know that $\int_{o(\gamma)<0} d\Omega(\gamma) < \infty$. To this end we present the next lemma.

Lemma 8. *For $o(\gamma) = o(\mu,p,q)$, $\mu = 1,2,3,4$,*

$$o(\gamma)_- \le 1 + k\hbar| < \mathbf{B} >_\rho | + | < \Phi_+ >_\rho |. \tag{30}$$

If $\Phi_+, |\mathbf{B}| \in L^{\frac{3}{2}}(\mathbb{R}^3)$ and $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$, then

$$\int_{o(\gamma)<0} d\Omega(\gamma) \lesssim \int_{\mathbb{R}^3} \{\Phi_+^{\frac{3}{2}} + (k\hbar)^{\frac{3}{2}}|\mathbf{B}|^{\frac{3}{2}} + |V|^3 + |V|^{\frac{3}{2}}\}dq.$$

[12]Note that $< f >_\rho (q) := \int_{\mathbb{R}^3} f(x) g_\rho(q-x)^2 dx$.

Proof. First, note that $o(\gamma)_- \le o_2(p,q)_-$ where

$$
\begin{aligned}
o_2(p,q) = \;& < (p-k\mathbf{a})^2 >_\rho + < V^2 - \Phi >_\rho \\
& -2\Big[< V(p-k\mathbf{a}) >_\rho^2 + < V >_\rho^2 + \tfrac{(k\hbar)^2}{4} | < \mathbf{B} >_\rho |^2 \\
& + k\hbar\sqrt{< V >_\rho^2 | < \mathbf{B} >_\rho |^2 + [< V(p-k\mathbf{a}) >_\rho \cdot < \mathbf{B} >_\rho]^2}\Big]^{\frac{1}{2}} \\
\ge \;& < (p-k\mathbf{a})^2 >_\rho + < V^2 - \Phi_+ >_\rho \\
& -2\Big[< V(p-k\mathbf{a}) >_\rho^2 + < V >_\rho^2 + \tfrac{(k\hbar)^2}{4} | < \mathbf{B} >_\rho |^2 \\
& + k\hbar | < \mathbf{B} >_\rho | \sqrt{< V >_\rho^2 + < V(p-k\mathbf{a}) >_\rho^2}\Big]^{\frac{1}{2}} \\
= \;& < (p-k\mathbf{a})^2 >_\rho + < V^2 - \Phi_+ >_\rho \\
& -2\big[\sqrt{< V >_\rho^2 + < V(p-k\mathbf{a}) >_\rho^2} + \tfrac{k\hbar}{2} | < \mathbf{B} >_\rho |\big].
\end{aligned}
\tag{31}
$$

Since

$$
< V(p-k\mathbf{a}) >_\rho^2 = \sum_{j=1}^{3} < V(p_j - ka_j) >_\rho^2 \le < V^2 >_\rho < (p-k\mathbf{a})^2 >_\rho
$$

and $< V >_\rho^2 \le < V^2 >_\rho$, then

$$
\begin{aligned}
o_2(p,q) \ge \;& < (p-k\mathbf{a})^2 >_\rho + < V^2 - \Phi_+ >_\rho \\
& -2\big[\sqrt{< V^2 >_\rho}\sqrt{1 + < (p-k\mathbf{a})^2 >_\rho} + \tfrac{k\hbar}{2} | < \mathbf{B} >_\rho |\big] \\
\ge \;& \big(\sqrt{1 + < (p-k\mathbf{a})^2 >_\rho} - \sqrt{< V^2 >_\rho}\big)^2 - \big(1 + < \Phi_+ >_\rho + k\hbar | < \mathbf{B} >_\rho |\big) \\
\ge \;& -\big(1 + < \Phi_+ >_\rho + k\hbar | < \mathbf{B} >_\rho |\big)
\end{aligned}
\tag{32}
$$

which implies (30). By (32) we have that $o(\gamma) \le 0$ implies that

$$
\sqrt{1 + < (p-k\mathbf{a})^2 >_\rho} \le [1 + < \Phi_+ >_\rho + k\hbar | < \mathbf{B} >_\rho |]^{\frac{1}{2}} + < V^2 >_\rho^{\frac{1}{2}} .
$$

Since

$$
< (p-k\mathbf{a})^2 >_\rho = |p - k < \mathbf{a} >_\rho |^2 + k^2 < \mathbf{a}^2 >_\rho - k^2 < \mathbf{a} >_\rho^2 \ge |p - k < \mathbf{a} >_\rho |^2
$$

then

$$
\begin{aligned}
|p - k < \mathbf{a} >_\rho |^2 \le \;& \Big([1 + < \Phi_+ >_\rho + k\hbar | < \mathbf{B} >_\rho |]^{\frac{1}{2}} + < V^2 >_\rho^{\frac{1}{2}}\Big)^2 - 1 \\
= \;& < \Phi_+ >_\rho + k\hbar | < \mathbf{B} >_\rho | + < V^2 >_\rho \\
& + 2[< V^2 >_\rho + < V^2 >_\rho < \Phi_+ >_\rho + k\hbar < V^2 >_\rho | < \mathbf{B} >_\rho |]^{\frac{1}{2}} \\
\lesssim \;& \big[< \Phi_+ >_\rho + k\hbar | < \mathbf{B} >_\rho | + < V^2 >_\rho + < V^2 >_\rho^{\frac{1}{2}} \big]
\end{aligned}
$$

Thus for some constant $C > 0$

$$
\begin{aligned}
\int_{o(\gamma)<0} d\Omega(\gamma) \le \;& C \int_{\mathbb{R}^3} dq \big\{ < \Phi_+ >_\rho^{\frac{3}{2}} + (k\hbar)^{\frac{3}{2}} | < \mathbf{B} >_\rho |^{\frac{3}{2}} + < V^2 >_\rho^{\frac{3}{2}} + < V^2 >_\rho^{\frac{3}{4}} \big\} \\
\le \;& C \int_{\mathbb{R}^3} dq \big\{ \Phi_+^{\frac{3}{2}} + (k\hbar)^{\frac{3}{2}} |\mathbf{B}|^{\frac{3}{2}} + |V|^3 + |V|^{\frac{3}{2}} \big\}
\end{aligned}
$$

since $\| < f >_\rho \|_p \le \|f\|_p$, $p \in [1, \infty)$. □

4.3. **A Convergence Theorem for the Density.** Recall that we let $\{\psi_\nu(x)\}_\nu$ be the eigenfunctions of $T_V(\mathbf{a})^2 - 1 + W$ (with $\Phi = -W$) corresponding to negative eigenvalues, and denote the sum of the density of these states by $n(x) := \sum_\nu |\psi_\nu(x)|^2$.

In order to emphasize the dependence of the eigenvalues $o(\gamma)$ and $u(\gamma)$ upon the parameters ρ, δ, and $\hbar$ we sometimes will write $o(\gamma) = o_{\rho,\hbar}(\gamma)$ and $u(\gamma) = u_{\delta,\hbar}(\gamma)$. These eigenvalues are computed in the appendix as

$$
\begin{aligned}
o_{\rho,\hbar}(\gamma) = \quad & <(p-k\mathbf{a})^2>_\rho + <V^2-\Phi>_\rho \\
& +s(\mu)2\Bigg[<V(p-k\mathbf{a})>_\rho^2 + <V>_\rho^2 + \tfrac{(k\hbar)^2}{4}|<\mathbf{B}>_\rho|^2 \\
& +(-1)^\mu k\hbar\sqrt{<V>_\rho^2 |<\mathbf{B}>_\rho|^2 + [<V(p-k\mathbf{a})>_\rho \cdot <\mathbf{B}>_\rho]^2}\Bigg]^{\frac{1}{2}}
\end{aligned} \tag{33}
$$

where $s(1)=s(2)=-1$ and $s(3)=s(4)=1$, and

$$
\begin{aligned}
u_{\delta,\hbar}(\gamma) = \quad & (1-\delta)(p-k\mathbf{a}(q))^2 + V(q)^2 - \Phi(q) \\
& +s(\mu)2\Bigg[V(q)^2((p-k\mathbf{a}(q))^2+1) + (1-\delta)^2\tfrac{(k\hbar)^2}{4}|\mathbf{B}(q)|^2 \\
& +(-1)^\mu(1-\delta)k\hbar|V(q)|\sqrt{|\mathbf{B}(q)|^2 + ((p-k\mathbf{a}(q))\cdot\mathbf{B}(q))^2}\Bigg]^{\frac{1}{2}}
\end{aligned} \tag{34}
$$

Lemma 9. *Assume that*

(i) $\mathbf{a}$ *satisfies (6) with* $\eta = 1$ *and* $\rho_0 > \rho = \hbar^s$, $s \in (0,1)$;
(ii) $k(\hbar) = O(\hbar^{-t})$ *for some* $t \in [0, s\eta)$;
(iii) $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ *and* $\nabla V \in L^\infty(\mathbb{R}^3)$; *and*
(iv) $|\mathbf{B}|, W, Z \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^4(\mathbb{R}^3)$.

Let $o(\gamma)$ *be given by (33) and let* $u^\epsilon(\gamma)$ *be given by (34) with* $\Phi := -W$ *and* $\Phi := -W+\epsilon Z$ *respectively. Then for all* $\epsilon > 0$

$$
\overline{\lim}_{\hbar\to 0}(2\pi\hbar)^3 \int_{\mathbb{R}^3} Z(x)n(x)dx \le \frac{1}{\epsilon}\overline{\lim}_{\hbar\to 0}\int_\Gamma (u^\epsilon(\gamma)_- - o(\gamma)_-)d\Omega(\gamma) \tag{35}
$$

and for all $\epsilon < 0$ *we obtain the reverse inequality.*

Proof. Let $d := \chi_{(-\infty,0)}(T_V(\mathbf{a})^2 - 1 + W)$. By the minimax principle and (14)

$$
-\operatorname{tr}(T_V(\mathbf{a})^2 - 1 + W - \epsilon Z)_- \le \operatorname{tr}[(T_V(\mathbf{a})^2 - 1 + W)d] - \epsilon\int_{\mathbb{R}^3} Z(x)n(x)dx
$$

since $\operatorname{tr}(Zd) = \int_{\mathbb{R}^3} Z(x)n(x)dx$. Since $Z \in L^{\frac{3}{2}}(\mathbb{R}^3)$ and each $\psi_\nu(x) \in H^1(\mathbb{R}^3)^4$ according to Corollary 1, then it follows from the Sobolev embedding theorem that

$$
\int_{\mathbb{R}^3} Z(x)n(x)dx < \infty
$$

and $\operatorname{tr}[(T_V(\mathbf{a})^2 - 1 + W)d] = -\operatorname{tr}(T_V(\mathbf{a})^2 - 1 + W)_- < \infty$ by (14) and Lemma 2. Therefore for $\epsilon \neq 0$

$$
\epsilon\int_{\mathbb{R}^3} Z(x)n(x)dx \le -\operatorname{tr}(T_V(\mathbf{a})^2 - 1 + W)_- + \operatorname{tr}(T_V(\mathbf{a})^2 - 1 + W - \epsilon Z)_-
$$

which implies the upper bound for $\epsilon > 0$

$$
\int_{\mathbb{R}^3} Z(x)n(x)dx \le [-\operatorname{tr}(T_V(\mathbf{a})^2 - 1 + W)_- + \operatorname{tr}(T_V(\mathbf{a})^2 - 1 + W - \epsilon Z)_-]/\epsilon \tag{36}
$$

and the lower bound for $\epsilon < 0$

$$
\int_{\mathbb{R}^3} Z(x)n(x)dx \ge [-\operatorname{tr}(T_V(\mathbf{a})^2 - 1 + W)_- + \operatorname{tr}(T_V(\mathbf{a})^2 - 1 + W - \epsilon Z)_-]/\epsilon. \tag{37}
$$

By choosing $\Phi := -W$ in Lemma 7

$$
-\operatorname{tr}(T_V(\mathbf{a})^2 - 1 + W)_- \le \int_{o(\gamma)<0}[o(\gamma) + \hbar^2\|\nabla g_\rho\|^2]\, d\Omega(\gamma). \tag{38}
$$

By choosing $\Phi = -W + \epsilon Z$ in Lemma 4 and in Lemma 6

$$
\begin{aligned}
& \operatorname{tr}(T_V(\mathbf{a})^2 - 1 + W - \epsilon Z)_- \le \textstyle\int_\Gamma u^\epsilon(\gamma)_- d\Omega(\gamma) \\
& \quad +K\left[\delta\hbar^2\left\{\int \mathcal{U}^{\frac{5}{2}}_{\delta,\hbar,\theta}(x)dx + \left(\tfrac{k}{\hbar}\right)^{\frac{3}{2}}\left(\int \mathbf{B}^2(x)dx\right)^{\frac{3}{4}}\left(\int \mathcal{U}^4_{\delta,\hbar,\theta}(x)dx\right)^{\frac{1}{4}}\right\} + \tfrac{1}{\hbar\rho^2} + \tfrac{k^2\rho^{2\eta}}{\hbar^3\delta\theta}\right].
\end{aligned} \tag{39}
$$

Now let $\mathcal{V}_{\delta,\hbar,\theta} := \hbar^2 \mathcal{U}_{\delta,\hbar,\theta}$ and substitute (38) and (39) into (36). We obtain the upper bound

$$\begin{aligned}(2\pi\hbar)^3 \int Z(x)n(x)dx \leq \tfrac{1}{\epsilon}\int_\Gamma (u^\epsilon(\gamma)_- - o(\gamma)_-)d\Omega(\gamma) + \tfrac{1}{\epsilon}\hbar^2\|\nabla g_\rho\|^2 \int_{o(\gamma)<0} d\Omega(\gamma) \\ +C\tfrac{1}{\epsilon}\left[\delta\left\{\int \mathcal{V}^{\frac{5}{2}}_{\delta,\hbar,\theta}(x)dx + (k\hbar)^{\frac{3}{2}}\left(\int \mathbf{B}^2(x)dx\right)^{\frac{3}{4}}\left(\int \mathcal{V}^4_{\delta,\hbar,\theta}(x)dx\right)^{\frac{1}{4}}\right\} + \tfrac{\hbar^2}{\rho^2} + \tfrac{k^2\rho^{2\eta}}{\delta\theta}\right]\end{aligned} \tag{40}$$

for all $\rho \in (0,\rho_0)$, $C > 0$, $\hbar > 0$, and $\epsilon > 0$, and for all positive δ and θ sufficiently small. Obviously by substituting (38) and (39) into (37) we obtain the corresponding lower bound

$$\begin{aligned}(2\pi\hbar)^3 \int Z(x)n(x)dx \geq \tfrac{1}{\epsilon}\int_\Gamma (u^\epsilon(\gamma)_- - o(\gamma)_-)d\Omega(\gamma) + \tfrac{1}{\epsilon}\hbar^2\|\nabla g_\rho\|^2 \int_{o(\gamma)<0} d\Omega(\gamma) \\ +C\tfrac{1}{\epsilon}\left[\delta\left\{\int \mathcal{V}^{\frac{5}{2}}_{\delta,\hbar,\theta}(x)dx + (k\hbar)^{\frac{3}{2}}\left(\int \mathbf{B}^2(x)dx\right)^{\frac{3}{4}}\left(\int \mathcal{V}^4_{\delta,\hbar,\theta}(x)dx\right)^{\frac{1}{4}}\right\} + \tfrac{\hbar^2}{\rho^2} + \tfrac{k^2\rho^{2\eta}}{\delta\theta}\right]\end{aligned} \tag{41}$$

for $\epsilon < 0$.

Therefore, it will suffice to show that

$$\begin{aligned}\overline{\lim}_{\hbar\to 0}\Bigg(\hbar^2\|\nabla g_\rho\|^2 \int_{o(\gamma)<0} d\Omega(\gamma) \\ +\left[\delta\left\{\int \mathcal{V}^{\frac{5}{2}}_{\delta,\hbar,\theta}(x)dx + (k\hbar)^{\frac{3}{2}}\left(\int \mathbf{B}^2(x)dx\right)^{\frac{3}{4}}\left(\int \mathcal{V}^4_{\delta,\hbar,\theta}(x)dx\right)^{\frac{1}{4}}\right\} + \tfrac{\hbar^2}{\rho^2} + \tfrac{k^2\rho^{2\eta}}{\delta\theta}\right]\Bigg) = 0.\end{aligned} \tag{42}$$

For the first term in (42) note that

$$\hbar^2 \int_{o(\gamma)<0} \|\nabla g_\rho\|^2 d\Omega(\gamma) \lesssim \frac{\hbar^2}{\rho^2}\int_{o(\gamma)<0} d\Omega(\gamma) \to 0 \qquad \text{as } \hbar \to 0$$

by Lemma 8. Next note that for $p = \frac{5}{2}$ or $p = 4$

$$\begin{aligned}\int \mathcal{V}^p_{\delta,\hbar,\theta}(x)dx \lesssim \ & \int \Big[\tfrac{1}{(\delta^2\theta)^p}[\mathfrak{d}_\rho(V)]^{2p} + \tfrac{1}{\delta^p}|\mathfrak{d}_\rho(V)|^p + \tfrac{1}{\delta^p}[\mathfrak{d}_\rho(V^2 + W - \epsilon Z)]^p_- \\ & + \left(\tfrac{\hbar k}{\delta}\right)^p (|\partial_\rho \mathbf{B}| + \delta\theta|\mathbf{B}|)^p + \left(\tfrac{k\rho^\eta}{\delta}\right)^p |V|^p\Big]dx.\end{aligned}$$

Consequently

$$\overline{\lim}_{\hbar\to 0}\int \mathcal{V}^p_{\delta,\hbar,\theta}(x)dx = 0.$$

□

Lemma 10. *Define*

$$u^\epsilon_0(\gamma) := p^2 + V(q)^2 + W(q) - \epsilon Z(q) + 2s(\mu)|V(q)|\sqrt{p^2+1}. \tag{43}$$

If the hypothesis of Lemma 9 holds then

$$\lim_{\delta\to 0}\lim_{\hbar\to 0}\int_\Gamma [u^\epsilon_{\delta,\hbar}(\gamma)]_- d\Omega(\gamma) = \int_\Gamma u^\epsilon_0(\gamma)_- d\Omega(\gamma). \tag{44}$$

Proof. We assume that $\epsilon > 0$. (The case for $\epsilon < 0$ is only a slight modification.) We have that

$$\begin{aligned}u^\epsilon_{\delta,\hbar}(\gamma) \geq \ & (1-\delta)(p - k\mathbf{a}(q))^2 + V(q)^2 + W(q) - \epsilon Z(q) \\ & -2\left(\left[|V(q)|\sqrt{((p-k\mathbf{a}(q))^2+1)} + (1-\delta)\tfrac{(k\hbar)}{2}|\mathbf{B}(q)|\right]^2\right)^{\frac{1}{2}} \\ \geq \ & (1-\delta)(p-k\mathbf{a}(q))^2 + |V(q)|^2 + W(q) - \epsilon Z(q) \\ & -2|V(q)|[|p - k\mathbf{a}(q)| + 1] - (1-\delta)k\hbar|\mathbf{B}| \\ \geq \ & (1-\delta)\Bigg[\left(|p - k\mathbf{a}(q)| - \tfrac{|V(q)|}{1-\delta}\right)^2 \\ & -(2V(q)^2 + 2W_-(q) + 2\epsilon Z_+(q) + 4|V(q)| + \hbar k|\mathbf{B}(q)|)\Bigg]\end{aligned}$$

for $\delta \leq \frac{1}{2}$. Therefore

$$u^\epsilon_{\delta,\hbar}(\gamma)_- \lesssim \left[|\mathbf{B}(q)| + W_-(q) + Z_+(q) + |V(q)| + V(q)^2\right] := M(p,q)$$

and

$$\operatorname{supp}[u^\epsilon_{\delta,\hbar}(\gamma)_-] \subseteq \{(p,q) : |p - k\mathbf{a}(q)| \lesssim \left[|\mathbf{B}(q)|^{\frac{1}{2}} + W_-(q)^{\frac{1}{2}} + Z_+(q)^{\frac{1}{2}} + |V(q)|^{\frac{1}{2}} + |V(q)|\right] := \Lambda(p,q).$$

Since

$$\int_{\Lambda(p,q)} M(p,q)dpdq < \infty,$$

then (44) follows by the dominated convergence theorem. □

Lemma 11. *Assume the hypothesis of Lemma 9 and let $o_\hbar(\gamma) := o_{\rho,\hbar}(\gamma)$, $\rho := \hbar^s$, be as in (33). In this case we have the inequality*

$$\underline{\lim}_{\hbar\to 0} \int_\Gamma [o_\hbar(\gamma)]_- d\Omega(\gamma) \geq \int_\Gamma u_0^0(\gamma)_- d\Omega(\gamma) \tag{45}$$

for $u_0^\epsilon(\gamma)$ defined in (43).

Proof. We make the substitution $\tilde{p} = p - k\mathbf{a}(q)$ and note that for all $\hbar$

$$\int_\Gamma [o_\hbar(\mu,p,q)]_- d\Omega(\gamma) = \sum_{\mu=1}^{4} \int_{\mathbb{R}^6} [\tilde{o}_\hbar(\mu,\tilde{p},q)]_- d\tilde{p}dq$$

for

$$\begin{aligned}\tilde{o}_\hbar(\mu,\tilde{p},q) = \quad & < \tilde{p} - k(\mathbf{a}(\cdot) - \mathbf{a}(q)) >_\rho^2 + < V^2 >_\rho + < W >_\rho \\ & + s(\mu) 2\Big[< V(\tilde{p} - k(\mathbf{a}(\cdot) - \mathbf{a}(q))) >_\rho^2 + < V >_\rho^2 + \tfrac{(k\hbar)^2}{4} < \mathbf{B} >_\rho^2 \\ & + (-1)^\mu k\hbar \sqrt{< V >_\rho^2 < \mathbf{B} >_\rho^2 + [< V(\tilde{p} - k(\mathbf{a}(\cdot) - \mathbf{a}(q))) >_\rho \cdot < \mathbf{B} >_\rho]^2}\Big]^{\frac{1}{2}}\end{aligned}$$

in which

$$< (\tilde{p} - k(\mathbf{a}(\cdot) - \mathbf{a}(q)) >_\rho^2 = \tilde{p}^2 + o(1)(|\tilde{p}| + 1)$$

and

$$< V(\tilde{p} - k(\mathbf{a}(\cdot) - \mathbf{a}(q))) >_\rho = < V >_\rho (q)(\tilde{p} + o(1))$$

as $\hbar \to 0$ by (ii) in the hypothesis of Lemma 9. Therefore as $\hbar \to 0$ we have

$$\begin{aligned}\tilde{o}_\hbar(\mu,\tilde{p},q) = \quad & \tilde{p}^2 + < V^2 + W >_\rho + o(1)(|\tilde{p}| + 1) + 2s(\mu)\big[< V >_\rho^2 (\tilde{p}^2 + 1)(1 + o(1)) \\ & + o(1) < \mathbf{B} >_\rho^2 + o(1)| < \mathbf{B} >_\rho || < V >_\rho | \sqrt{(1 + \tilde{p}^2)(1 + o(1))}\big]^{\frac{1}{2}}.\end{aligned} \tag{46}$$

Thus, as $\hbar \to 0$ through some subsequence

$$\tilde{o}_\hbar(\mu,\tilde{p},q) \to \tilde{p}^2 + V(q)^2 + W(q) + 2s(\mu)|V(q)|\sqrt{\tilde{p}^2 + 1} = u_0^0(\mu,\tilde{p},q)$$

since $< f >_{\hbar^s} \to f$, a.e. through some subsequence, for any $f \in L^p$, $p \in [1,\infty)$.

Since

$$\int_{\mathbb{R}^6} [\tilde{o}_\hbar(\mu,\tilde{p},q)]_- d\tilde{p}dq \geq \int_{u_0^0 < 0} [\tilde{o}_\hbar(\mu,\tilde{p},q)]_- d\tilde{p}dq$$

it suffices to show that

$$R_\hbar := \lim_{\hbar\to 0} \int_{u_0^0 < 0} \big([\tilde{o}_\hbar(\mu,\tilde{p},q)]_- - [u_0^0(\mu,\tilde{p},q)]_-\big) d\tilde{p}dq = 0.$$

¿From $u_0^0(\mu,\tilde{p},q) = (\sqrt{\tilde{p}^2 + 1} \pm |V|)^2 + W - 1$, it follows that

$$\operatorname{supp}[u_0^0]_- \subseteq \{(\tilde{p},q) : |\tilde{p}| \lesssim (|V| + |V|^{\frac{1}{2}} + W_-^{\frac{1}{2}})\}. \tag{47}$$

¿From (46) we may simplify the expression

$$\begin{aligned}\tilde{o}_\hbar(\mu,\tilde{p},q) = \quad & \tilde{p}^2 + < V^2 + W >_\rho + o(1)(|\tilde{p}| + 1) \\ & + 2s(\mu)\sqrt{\big[< V >_\rho^2 (\tilde{p}^2 + 1) + o(1)[(\tilde{p}^2 + 1) < V >_\rho^2 + < \mathbf{B} >_\rho^2]\big]_+}.\end{aligned} \tag{48}$$

Now we have the estimate[13]

$$\begin{array}{rcl} |[\tilde{o}_\hbar(\mu,\tilde{p},q)]_- - [u_0^0(\mu,\tilde{p},q)]_-| & \leq & |\tilde{o}_\hbar(\mu,\tilde{p},q) - u_0^0(\mu,\tilde{p},q)| \\ & \leq & |-\mathfrak{d}_\rho(V^2+W) - 2s(\mu)\sqrt{\tilde{p}^2+1}(|V| - |<V>_\rho|)| \\ & & +o(1)\{(|\tilde{p}|+1)(1+|<V>_\rho|) + |<\mathbf{B}>_\rho|\} \\ & \lesssim & |\mathfrak{d}_\rho(V^2+W)| + (|\tilde{p}|+1)|\mathfrak{d}_\rho(V)| \\ & & +o(1)\{(|\tilde{p}|+1)(1+|<V>_\rho|) + |<\mathbf{B}>_\rho|\}. \end{array}$$

Hence, we have

$$|R_\hbar| \lesssim \int_{\mathbb{R}^3} \Big\{ \big(|\mathfrak{d}_\rho(V^2+W)| + |\mathfrak{d}_\rho(V)| + o(1)(1+|<V>_\rho| + |<\mathbf{B}>_\rho|)\big)(|V| + |V|^{\frac{1}{2}} + W_-^{\frac{1}{2}})^3$$
$$+ \big(|\mathfrak{d}_\rho(V)| + o(1)(1+|<V>_\rho|)\big)(|V| + |V|^{\frac{1}{2}} + W_-^{\frac{1}{2}})^4 \Big\} dq \to 0$$

as $\hbar \to 0$ which completes the proof. □

Proof of Theorem 3. Combining the results of (35), (44), and (45) we can conclude that for $Z = Z_+$ and $\epsilon > 0$

$$\begin{array}{rcl} \overline{\lim}_{\hbar\to 0}(2\pi\hbar)^3 \int_{\mathbb{R}^3} Z(x)n(x)dx & \leq & \frac{1}{\epsilon}\overline{\lim}_{\hbar\to 0} \int_\Gamma (u^\epsilon(\gamma)_- - o(\gamma)_-)d\Omega(\gamma) \\ & \leq & \frac{1}{\epsilon}\int_\Gamma \left[u_0^\epsilon(\gamma)_- - u_0^0(\gamma)_-\right] d\Omega(\gamma) \\ & = & \frac{1}{\epsilon}\{-\int_{u_0^0(\gamma)\leq \epsilon Z}[u_0^0(\gamma) - \epsilon Z]d\Omega(\gamma) + \int_{u_0^0(\gamma)\leq 0} u_0^0(\gamma)d\Omega(\gamma)\} \\ & = & \int_{u_0^0(\gamma)<0} Z d\Omega(\gamma) + \int_\Gamma \frac{-u_0^0(\gamma)+\epsilon Z}{\epsilon}\chi_S d\Omega(\gamma) \end{array}$$

where $S := \{\gamma \in \Gamma : 0 \leq u_0^0(\gamma) \leq \epsilon Z\}$. As was done with (47) we can show that

$$S \subseteq T := \{\gamma : |p| \lesssim (|V| + |V|^{\frac{1}{2}} + W_-^{\frac{1}{2}} + Z_+^{\frac{1}{2}})\}.$$

If the hypothesis of Theorem 3 holds then

$$0 \leq \frac{-u_0^0(\gamma)+\epsilon Z}{\epsilon}\chi_S \leq Z\chi_S \leq Z\chi_T \in L^1(\mathbb{R}^6).$$

Since $Z\chi_S \to 0$ as $\epsilon \to 0$, then

$$\overline{\lim}_{\hbar\to 0}(2\pi\hbar)^3 \int_{\mathbb{R}^3} Z(x)n(x)dx \leq \int_{u_0^0(\gamma)<0} Z(q)d\Omega(\gamma)$$

by the dominated convergence theorem. By following the above analysis for the case of $\epsilon < 0$ we obtain the reverse inequality. Therefore we conclude that

$$\overline{\lim}_{\hbar\to 0}(2\pi\hbar)^3 \int_{\mathbb{R}^3} Z(x)n(x)dx = \int_{u_0^0(\gamma)<0} Z(q)d\Omega(\gamma) \tag{49}$$

in the case that $Z = Z_+$. However the analogous argument for $Z = Z_-$ gives the same equality for (49) which allows us to conclude that (49) holds for arbitrary $Z \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^4(\mathbb{R}^3)$.

Therefore

$$\int_{\mathbb{R}^3} Z(x)n(x)dx = (2\pi\hbar)^{-3}\int_{\mathbb{R}^6} Z(q)\sum_{\mu=1}^4 \chi_{\{u(\mu,p,q)<0\}}dpdq + o(\hbar^{-3})$$

where $u(\mu,p,q) := u_0^0(\mu,p,q)$, $\mu = 1,2,3,4$, are the eigenvalues of $p^2 + V(q)^2 + W(q) + 2V(q)(\alpha\cdot p + \beta)$. Consequently

$$\sum_{\mu=1}^4 \chi_{\{u(\mu,p,q)<0\}} = \mathrm{tr}\,\chi_{(-\infty,0)}[p^2 + V(q)^2 + W(q) + 2V(q)(\alpha\cdot p + \beta)]$$

and this completes the proof of Theorem 3. □

[13] We have used the fact that $|\sqrt{(x+y)_+} - \sqrt{x}| \leq \sqrt{|y|}$ for all $x \geq 0$.

5. Proof of Theorem 4

It is convenient first to prove Theorem 4 with a more restrictive hypothesis.

Lemma 12. *The conclusion of Theorem 4 is valid if (13)(i) holds and $V, W \in C_0^\infty(\mathbb{R}^3)$.*

Proof. Choose two functions $I \in C_0^\infty(\mathbb{R}^3)$ and $O \in C^\infty(\mathbb{R}^3)$ such that

$$(50) \qquad \begin{array}{l} (i)\ I(x)^2 + O(x)^2 = 1, \qquad x \in \mathbb{R}^3, \\ (ii)\ \operatorname{supp} V \cup \operatorname{supp} W \subset \operatorname{supp} I, \\ (iii)\ \operatorname{distance}(\operatorname{supp} V \cup \operatorname{supp} W, \operatorname{supp} O) \geq 1. \end{array}$$

Calculations show that (for $D = \frac{\hbar}{i}\nabla$)

$$OT_V^2(\mathbf{a})O = O^2 T_V(\mathbf{a})^2 + 2O[(\alpha \cdot D)O]T_V(\mathbf{a}) - \hbar^2(O\Delta O)$$

and similarly for I. Then, using the identity $I\partial_\nu I + O\partial_\nu O \equiv 0$, $\nu = 1, 2, 3$, we have the localization formula

$$T_V(\mathbf{a})^2 = OT_V(\mathbf{a})^2 O + IT_V(\mathbf{a})^2 I + \hbar^2(O\Delta O + I\Delta I).$$

Let

$$P := T_V(\mathbf{a})^2 - 1 + W - \hbar^2(|\nabla I|^2 + |\nabla O|^2).$$

Since $I\Delta I + |\nabla I|^2 + O\Delta O + |\nabla O|^2 \equiv 0$ then

$$(51) \qquad T_V(\mathbf{a})^2 - 1 + W = P_I + P_O \qquad \text{for } P_O := OPO \text{ and } P_I := IPI.$$

From (50)(ii) it follows that

$$P_O = O\left(T_0(\mathbf{a})^2 - 1 - \hbar^2[|\nabla I|^2 + |\nabla O|^2]\right) O.$$

It follows (as in (21) of [7]) that

$$(52) \qquad N(P_O) \leq N(T_0(\mathbf{a})^2 - 1 - \hbar^2[|\nabla I|^2 + |\nabla O|^2]) := C < \infty$$

by Lemma 2 (where $N(P_O)$ denotes the number of negative eigenvalues of P_O.)

By (51) and (52)

$$(53) \qquad \begin{array}{rcl} N(T_V(\mathbf{a})^2 - 1 + W) & \leq & N(P_I) + N(P_O) \\ & \leq & N(P|_{H_0^1(supp(I))}) + C \\ & \leq & \frac{1}{\epsilon}\big[-\operatorname{tr}(P|_{H_0^1(supp(I))})_- + \operatorname{tr}(P|_{H_0^1(supp(I))} - \epsilon)_-\big] + C \\ & \leq & \frac{1}{\epsilon}\big[-\operatorname{tr}(P_I)_- + \operatorname{tr}[(P - \epsilon\chi_{supp(I)})|_{H_0^1(supp(I))}]_-\big] + C \\ & \leq & \frac{1}{\epsilon}\big[\operatorname{tr}(P_I\tilde{d}) + \operatorname{tr}(P - \epsilon\chi_{supp(I)})_-\big] + C \end{array}$$

on using $-\operatorname{tr}[P_I]_- \leq \operatorname{tr}[P_I\tilde{d}]$ as given by (14) in which $\tilde{d}$ is to be determined. (See [7] for a similar argument.) If $\operatorname{dist}(q, \operatorname{supp}(V) \cup \operatorname{supp}(W)) > \rho$, then

$$O(p, q) = < (p - k\mathbf{a})^2 >_\rho - \hbar k < \mathbf{B} >_\rho$$

and from (28) and (29)

$$o_{\rho,\hbar}(\mu, p, q) + \hbar^2\|\nabla g_\rho\|^2 \geq 0.$$

Hence with

$$\tilde{M} := \chi_{\{\gamma : o(\gamma) \leq -\hbar^2\|\nabla g_\rho\|^2\}},$$

we have that $\operatorname{dist}(q, \operatorname{supp}(V) \cup \operatorname{supp}(W)) \leq \rho$ for $(\mu, p, q) \in \operatorname{supp}(\tilde{M})$. It follows that if $\rho < \frac{1}{2}$ and $\tilde{d}$ is defined as in (23) with $M(\gamma)$ replaced by $\tilde{M}(\gamma)$ then $I\tilde{d}I = \tilde{d}$ and therefore $P_I\tilde{d} = P\tilde{d}$. Consequently

$$(54) \qquad N(T_V(\mathbf{a})^2 - 1 + W) \leq \frac{1}{\epsilon}\big[\operatorname{tr}(P\tilde{d}) + \operatorname{tr}(P - \epsilon\chi_{supp(I)})_-\big] + C.$$

As in Lemma 7 with $\Phi := -W$ we have that

$$(55) \qquad \begin{array}{rcl} \operatorname{tr}(P\tilde{d}) & = & (2\pi\hbar)^{-3}\int_{o(\gamma) \leq -\hbar^2\|\nabla g_\rho\|^2}[o(\gamma) + \hbar^2\|\nabla g_\rho\|^2]d\Omega(\gamma) \\ & \leq & (2\pi\hbar)^{-3}\int_{o(\gamma)<0}[o(\gamma) + \hbar^2\|\nabla g_\rho\|^2]d\Omega(\gamma) \\ & = & -(2\pi\hbar)^{-3}\int_\Gamma o(\gamma)_- d\Omega(\gamma) + \frac{1}{8\pi^3\hbar}\int_{o(\gamma)<0}\|\nabla g_\rho\|^2 d\Omega(\gamma). \end{array}$$

Similarly we may let $\Phi := -W + \hbar^2(|\nabla I|^2 + |\nabla A|^2) + \epsilon\chi_{\mathrm{supp}(I)}$ in Lemma 4 and Lemma 6 and conclude that

$$
\begin{aligned}
&\mathrm{tr}(P - \epsilon\chi_{\mathrm{supp}(I)})_- \le (2\pi\hbar)^{-3} \textstyle\int_\Gamma u(\gamma)_- d\Omega(\gamma) \\
&+K\hbar^{-3}\left[\delta\left\{\int \mathcal{V}_{\delta,\hbar,\theta}^{\frac{5}{2}}(x)dx + (k\hbar)^{\frac{3}{2}}\left(\int \mathbf{B}^2(x)dx\right)^{\frac{3}{4}}\left(\int \mathcal{V}_{\delta,\hbar,\theta}^4(x)dx\right)^{\frac{1}{4}}\right\} + \tfrac{\hbar^2}{\rho^2} + \tfrac{k^2\rho^{2\eta}}{\delta\theta}\right]
\end{aligned}
\tag{56}
$$

(for $\mathcal{V}_{\delta,\hbar,\theta} = \hbar^2\mathcal{U}_{\delta,\hbar,\theta}$) which simplifies according to (42) upon letting $\hbar \to 0$ and using (ii) of Lemma 9.

In light of the inequality in (26) the first two terms on the right side of (54) compare with the right side of (36) with $-\epsilon Z$ replaced by $-\hbar^2(|\nabla I|^2 + |\nabla A|^2) - \epsilon\chi_{\mathrm{supp}(I)}$. Similarly (55) and (56) compare to (38) and (39), respectively. Hence, (40) holds for $\epsilon > 0$ (and (41) holds for $\epsilon < 0$) with the left-hand-side $(2\pi\hbar)^3 \int Z(x)n(x)dx$ replaced by $(2\pi\hbar)^3(N(T_V(\mathbf{a})^2 - 1 + W) - C)$. For $\rho = \hbar^s$ and $\epsilon > 0$ we obtain the identity

$$
\overline{\lim}_{\hbar\to 0}(2\pi\hbar)^3 N(T_V(\mathbf{a})^2 - 1 + W) \le \frac{1}{\epsilon}\left[\overline{\lim}_{\delta\to 0}\overline{\lim}_{\hbar\to 0}\int_\Gamma u_{\delta,\hbar}^\epsilon(\gamma)_- d\Omega(\gamma) - \underline{\lim}_{\hbar\to 0}\int_\Gamma o_\hbar(\gamma)_- d\Omega(\gamma)\right]
$$

in which $u_{\delta,\hbar}^\epsilon(\gamma)$ is given by (34) with $\Phi := -W + \hbar^2(|\nabla I|^2 + |\nabla A|^2) + \epsilon\chi_{\mathrm{supp}(I)}$. Continuing as in Lemma 10 and Lemma 11 for

$$
u_0^\epsilon(\gamma) := p^2 + V(q)^2 + W(q) - \epsilon\chi_{\mathrm{supp}(I)} + 2s(\mu)|V(q)|\sqrt{p^2+1}.
$$

we have that for $\epsilon > 0$

$$
\overline{\lim}_{\hbar\to 0}(2\pi\hbar)^3 N(T_V(\mathbf{a})^2 - 1 + W) \le \frac{1}{\epsilon}\int_\Gamma [u_0^\epsilon(\gamma)_- - u_0^0(\gamma)_-]d\Omega(\gamma).
$$

However, for $\epsilon > 0$

$$
\begin{aligned}
\tfrac{1}{\epsilon}\textstyle\int_\Gamma (u_0^\epsilon(\gamma)_- - u_0^0(\gamma)_-)d\Omega(\gamma) = \;& \textstyle\int_{u_0^0(\gamma)<0} \chi_{\mathrm{supp}(I)} d\Omega(\gamma) \\
&+ \tfrac{1}{\epsilon}\textstyle\int_{0\le u_0^0(\gamma)<\epsilon\chi_{\mathrm{supp}(I)}} [-u_0^0(\gamma) + \epsilon\chi_{\mathrm{supp}(I)}]d\Omega(\gamma) \\
&\to \textstyle\int_{u_0^0(\gamma)<0} \chi_{\mathrm{supp}(I)} d\Omega(\gamma) \qquad \text{as } \epsilon \to 0
\end{aligned}
$$

by the dominated convergence theorem. Thus, as $\hbar \to 0$

$$
N(T_V(\mathbf{a})^2 - 1 + W) \le (2\pi\hbar)^{-3}\int_{u_0^0(\gamma)<0} d\Omega(\gamma) + o(\hbar^{-3}).
$$

By Theorem 3, as $\hbar \to 0$

$$
N(T_V(\mathbf{a})^2 - 1 + W) \ge \int_{\mathbb{R}^3} \chi_{\mathrm{supp}(V)\cup\mathrm{supp}(W)}(x)n(x)dx = \frac{1}{(2\pi\hbar)^3}\int_{u_0^0(\gamma)<0} d\Omega(\gamma) + o(\hbar^{-3})
$$

since $q \notin \mathrm{supp}(V) \cup \mathrm{supp}(W)$ implies that $u_0^0(\gamma) \ge 0$.

In conclusion we have that as $\hbar \to 0$

$$
N(T_V(\mathbf{a})^2 - 1 + W) = (2\pi\hbar)^{-3}\sum_{\mu=1}^4 \int_{\mathbb{R}^6} \chi_{\{(p,q):u_0^0(\mu,p,q)<0\}}dpdq + o(\hbar^{-3}) \tag{57}
$$

since $\mathrm{supp}(V), \mathrm{supp}(W) \subset \mathrm{supp}(I)$. □

Next we seek to prove Theorem 4 for the case in which $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$, $W \in L^{\frac{3}{2}}(\mathbb{R}^3)$, and either (13) (i) or (ii) holds. To this end we first prove the following

Lemma 13. *Assume that $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$ and $W \in L^{\frac{3}{2}}(\mathbb{R}^3)$. Choose $V_0, W_0 \in C_0^\infty(\mathbb{R}^3)$ for which $V = V_0 + V_\infty$, $W = W_0 + W_\infty$, and*

$$
\|V_\infty\|_3 + \|V_\infty\|_{\frac{3}{2}} + \|W_\infty\|_{\frac{3}{2}} < \delta
$$

for a given $\delta > 0$.

(a) *If (13)(i) holds, then for each $\epsilon \in (0, \frac{1}{2})$ and $T_1 := (1-\epsilon)\alpha \cdot (\frac{\hbar}{i}\nabla - k\mathbf{a}) + \beta + V_0$*

$$
N(T_V(\mathbf{a})^2 - 1 + W) \le N(T_1^2 - 1 + W_0 - 2\frac{\epsilon}{1-\epsilon}V_0^2) + const\ (\hbar^{-\frac{3}{2}(t+1)} + \frac{\delta(1+\epsilon^{\frac{3}{2}})}{\epsilon^3\hbar^3}).
$$

(b) *If (13)(ii) holds, then for* $\mathbf{a} = \mathbf{a}^0 + \mathbf{a}^\infty$ *with* $\mathbf{a}^0, \mathbf{B}^0 \in C_0^\infty(\mathbb{R}^3)^3$ *and* $\|\mathbf{a}^\infty\|_3 + \|\mathbf{B}^\infty\|_{\frac{3}{2}} < \delta$, *we have that* [14]

$$N(T_V(\mathbf{a})^2 - 1 + W) \le N(T_2^2 - 1 + W_0 - 2\tfrac{\epsilon}{1-\epsilon}[|\mathbf{a}^0| + |V_0|]^2]) + const\tfrac{\delta^{\frac{3}{2}}}{\epsilon^3\hbar^3}[1 + (k\hbar)^{\frac{3}{2}}]$$

for each $\epsilon \in (0, \frac{1}{2})$ *and* $T_2 := \alpha \cdot ((1-\epsilon)\frac{\hbar}{i}\nabla - k\mathbf{a}^0) + \beta + V_0$.

Proof. First we prove part (b).

For $\tilde{D}_{\mathbf{a}} := (\frac{\tilde{h}}{i}\nabla - k\mathbf{a})$ and $\tilde{h}$ a real number to be chosen, define $\tilde{T}_{V_0}(\mathbf{a}^0) := \alpha \cdot \tilde{D}_{\mathbf{a}^0} + \beta + V_0$. Let $\hat{D}_{\mathbf{a}^\infty} := \frac{\hbar - \tilde{h}}{i}\nabla - k\mathbf{a}^\infty$ and $\tilde{S} := \alpha \cdot \hat{D}_{\mathbf{a}^\infty} + \beta + V_\infty$. We have that

$$\begin{aligned}
([T_V(\mathbf{a})^2 - 1 + W]\psi, \psi) = \;& \|T_V(\mathbf{a})\psi\|^2 + ([-1+W]\psi,\psi) \\
=\;& \|[\tilde{T}_{V_0}(\mathbf{a}^0) + \alpha \cdot \hat{D}_{\mathbf{a}^\infty} + V_\infty]\psi\|^2 + ([-1+W]\psi,\psi) \\
=\;& \|\tilde{T}_{V_0}(\mathbf{a}^0)\psi\|^2 + 2\mathfrak{Re}(\tilde{T}_{V_0}(\mathbf{a}^0)\psi, (\tilde{S}-\beta)\psi) \\
&+ \|(\tilde{S}-\beta)\psi\|^2 + ([-1+W]\psi,\psi) \\
=\;& ([\tilde{T}_{V_0}(\mathbf{a}^0)^2 - 1 + W_0]\psi,\psi) + 2\mathfrak{Re}(\tilde{T}_{V_0}(\mathbf{a}^0)\psi, (\tilde{S}-\beta)\psi) \\
&+ \|(\tilde{S}-\beta)\psi\|^2 + (W_\infty\psi,\psi).
\end{aligned} \tag{58}$$

Since $\mathfrak{Re}(\alpha \cdot \hat{D}_{\mathbf{a}^\infty}\psi, \beta\psi) = 0$ then

$$\begin{aligned}
\|(\tilde{S}-\beta)\psi\|^2 = \;& \|\tilde{S}\psi\|^2 - 2\mathfrak{Re}(\tilde{S}\psi,\beta\psi) + \|\psi\|^2 \\
=\;& \|\tilde{S}\psi\|^2 - 2\mathfrak{Re}((\beta+V_\infty)\psi,\beta\psi) + \|\psi\|^2 \\
=\;& ((\tilde{S}^2 - 1)\psi,\psi) - 2(V_\infty\beta\psi,\psi).
\end{aligned}$$

Therefore $R := [T_V(\mathbf{a})^2 - 1 + W] - [\tilde{T}_{V_0}(\mathbf{a}^0)^2 - 1 + W_0]$ satisfies

$$(R\psi,\psi) = ((\tilde{S}^2 - 2V_\infty\beta + W_\infty - 1)\psi,\psi) + 2\mathfrak{Re}(\tilde{T}_{V_0}(\mathbf{a}^0)\psi, (\tilde{S}-\beta)\psi)$$

in which

$$\begin{aligned}
\mathfrak{Re}(\tilde{T}_{V_0}(\mathbf{a}^0)\psi, (\tilde{S}-\beta)\psi) = \;& \mathfrak{Re}\big\{\tfrac{\hbar-\tilde{h}}{\tilde{h}}\|\alpha\cdot\tfrac{\tilde{h}}{i}\nabla\psi\|^2 + (\alpha\cdot\tfrac{\tilde{h}}{i}\nabla\psi, (-\alpha\cdot\mathbf{a}^\infty + V_\infty)\psi) \\
&+ ((-\alpha\cdot\mathbf{a}^0 + V_0)\psi, \tilde{S}\psi) + ((V_\infty - V_0)\beta\psi,\psi)\big\}.
\end{aligned}$$

As a consequence we have for $\hat{h} := \frac{\hbar-\tilde{h}}{\tilde{h}}$ and any positive γ_1, γ_2,

$$\begin{aligned}
(R\psi,\psi) = \;& ((\tilde{S}^2 - 2V_\infty\beta + W_\infty - 1)\psi,\psi) \\
&+ 2\hat{h}\|\alpha\cdot\tfrac{\tilde{h}}{i}\nabla\psi\|^2 + 2\mathfrak{Re}\big\{(\alpha\cdot\tfrac{\tilde{h}}{i}\nabla\psi, (-\alpha\cdot\mathbf{a}^\infty + V_\infty)\psi) \\
&+ ((-\alpha\cdot\mathbf{a}^0 + V_0)\psi, [\hat{h}\alpha\cdot\tfrac{\tilde{h}}{i}\nabla - \alpha\cdot\mathbf{a}^\infty + V_\infty]\psi) + (V_\infty\beta\psi,\psi)\big\} \\
\ge\;& ((\tilde{S}^2 - 2V_\infty\beta + W_\infty - 1)\psi,\psi) + 2\hat{h}\tilde{h}^2\|\alpha\cdot\tfrac{1}{i}\nabla\psi\|^2 - (|V_\infty|\psi,\psi) \\
&- \gamma_1\tilde{h}^2\|\alpha\cdot\tfrac{1}{i}\nabla\psi\|^2 - \tfrac{1}{\gamma_1}([|\mathbf{a}^\infty| + |V_\infty|]^2\psi,\psi) - \gamma_2\hat{h}\tilde{h}^2\|\alpha\cdot\tfrac{1}{i}\nabla\psi\|^2 \\
&- \hat{h}\tfrac{1}{\gamma_2}([|\mathbf{a}^0| + |V_0|]^2\psi,\psi) - ([|\mathbf{a}^0| + |V_0|][|\mathbf{a}^\infty| + |V_\infty|]\psi,\psi).
\end{aligned}$$

Given $\epsilon \in (0,\frac{1}{2})$ choose $\tilde{h} = (1-\epsilon)\hbar$ ($\implies$ $\hat{h} = \epsilon/(1-\epsilon)$), $\gamma_1 = \epsilon/2(1-\epsilon)$, and $\gamma_2 = 1/2$. This choice of parameters implies that

$$\begin{aligned}
(R\psi,\psi) \ge \;& ((\tilde{S}^2 - 2V_\infty\beta + W_\infty - 1)\psi,\psi) + \epsilon(1-\epsilon)\hbar^2(-\Delta\psi,\psi) - (|V_\infty|\psi,\psi) \\
&- 2\tfrac{1-\epsilon}{\epsilon}([|\mathbf{a}^\infty| + |V_\infty|]^2\psi,\psi) - 2\tfrac{\epsilon}{1-\epsilon}([|\mathbf{a}^0| + |V_0|]^2\psi,\psi) \\
&- ([|\mathbf{a}^0| + |V_0|][|\mathbf{a}^\infty| + |V_\infty|]\psi,\psi).
\end{aligned}$$

In summary we have that

$$T_V(\mathbf{a})^2 - 1 + W = [\tilde{T}_{V_0}(\mathbf{a}^0)^2 - 1 + W_0 - 2\frac{\epsilon}{1-\epsilon}[|\mathbf{a}^0| + |V_0|]^2] + \hat{R}$$

for

$$\hat{R} \ge \tilde{S}^2 - 2|V_\infty| - |W_\infty| - 1 + \epsilon(1-\epsilon)\hbar^2(-\Delta) - |V_\infty| - 2\frac{(1-\epsilon)}{\epsilon}[|\mathbf{a}^\infty| + |V_\infty|]^2 - [|\mathbf{a}^0| + |V_0|][|\mathbf{a}^\infty| + |V_\infty|].$$

Then

$$N(T_V(\mathbf{a})^2 - 1 + W) \le N(\tilde{T}_{V_0}(\mathbf{a}^0)^2 - 1 + W_0 - 2\frac{\epsilon}{1-\epsilon}[|\mathbf{a}^0| + |V_0|]^2]) + N(\hat{R}).$$

[14] Note that $\mathbf{B}^0 := \nabla \times \mathbf{a}^0$ and $\mathbf{B}^\infty := \nabla \times \mathbf{a}^\infty$.

By an application of Lemma 2 to $\tilde{S} = \alpha \cdot \left(\frac{\epsilon\hbar}{i}\nabla - k\mathbf{a}^\infty\right) + \beta + V_\infty$ and the Cwikel-Lieb-Rosenblum inequality we have the estimate

$$\begin{aligned}
N(\hat{R}) \leq\ & N[\tilde{S}^2 - 2|V_\infty| - |W_\infty| - 1] \\
& + N\big[-\epsilon(1-\epsilon)\hbar^2\Delta - \big(2\tfrac{(1-\epsilon)}{\epsilon}[|\mathbf{a}^\infty| + |V_\infty|]^2 + [|\mathbf{a}^0| + |V_0|][|\mathbf{a}^\infty| + |V_\infty|] + |V_\infty|\big)\big] \\
\lesssim\ & \tfrac{1}{(\epsilon\hbar)^3}\int_{\mathbb{R}^3}\big[|V_\infty| + |V_\infty|^2 + |W_\infty| + k\epsilon\hbar|\mathbf{B}^\infty|\big]^{\frac{3}{2}}dx \\
& + const\tfrac{1}{(\epsilon(1-\epsilon)\hbar^2)^{\frac{3}{2}}}\int_{\mathbb{R}^3}\big[\tfrac{1}{\epsilon}[|\mathbf{a}^\infty| + |V_\infty|]^2 + [|\mathbf{a}^0| + |V_0|][|\mathbf{a}^\infty| + |V_\infty|] + |V_\infty|\big]^{\frac{3}{2}}dx \\
\lesssim\ & \tfrac{1}{(\epsilon\hbar)^3}\big[\|V_\infty\|_{\frac{3}{2}}^{\frac{3}{2}} + \|V_\infty\|_3^3 + \|W_\infty\|_{\frac{3}{2}}^{\frac{3}{2}} + (k\epsilon\hbar)^{\frac{3}{2}}\|\mathbf{B}^\infty\|_{\frac{3}{2}}^{\frac{3}{2}}\big] \\
& + const\tfrac{1}{(\epsilon\hbar^2)^{\frac{3}{2}}}\big[\epsilon^{-\frac{3}{2}}[\|\mathbf{a}^\infty\|_3^3 + \|V_\infty\|_3^3] + \|[|\mathbf{a}^0| + |V_0|]^{\frac{3}{2}}\|_2[\|\mathbf{a}^\infty\|_3^3 + \|V_\infty\|_3^3]^{\frac{1}{2}} + \|V_\infty\|_{\frac{3}{2}}^{\frac{3}{2}}\big] \\
\lesssim\ & \tfrac{\delta^{\frac{3}{2}}}{\epsilon^3\hbar^3}[1 + (k\hbar)^{\frac{3}{2}}]
\end{aligned}$$

by the hypothesis. Therefore part (b) is proved with $T_2 = \tilde{T}_{V_0}(\mathbf{a}^0)$.

The proof for part (a) is similar to the above analysis. For $\tilde{h}$ a real number to be chosen, define $\tilde{T} := \frac{\tilde{h}}{\hbar}\mathcal{D}_\mathbf{a} + \beta + V_0$. As in (58)

$$([T_V(\mathbf{a})^2 - 1 + W]\psi, \psi) = ([\tilde{T}^2 - 1 + W_0]\psi, \psi) + 2\mathfrak{Re}(\tilde{T}\psi, \tilde{L}\psi) + \|\tilde{L}\psi\|^2 + (W_\infty\psi, \psi).$$

in which $\tilde{L} := \frac{\hbar - \tilde{h}}{\hbar}\mathcal{D}_\mathbf{a} + V_\infty$. Set $\hat{h} := \frac{\hbar - \tilde{h}}{\tilde{h}}$. Then

$$\begin{aligned}
([T_V(\mathbf{a})^2 - 1 + W]\psi, \psi) =\ & ([\tilde{T}^2 - 1 + W_0]\psi, \psi) + (W_\infty\psi, \psi) + 2\hat{h}\|\tfrac{\tilde{h}}{\hbar}\mathcal{D}_\mathbf{a}\psi\|^2 \\
& + 2\mathfrak{Re}\big[(\tfrac{\tilde{h}}{\hbar}\mathcal{D}_\mathbf{a}\psi, V_\infty\psi) + \hat{h}(V_0\psi, \tfrac{\tilde{h}}{\hbar}\mathcal{D}_\mathbf{a}\psi) + ((\beta + V_0)\psi, V_\infty\psi)\big] \\
& + \|(\tfrac{\hbar - \tilde{h}}{\hbar}\mathcal{D}_\mathbf{a} + V_\infty)\psi\|^2
\end{aligned}$$

and for any positive γ_1, γ_2, $R := [T_V(\mathbf{a})^2 - 1 + W] - [\tilde{T}^2 - 1 + W_0]$ satisfies

$$\begin{aligned}
(R\psi, \psi) \geq\ & 2\hat{h}\|\tfrac{\tilde{h}}{\hbar}\mathcal{D}_\mathbf{a}\psi\|^2 - \gamma_1\|(\tfrac{\tilde{h}}{\hbar}\mathcal{D}_\mathbf{a}\psi\|^2 - \tfrac{1}{\gamma_1}\|V_\infty\psi\|^2 \\
& - \hat{h}\tfrac{1}{\gamma_2}\|V_0\psi\|^2 - \hat{h}\gamma_2\|\tfrac{\tilde{h}}{\hbar}\mathcal{D}_\mathbf{a}\psi\|^2 - 2((1 + |V_0|)|V_\infty|\psi, \psi) + (W_\infty\psi, \psi) \\
=\ & (2\hat{h} - \gamma_1 - \hat{h}\gamma_2)\|\tfrac{\tilde{h}}{\hbar}\mathcal{D}_\mathbf{a}\psi\|^2 + ([W_\infty - \tfrac{1}{\gamma_1}{V_\infty}^2 - \hat{h}\tfrac{1}{\gamma_2}V_0^2 - 2(1 + |V_0|)|V_\infty|]\psi, \psi).
\end{aligned}$$

Now choose $\tilde{h} = (1-\epsilon)\hbar$ for $\epsilon \in (0, \frac{1}{2})$, $\gamma_1 = \hat{h}/2$, and $\gamma_2 = 1/2$, which implies that $\hat{h} = \frac{\epsilon}{(1-\epsilon)}$. Consequently

$$(R\psi, \psi) \geq \tfrac{\epsilon}{1-\epsilon}\|\tfrac{\tilde{h}}{\hbar}\mathcal{D}_\mathbf{a}\psi\|^2 + ([W_\infty - \tfrac{2(1-\epsilon)}{\epsilon}{V_\infty}^2 - \tfrac{2\epsilon}{1-\epsilon}V_0^2 - 2(1 + |V_0|)|V_\infty|]\psi, \psi)$$

or alternatively we may write

$$T_V(\mathbf{a})^2 - 1 + W \geq [\tilde{T}^2 - 1 + W_0 - \frac{2\epsilon}{1-\epsilon}V_0^2] + \hat{R} \tag{59}$$

for

$$\hat{R} := \epsilon(1-\epsilon)\big((D - k\mathbf{a})^2 - \hbar k\Sigma \cdot \mathbf{B}\big) - |W_\infty| - \frac{2(1-\epsilon)}{\epsilon}{V_\infty}^2 - 2|1 + V_0||V_\infty|.$$

By the diamagnetic inequality

$$\begin{aligned}
N(\hat{R}) =\ & N\big[\big((D - k\mathbf{a})^2 - \hbar k\Sigma \cdot \mathbf{B}\big) - \tfrac{1}{\epsilon(1-\epsilon)}\big(|W_\infty| + \tfrac{2(1-\epsilon)}{\epsilon}{V_\infty}^2 + 2|1 + V_0||V_\infty|\big)\big] \\
\leq\ & N\big[(D - k\mathbf{a})^2 - \hbar|k||\mathbf{B}| - \tfrac{2}{\epsilon^2}{V_\infty}^2 - \tfrac{1}{\epsilon(1-\epsilon)}\big(|W_\infty| + 2|1 + V_0||V_\infty|\big)\big] \\
\lesssim\ & \tfrac{1}{\hbar^3}\int_{\mathbb{R}^3}\big[\hbar|k||\mathbf{B}| + \tfrac{2}{\epsilon^2}{V_\infty}^2 + \tfrac{1}{\epsilon(1-\epsilon)}\big(|W_\infty| + 2|1 + V_0||V_\infty|\big)\big]^{\frac{3}{2}}dx \\
\lesssim\ & \tfrac{1}{[\epsilon(1-\epsilon)\hbar^2]^{\frac{3}{2}}}\int_{\mathbb{R}^3}\big[\epsilon\hbar^{1-t}|\mathbf{B}| + \epsilon^{-1}{V_\infty}^2 + |W_\infty| + |V_\infty| + |V_0||V_\infty|\big]^{\frac{3}{2}}dx \\
\lesssim\ & \tfrac{1}{[\epsilon\hbar^2]^{\frac{3}{2}}}\big[\epsilon^{\frac{3}{2}}\hbar^{3(1-t)/2}\|\mathbf{B}\|_{\frac{3}{2}}^{\frac{3}{2}} + \epsilon^{-\frac{3}{2}}\|V_\infty\|_3^3 + \|W_\infty\|_{\frac{3}{2}}^{\frac{3}{2}} + \|V_\infty\|_{\frac{3}{2}}^{\frac{3}{2}} + \|V_0\|_3^{\frac{3}{2}}\|V_\infty\|_3^{\frac{3}{2}}\big] \\
\lesssim\ & \tfrac{1}{[\epsilon\hbar^2]^{\frac{3}{2}}}[\epsilon^{\frac{3}{2}}\hbar^{3(1-t)/2} + \delta(1 + \epsilon^{-\frac{3}{2}})]
\end{aligned}$$

since $k(\hbar) = O(\hbar^{-t})$ for $t \in (0, 1)$. By (59) the proof of part (a) is complete. ∎

In part (a) of Lemma 13 we set $\epsilon' := \epsilon/(1-\epsilon)$ and make the appropriate substitutions[15] in (57) to show that (for $\tilde{h} := (1-\epsilon)\hbar$)

$$N(T_1 - 1 + W_0 - 2\epsilon' V_0^2) = (2\pi\tilde{h})^{-3} \sum_{\mu=1}^{4} \int_{\mathbb{R}^6} \chi_{\{(p,q): v_\epsilon^\delta(\mu,p,q)<0\}} dpdq + o(\hbar^{-3}) \tag{60}$$

for

$$v_\epsilon^\delta(\mu,p,q) := p^2 + V_0(q)^2 + W_0(q) - 2\epsilon' V_0^2 + 2s(\mu)|V_0(q)|\sqrt{p^2+1}$$

(compare to u_0^0 defined in (43)) in which we remind the reader of the dependence of V_0 and W_0 upon δ.

Similarly in part (b) of Lemma 13 we set $\epsilon' := \epsilon/(1-\epsilon)$ and make the appropriate substitutions in (57) to show that

$$N(T_2 - 1 + W_0 - 2\epsilon'[|\mathbf{a}^0| + |V_0|]^2) = (2\pi\tilde{h})^{-3} \sum_{\mu=1}^{4} \int_{\mathbb{R}^6} \chi_{\{(p,q): w_\epsilon^\delta(\mu,p,q)<0\}} dpdq + o(\hbar^{-3}) \tag{61}$$

for

$$w_\epsilon^\delta(\mu,p,q) := p^2 + V_0(q)^2 + W_0(q) - 2\epsilon'[|\mathbf{a}^0| + |V_0|]^2 + 2s(\mu)|V_0(q)|\sqrt{p^2+1}.$$

If $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$, and $W \in L^{\frac{3}{2}}(\mathbb{R}^3)$, then it follows from part (a) of Lemma 13 and (60) that

$$\overline{\lim}_{\hbar\to 0}(2\pi\hbar)^3 N(T_V(\mathbf{a})^2 - 1 + W) \le \underline{\lim}_{\epsilon\to 0}\underline{\lim}_{\delta\to 0} \int_{v_\epsilon^\delta(\gamma)<0} d\Omega(\gamma)$$

provided (13)(i) holds, and it follows from part (b) of Lemma 13 and (61) that

$$\overline{\lim}_{\hbar\to 0}(2\pi\hbar)^3 N(T_V(\mathbf{a})^2 - 1 + W) \le \underline{\lim}_{\epsilon\to 0}\underline{\lim}_{\delta\to 0} \int_{w_\epsilon^\delta(\gamma)<0} d\Omega(\gamma)$$

provided (13)(ii) holds.

We claim that

$$\underline{\lim}_{\epsilon\to 0}\underline{\lim}_{\delta\to 0} \int_{v_\epsilon^\delta(\gamma)<0} d\Omega(\gamma) = \int_{v_0^0(\gamma)<0} d\Omega(\gamma) = \underline{\lim}_{\epsilon\to 0}\underline{\lim}_{\delta\to 0} \int_{w_\epsilon^\delta(\gamma)<0} d\Omega(\gamma) \tag{62}$$

for $v_0^0(\mu,p,q) := p^2 + V(q)^2 + W(q) + 2s(\mu)|V(q)|\sqrt{p^2+1}$.

We indicate the proof for the first limit in (62). The second limit follows in the same manner. Note that

$$\begin{aligned} \int_{v_\epsilon^\delta(\gamma)<0} d\Omega(\gamma) = & \int_{v_0^0(\gamma)<0} d\Omega(\gamma) - \int_{v_0^0(\gamma)<0\le v_\epsilon^\delta(\gamma)} d\Omega(\gamma) + \int_{v_0^0(\gamma)\ge 0 > v_\epsilon^\delta(\gamma)} d\Omega(\gamma) \\ \le & \int_{v_0^0(\gamma)<0} d\Omega(\gamma) + \int_{v_0^0(\gamma)\ge 0 > v_\epsilon^\delta(\gamma)} d\Omega(\gamma). \end{aligned}$$

Therefore we need to show that

$$\underline{\lim}_{\epsilon\to 0}\underline{\lim}_{\delta\to 0} \int_{v_0^0(\gamma)\ge 0 > v_\epsilon^\delta(\gamma)} d\Omega(\gamma) = 0. \tag{63}$$

As $\delta \to 0$, $V_0 = V_0^\delta \to V$ in $L^3(\mathbb{R}^3)$. This implies that $V_0^\delta \to V$ in measure. Therefore there is a subsequence $\delta_n \to 0$ such that $V_0^{\delta_n} \to V$ almost everywhere in $\mathbb{R}^3$ and similarly for $W_0^\delta \to W$. Equivalently, $V_\infty \to 0$ and $W_\infty \to 0$ almost everywhere in $\mathbb{R}^3$. Thus as $\epsilon \to 0$ and some subsequence $\delta \to 0$ we have

$$\chi_{\{v_0^0>0,\, v_\epsilon^\delta<0\}} \to 0, \qquad \text{a.e. in } \mathbb{R}^3 \times \mathbb{R}^3$$

for each $\mu = 1,2,3,4$. Moreover

$$\chi_{\{v_0^0>0,\, v_\epsilon^\delta<0\}} < \chi_{\{v_\epsilon^\delta<0\}} \le \chi_{S_{\epsilon,\delta}}$$

for

$$S_{\epsilon,\delta} := \{(p,q) : |p|^2 \le 2(|V_0| + |V_0|^2 + |W_0| + 2\epsilon V_0^2)\},$$

[15] i.e., V_0 for V, $\tilde{D}_{\mathbf{a}} = \frac{\tilde{h}}{i}\nabla - (1-\epsilon)k\mathbf{a}$ for $\mathcal{D}_{\mathbf{a}}$, and $W_0 - 2\epsilon' V_0^2$ for W.

and as $\epsilon \to 0$ and some subsequence $\delta \to 0$

$$\chi_{S_{\epsilon,\delta}} \to \chi_{S_0} \qquad \text{for} \quad S_0 := \{(p,q) : |p|^2 \leq 2(|V| + |V|^2 + |W|)\}.$$

Since $V \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$ and $W \in L^{\frac{3}{2}}(\mathbb{R}^3)$ then χ_{S_0} is integrable. Also,

$$\int_{\mathbb{R}^6} \chi_{S_{\epsilon,\delta}} dpdq \to \int_{\mathbb{R}^6} \chi_{S_0} dpdq.$$

As a consequence it follows from the generalized Lebesgue dominated convergence theorem[16] that

$$\int_{\mathbb{R}^6} \chi_{\{v_0^0 > 0, v_\epsilon^\delta < 0\}} dpdq \to 0,$$

i.e., (63) holds.

Therefore the conclusion of Theorem 4 holds if we replace the equality with an inequality. However, to prove the reverse inequality we need only establish lower bounds similar to parts (a) and (b) of Lemma 13 the proof of which follows in an analogous manner to the proof of Lemma 13.

6. Appendix

In this section we compute the eigenvalues of the matrices $U(p,q) = U_\delta(p,q)$ introduced in (17) and $O(p,q)$ given in (25).

Let $M := \alpha \cdot \mathbf{r} + \beta - \Sigma \cdot \mathbf{C}$ for vectors $\mathbf{r}, \mathbf{C} \in \mathbb{R}^3$. Then we see that

$$M^2 = \mathbf{r}^2 + 1 + |\mathbf{C}|^2 - 2N$$

for

$$N := \sum_{\mu=1}^{3} C_\mu \begin{pmatrix} \sigma_\mu & r_\mu I_2 \\ r_\mu I_2 & -\sigma_\mu \end{pmatrix}.$$

It follows that

$$N^2 = (|\mathbf{C}|^2 + (\mathbf{r} \cdot \mathbf{C})^2) I_4.$$

Therefore we have that

(i) N has eigenvalues $\pm[|\mathbf{C}|^2 + (\mathbf{r}\cdot\mathbf{C})^2]^{\frac{1}{2}}$, each of multiplicity 2;

(ii) M^2 has eigenvalues $\mathbf{r}^2 + 1 + |\mathbf{C}|^2 \mp 2[|\mathbf{C}|^2 + (\mathbf{r}\cdot\mathbf{C})^2]^{\frac{1}{2}}$, each of multiplicity 2; and

(iii) M has eigenvalues $\pm\big[\mathbf{r}^2 + 1 + |\mathbf{C}|^2 \mp 2[|\mathbf{C}|^2 + (\mathbf{r}\cdot\mathbf{C})^2]^{\frac{1}{2}}\big]^{\frac{1}{2}}$.

We now note that we may write

$$\begin{aligned} U(p,q) :=&\ (1-\delta)\{(p - k\mathbf{a}(q))^2 - \hbar k \Sigma \cdot \mathbf{B}(q)\} + V(q)^2 - \Phi(q) + 2V(q)\{\alpha \cdot (p - k\mathbf{a}(q)) + \beta\} \\ =&\ 2V(q)(M + c) \end{aligned}$$

for

$$\mathbf{r} := p - k\mathbf{a}(q), \quad \mathbf{C} := \frac{(1-\delta)\hbar k}{2V(q)} \mathbf{B}(q), \quad c := \frac{1}{2V(q)} \left\{(1-\delta)(p - k\mathbf{a}(q))^2 + V(q)^2 - \Phi(q)\right\}.$$

It now follows from the analysis above that U has eigenvalues

$$\begin{aligned} u_{\delta,\hbar}(\gamma) =&\ (1-\delta)(p - k\mathbf{a}(q))^2 + V(q)^2 - \Phi(q) \\ &+ s(\mu) 2\Big[V(q)^2((p - k\mathbf{a}(q))^2 + 1) + (1-\delta)^2 \tfrac{(k\hbar)^2}{4} |\mathbf{B}(q)|^2 \\ &+ (-1)^\mu (1-\delta) k\hbar |V(q)| \sqrt{|\mathbf{B}(q)|^2 + ((p - k\mathbf{a}(q)) \cdot \mathbf{B}(q))^2}\Big]^{\frac{1}{2}} \end{aligned}$$

for $s(1) = s(2) = -1$ and $s(3) = s(4) = 1$.

Next, we consider the matrix

$$\begin{aligned} O(p,q) =&\ < (p - k\mathbf{a})^2 >_\rho - \hbar k \Sigma \cdot < \mathbf{B} >_\rho + 2 < V\{\alpha \cdot (p - k\mathbf{a}) + \beta\} >_\rho + < V^2 - \Phi >_\rho \\ =&\ 2 < V >_\rho \{\alpha \cdot \mathbf{r} + \beta - \Sigma \cdot \mathbf{C} + c\} \end{aligned}$$

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[16] This can be found in [15].

for

$$\mathbf{r} := p - k\frac{< V\mathbf{a} >_\rho}{< V >_\rho},\ \mathbf{C} := \frac{\hbar k}{2 < V >_\rho} < \mathbf{B} >_\rho,\ c := \frac{1}{2 < V >_\rho}\{< (p - k\mathbf{a})^2 >_\rho + < V^2 - \Phi >_\rho\}.$$

Consequently the same analysis as above shows that the eigenvalues of $O(p, q)$ are given by

$$\begin{aligned} o_{\rho,\hbar}(\gamma) = \quad & < (p - k\mathbf{a})^2 >_\rho + < V^2 - \Phi >_\rho \\ & + s(\mu) 2 \Big[< V(p - k\mathbf{a}) >_\rho^2 + < V >_\rho^2 + \tfrac{(k\hbar)^2}{4} | < \mathbf{B} >_\rho |^2 \\ & + (-1)^\mu k\hbar \sqrt{< V >_\rho^2 | < \mathbf{B} >_\rho |^2 + [< V(p - k\mathbf{a}) >_\rho \cdot < \mathbf{B} >_\rho]^2} \Big]^{\frac{1}{2}}. \end{aligned}$$

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