On the Asymptotics of the Spectral Density of Radial Dirac Operators with Divergent Potential

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Dedicated to the memory of Michael S. P. Eastham

Abstract. The radial Dirac operator with a potential tending to infinity at infinity and satisfying a mild regularity condition is known to have a purely absolutely continuous spectrum covering the whole real line. Although having two singular end-points in the limit-point case, the operator has a simple spectrum and a generalised Fourier expansion in terms of a single solution. In the present paper, a simple formula for the corresponding spectral density is derived, and it is shown that, under certain conditions on the potential, the spectral function is convex for large values of the spectral parameter. This settles a question considered in earlier work by M. S. P. Eastham and the author.

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1. Introduction

The one-dimensional Dirac operator (2.1) with a potential q tending to $-\infty$ (or ∞) at infinity and satisfying the Erdélyi condition, which essentially says that $1/q$ has bounded variation at infinity, is known to have a purely absolutely continuous spectrum covering the whole real line ([6], [12], [13]). In [3], the properties of the spectral density were studied in greater detail for the case of a regular end-point 0 (corresponding to angular momentum quantum number $k = 0$). It was shown that under certain regularity and growth conditions on the potential function, the spectral density has no local extrema for large spectral parameter; this can be interpreted as an absence of high-energy points of spectral concentration. In [4], an analogous study was undertaken for the operator with angular momentum, a differential expression with two singular end-points in the limit-point case. Asymptotics for the spectral matrix with respect to expansion in terms of the canonical fundamental system at an arbitrary intermediate point c were derived, under slightly less restrictive conditions on the potential q than in the regular case; however, the resulting spectral density shows oscillatory behaviour for large spectral parameter and, moreover, depends in an essential way on the choice of c, which stands in the way of a clear interpretation of the result. It is the purpose of the present note to amend this unsatisfactory outcome and indeed prove the absence of high-energy local extrema of an appropriately defined spectral density.

The key observation is that, despite the two singular end-points, this operator has a simple spectrum and admits a generalised Fourier expansion in terms of a single solution, with a real-valued spectral function, as opposed to the general case of expansion in terms of a fundamental system of solutions, with a corresponding matrix-valued spectral function. Differential operators (mostly of Sturm-Liouville type) with this property have, after an early observation by I. S. Kac on the Bessel equation [10], attracted considerable attention in recent years. The existence of a solution square-integrable at one of the singular end-points and analytic in the spectral parameter was identified as an important indicator in [9], [11]; see also [7], [8], [1] and references cited therein.

In contrast to these studies, which involve a generalised Titchmarsh-Weyl function for the singular boundary value problem in one way or another, the present paper uses oscillation theory for real spectral parameter only. Section 2 reviews the required tools from [4], in particular (Theorem 2.1) the existence of a distinguished solution at the singular end-point 0. In analogy to the regular case, where a λ-independent initial condition is used, we normalise the solutions for different values of the spectral parameter λ by imposing the condition of a particular, λ-independent leading asymptotic at 0. (Clearly, a λ-dependent boundary condition would be reflected directly in the shape of the spectral function.) In Section 3, we derive (Theorem 3.1) a neat formula for the spectral density for expansion in terms of the distinguished solution and show how it relates to the spectral matrix of [4]. In Section 4, we state and prove the main result (Theorem 4.1) on the absence of local extrema of the spectral density.

2. Preliminaries

Consider the one-dimensional radial Dirac operator

$$-i\sigma_2\frac{d}{dr} + m\sigma_3 + \frac{k}{r}\,\sigma_1 + q(r) \qquad (r \in (0,\infty)), \tag{2.1}$$

where

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

are the Pauli matrices. This operator arises from variable separation in polar coordinates of the Dirac operator in $\mathbb{R}^n$ ($n \geq 3$) with mass m and rotationally symmetric potential $V(x) = q(|x|)$ ($x \in \mathbb{R}^n$). The angular momentum quantum number k takes non-zero integer values if n is odd, half-integer values if n is even, so $|k| \geq \frac{1}{2}$ in all cases. The results of the present paper hold for all real $k > 0$; we focus on the case of positive k for definiteness and convenience, but note that analogous, qualitatively identical results hold true for $k < 0$.

We take m to be a positive constant. Regarding the potential function q, we assume that $\lim_{r\to\infty} q(r) = -\infty$, that $q \in AC_{\rm loc}(0,\infty)$ and that the Erdélyi condition $\int^\infty \frac{|q'|}{q^2} < \infty$ ([6]) is satisfied. For our main result, Theorem 4.1, we assume furthermore that q is constant on the interval $[0, r_0]$, for some $r_0 > 0$; and that it satisfies further regularity and growth conditions, see conditions (P) and (E) in Section 4. (Similar, though slightly stronger conditions were shown in [3] to imply the high-energy concavity or convexity of the spectral function of the half-line Dirac equation without the angular momentum term and with a regular boundary condition at 0.)

Under these assumptions, for $|k| \geq \frac{1}{2}$, the formal differential expression (2.1) is in the limit-point case both at 0 and at ∞ and therefore gives rise to a unique self-adjoint operator H in the Hilbert space $L^2(0,\infty)^2$. If $|k| \in (0, \frac{1}{2})$, the end-point 0 is in the limit-circle case, and we impose the boundary condition (3.1) corresponding to the distinguished solution of Theorem 2.1 to obtain a self-adjoint operator H.

We shall use the Prüfer transformation, writing an $\mathbb{R}^2$-valued solution of the Dirac equation (2.3) in the (polar-coordinate) form

$$u(r) = |u(r)| \begin{pmatrix} \sin\vartheta(r) \\ \cos\vartheta(r) \end{pmatrix} \qquad (r > 0)$$

with the Prüfer angle function ϑ, which is uniquely defined up to an additive offset of an integer multiple of 2π. The Dirac equation (2.3) is then equivalent to the Prüfer equations

$$\begin{aligned} \vartheta'(r) &= \lambda - q(r) + m\cos 2\vartheta(r) - \frac{k}{r}\sin 2\vartheta(r), \\ (\log|u|)'(r) &= \frac{k}{r}\cos 2\vartheta(r) + m\sin\vartheta(r); \end{aligned} \tag{2.2}$$

clearly the latter equation can easily be integrated to give $|u|$ in terms of ϑ.

The starting point for the present study is the following fundamental observation on the existence of a distinguished solution of the eigenvalue equation (2.3) for the radial Dirac operator, proved as Theorem 1 of [4] (where $k \geq \frac{1}{2}$ is assumed, but the proof is identical for $k > 0$).

Theorem 2.1. *Let $m > 0$, $q \in L^1_{\mathrm{loc}}[0,\infty)$ and $k > 0$. Then, for each $\lambda \in \mathbb{R}$, the Dirac equation*

$$\left(-i\sigma_2 \frac{d}{dr} + m\,\sigma_3 + \frac{k}{r}\,\sigma_1 + q(r)\right) u(r) = \lambda\, u(r) \qquad (r \in (0,\infty)) \tag{2.3}$$

has a unique ($\mathbb{R}^2$-valued) solution $w(\cdot,\lambda)$ such that

$$w(r,\lambda) = \begin{pmatrix} o(1) \\ 1 + o(1) \end{pmatrix} r^k \qquad (r \to 0).$$

For each $r > 0$, $w(r,\cdot)$ is differentiable, and

$$\frac{\partial}{\partial\lambda} w(r,\lambda) = o(r^k) \qquad (r \to 0).$$

The Prüfer angle ϑ of w, with suitably chosen offset, has the properties

$$\lim_{r\to 0} \vartheta(r,\lambda) = 0, \qquad \lim_{r\to 0} \frac{\partial\vartheta}{\partial\lambda}(r,\lambda) = 0.$$

The following formulae can be shown by integration of the variational equation obtained by formal differentiation of the differential equation for the Prüfer angle with respect to λ, and using the asymptotics of Theorem 2.1. They can be found in Lemma 1 and Corollary 1 of [4], respectively.

Lemma 2.2. *Let ϑ be the Prüfer angle of the distinguished solution w of Theorem 2.1, and let $x_0 > 0$. Then*

(a) $$\frac{\partial\vartheta}{\partial\lambda}(x,\lambda) = \frac{|w(x_0,\lambda)|^2}{|w(x,\lambda)|^2} \frac{\partial\vartheta}{\partial\lambda}(x_0,\lambda) + \int_{x_0}^{x} \frac{|w(t,\lambda)|^2}{|w(x,\lambda)|^2}\, dt \qquad (x > 0, \lambda \in \mathbb{R});$$

(b) $$\frac{\partial\vartheta}{\partial\lambda}(x,\lambda) = \frac{1}{|w(x,\lambda)|^2} \int_0^x |w(t,\lambda)|^2\, dt \qquad (x > 0, \lambda \in \mathbb{R}).$$

In the following we fix $\lambda_0 > m + \frac{|k|}{r_0} + \sup q$.

Lemma 2.3. *Let w be the distinguished solution of Theorem 2.1. There is a constant $C > 1$ such that*

$$\frac{1}{C} \le \frac{|w(r,\lambda)|}{|w(r_0,\lambda)|} \le C \qquad (r \ge r_0, \lambda \ge \lambda_0).$$

Moreover, the limit $|w(\infty,\lambda)| = \lim_{r\to\infty} |w(r,\lambda)|$ exists for all $\lambda \ge \lambda_0$.

These statements are proved as part of Lemma 4 in [4]. We remark that the following asymptotics for $\lambda \to \infty$ hold (cf. Theorem 2, Lemma 4 of [4]),

$$\frac{\partial\vartheta}{\partial\lambda}(r,\lambda) = r\,(1 + o(1)), \qquad \frac{|w(r,\lambda)|}{|w(r_0,\lambda)|} = 1 + o(1),$$

both with $o(1)$ term uniform in $r \ge r_0$, and

$$\frac{|w(\infty,\lambda)|}{|w(r_0,\lambda)|} = 1 + o(1).$$

These asymptotics are used in the proof (detailed in [4]) of Lemma 4.2 below.

3. The spectral density of the half-line operator

We now consider a self-adjoint realisation H of the Dirac operator (2.1) in the Hilbert space $L^2(0,\infty)^2$. If $k \geq \frac{1}{2}$, then the differential expression is in the limit-point case both at 0 and at ∞, so there is a unique self-adjoint realisation; if $k \in (0,2)$, we have the limit-circle case at 0 and impose the boundary condition

$$\lim_{r\to 0}[u,w](r) = 0, \tag{3.1}$$

where w is the distinguished solution of Theorem 2.1 and $[u,w] = \det(u,w)$ is the Liouville bracket.

Theorem 3.1. *The self-adjoint operator H has purely absolutely continuous spectrum in (λ_0,∞) with spectral density*

$$\varrho'(\lambda) = \frac{1}{\pi|w(\infty,\lambda)|^2} \qquad (\lambda \geq \lambda_0),$$

where w is the distinguished solution of Theorem 2.1*.*

Note that here ϱ is the spectral function for expansion with respect to the solution w, in the form

$$f(x) = \int_{\mathbb{R}} \left(\int_0^\infty f(y)^T w(y,\lambda)\,dy\right) w(x,\lambda)\,d\varrho(\lambda) \qquad (x \in \mathbb{R}; f \in L^2(0,\infty)^2).$$

Proof. We start from the boundary-value problem on $(0,b)$ with boundary condition

$$u(b)^T \begin{pmatrix} \cos\beta \\ -\sin\beta \end{pmatrix} = 0 \tag{3.2}$$

for some $\beta \in [0,\pi)$ (and with the boundary condition (3.1) at 0 if $k \in (0,\frac{1}{2})$). The spectrum of this boundary-value problem is purely discrete, with simple eigenvalues determined by the condition $\vartheta(b,\lambda) = \beta \bmod \pi$. (Indeed, for the other values of λ, the solution w and the solution y such that $y(b) = \begin{pmatrix} \sin\beta \\ \cos\beta \end{pmatrix}$ are linearly independent and can be used to construct the resolvent $(H_b - l)^{-1}$, where H_b is the self-adjoint operator on $(0,b)$ with the boundary condition (3.2) at the right-hand end-point.)

The eigenvalues can be indexed as $\{\lambda_j \mid j \in \mathbb{Z}\}$, where $\vartheta(b,\lambda_j) = \beta + j\pi$. For the eigenvalue λ_j, clearly

$$\frac{w(\cdot,\lambda_j)}{\sqrt{\int_0^b |w(t,\lambda_j)|^2\,dt}}$$

is a normalised eigenfunction, so we obtain the expansion formula for $f \in L^2(0,b)^2$,

$$\begin{aligned} f &= \sum_{j\in\mathbb{Z}} \frac{1}{\sqrt{\int_0^b |w(t,\lambda_j)|^2\,dt}} \left(\int_0^b f(t)^T w(t,\lambda_j)\,dt\right) w(\cdot,\lambda_j) \\ &= \int_{\mathbb{R}} \left(\int_0^b f(t)^T w(t,\lambda)\,dt\right) w(\cdot,\lambda)\,d\varrho_b(\lambda) \end{aligned}$$

with the spectral function

$$\varrho_b(\lambda) = \begin{cases} \sum\limits_{\lambda_j\in\sigma(H_b)\cap(\lambda_0,\lambda]} \left(\int_0^b |w(t,\lambda_j)|^2\,dt\right)^{-1} & \text{if } \lambda \geq \lambda_0, \\ -\sum\limits_{\lambda_j\in\sigma(H_b)\cap(\lambda,\lambda_0]} \left(\int_0^b |w(t,\lambda_j)|^2\,dt\right)^{-1} & \text{if } \lambda < \lambda_0. \end{cases}$$

Now consider the spectral function averaged over the boundary condition parameter β,

$$\tilde{\varrho}_b(\lambda) = \frac{1}{\pi}\int_0^\pi \varrho_b(\lambda)\,d\beta.$$

As the jth eigenvalue branch $\Lambda_j(\beta)$ satisfies $\vartheta(b,\Lambda_j(\beta)) = \beta + j\pi$, it follows, using Lemma 2.2 (b), that

$$1 = \frac{\partial}{\partial\lambda}\vartheta(b,\Lambda_j(\beta))\,\Lambda_j'(\beta) = \frac{\Lambda_j'(\beta)}{|w(b,\Lambda_j(\beta))|^2}\int_0^b |w(t,\Lambda_j(\beta))|^2\,dt,$$

and hence by a change of integration variables

$$\tilde{\varrho}_b(\lambda) = \frac{1}{\pi}\int_0^\pi \sum_{j:\Lambda_j(\beta)\in(\lambda_0,\lambda]} \frac{\Lambda_j'(\beta)}{|w(b,\Lambda_j(\beta))|^2}\,d\beta = \frac{1}{\pi}\int_{\lambda_0}^\lambda \frac{d\mu}{|w(b,\mu)|^2} \qquad (\lambda \geq \lambda_0).$$

As the Dirac equation (2.3) is in the limit-point case at ∞ (see e.g. Theorem 6.8 in [14]), the spectral function for the half-line problem will be the limit $\varrho(\lambda) = \lim\limits_{b\to\infty} \varrho_b(\lambda)$ $(\lambda \geq \lambda_0)$ for *any* choice of boundary condition β. This implies $\varrho(\lambda) = \lim\limits_{b\to\infty} \tilde{\varrho}_b(\lambda)$ $(\lambda \geq \lambda_0)$ by the Lebesgue dominated convergence theorem, as there is a locally integrable majorant of ϱ_b which is independent of b and of β. (Indeed, the number of eigenvalues in $(\lambda_0,\lambda]$ can be estimated above by

$$\begin{aligned} 1 + \frac{1}{\pi}(\vartheta(b,\lambda) - \vartheta(b,\lambda_0)) &= 1 + \frac{1}{\pi}\int_{\lambda_0}^\lambda \frac{\partial\vartheta}{\partial\lambda}(b,\mu)\,d\mu \\ &= 1 + \frac{1}{\pi}\int_{\lambda_0}^\lambda \left(\frac{|w(r_0,\mu)|^2}{|w(b,\mu)|^2}\,\frac{\partial\vartheta}{\partial\lambda}(r_0,\mu) + \int_{r_0}^b \frac{|w(t,\mu)|^2}{|w(r_0,\mu)|^2}\,\frac{|w(r_0,\mu)|^2}{|w(b,\mu)|^2}\,dt\right) d\mu \\ &\leq 1 + \frac{1}{\pi}(C^2(\vartheta(r_0,\lambda) - \vartheta(r_0,\lambda_0)) + C^4(b-r_0)(\lambda-\lambda_0)), \end{aligned}$$

where we used Lemma 2.2 (a) and Lemma 2.3. The latter lemma also gives a lower estimate for $\int_{r_0}^{b} |w(t,\mu)|^2\,dt$, and hence

$$\varrho_b(\mu) \leq \frac{1 + \frac{1}{\pi}(C^2(\vartheta(r_0,\mu) - \vartheta(r_0,\lambda_0)) + C^4(b-r_0)(\mu-\lambda_0))}{\int_0^{r_0} |w(t,\mu)|^2\,dt + C^{-2}|w(r_0,\mu)|^2(b-r_0)};$$

this bound is independent of β and remains bounded as $b \to \infty$.)

Thus we have

$$\varrho(\lambda) = \lim_{b\to\infty} \tilde{\varrho}_b(\lambda) = \frac{1}{\pi}\int_{\lambda_0}^{\lambda} \frac{d\mu}{|w(b,\mu)|^2} = \frac{1}{\pi}\int_{\lambda_0}^{\lambda} \frac{d\mu}{|w(\infty,\mu)|^2} \qquad (\lambda \geq \lambda_0),$$

using Lebesgue's dominated convergence theorem again with the estimate from Lemma 2.3,

$$\frac{1}{|w(b,\mu)|^2} \leq \frac{C^2}{|w(r_0,\mu)|^2} \qquad (b \geq r_0). \qquad \square$$

Remark. In [4] Theorem 3, it was shown that the spectral matrix for expansion with respect to the canonical fundamental system Φ at some point $c \in (0,\infty)$ (according to the treatment of the boundary-value problem with two singular end-points as outlined e.g. in [2]) has the matrix density

$$\varrho_\Phi'(\lambda) = \frac{w(c,\lambda)w(c,\lambda)^T}{\pi|w(\infty,\lambda)|^2} \qquad (\lambda \geq \lambda_0).$$

This corresponds to the expansion of $f \in L^2(0,\infty)^2$,

$$f = \int_{\mathbb{R}} \Phi(\cdot,\lambda)\,d\varrho_\Phi(\lambda) \int_0^\infty \Phi(y,\lambda)^T f(y)\,dy,$$

where

$$\Big(-i\sigma_2 + m\sigma_3 + \frac{k}{r}\sigma_1 - \lambda\Big)\Phi(\cdot,\lambda) = 0, \qquad \Phi(c,\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Let Ψ be the fundamental system

$$\Psi = \begin{pmatrix} w_1 & z_1 \\ w_2 & z_2 \end{pmatrix},$$

where w is the special solution of Theorem 2.1 and z is another solution of (2.3) such that the Wronskian $\det\Psi = 1$. Then $\Psi(x,\lambda) = \Phi(x,\lambda)\Psi(c,\lambda)$ $(x > 0)$, and we can rewrite the expansion formula as

$$\begin{aligned} f &= \int_{\mathbb{R}} \Psi(\cdot,\lambda)\Psi(c,\lambda)^{-1}\,d\varrho_\Phi(\lambda) \int_0^\infty (\Psi(c,\lambda)^{-1})^T \Psi(y,\lambda)^T f(y)\,dy \\ &= \int_{\mathbb{R}} \Psi(\cdot,\lambda)\,d\varrho_\Psi(\lambda) \int_0^\infty \Psi(y,\lambda)^T f(y)\,dy, \end{aligned}$$

where

$$
\begin{aligned}
d\varrho_\Psi(\lambda) &= \Psi(c,\lambda)^{-1}\, d\varrho_\Phi(\lambda)\, (\Psi(c,\lambda)^{-1})^T \\
&= \begin{pmatrix} z_2 & -z_1 \\ -w_2 & w_1 \end{pmatrix}(c,\lambda) \begin{pmatrix} w_1^2 & w_1 w_2 \\ w_1 w_2 & w_s^2 \end{pmatrix}(c,\lambda) \begin{pmatrix} z_2 & -w_2 \\ -z_1 & w_1 \end{pmatrix}(c,\lambda) \frac{d\lambda}{\pi |w(\infty,\lambda)|^2} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \frac{d\lambda}{\pi |w(\infty,\lambda)|^2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} d\varrho(\lambda),
\end{aligned}
$$

with ϱ as in Theorem 3.1 above. This shows clearly how the spectral matrix degenerates to a single spectral function for an expansion in terms of w only.

4. High-energy convexity of the spectral function

In addition to the general hypotheses on q, we shall use either of the following growth conditions, roughly corresponding to polynomial growth (P) or exponential growth (E). These conditions are identical to those used in [4]; in the case of a regular end-point 0, analogous conditions on the third derivative of q were required in addition [3].

Condition (P). Assume $q, q' \in AC_{\mathrm{loc}}(0,\infty)$ and that there are positive constants a, C_1, C_2 such that

$$
-q(r) \geq C_1 r^a, \qquad |q'(r)| \leq C_2 r^{a-1}, \qquad |q''(r)| \leq C_2 r^{a-2}
$$

for sufficiently large $r > 0$.

Condition (E). Assume $q, q' \in AC_{\mathrm{loc}}(0,\infty)$ and that there are positive constants a, C_1 such that

$$
-q(r) \geq C_1 r^a
$$

for sufficiently large $r > 0$. Moreover, assume that for some $\delta \in (0,1)$ and any $\varepsilon > 0$,

$$
\int^\infty \frac{r|q'(r)|}{|q(r)|^{1+\delta}}\, dr < \infty, \qquad \int^\infty \frac{r|q''(r)|}{|q(r)|^{1+\delta}}\, dr < \infty
$$

and

$$
\frac{q'(r)}{|q(r)|^{1+\varepsilon}} = O(1) \qquad (r \to \infty).
$$

Theorem 4.1. *Suppose that q is constant on $[0, r_0]$ and satisfies either* (P) *or* (E)*. Let $k > 0$. Then there is $\lambda_1 \geq \lambda_0$ such that the spectral function ϱ is strictly convex on $[\lambda_1, \infty)$.*

By Theorem 3.1 and the Prüfer equation (2.2),

$$\varrho'(\lambda) = \frac{1}{\pi} \exp\Bigg(-2\log|w(r_0,\lambda)| \\ - 2\int_{r_0}^{\infty} \Big(\frac{k}{r}\cos 2\vartheta(r,\lambda) + m\sin 2\vartheta(r,\lambda)\Big)\,dr\Bigg) > 0,$$

so

$$\frac{\varrho''(\lambda)}{\varrho'(\lambda)} = -2\Bigg(\frac{d}{d\lambda}\log|w(r_0,\lambda)| \\ + \frac{d}{d\lambda}\int_{r_0}^{\infty}\Big(\frac{k}{r}\cos 2\vartheta(r,\lambda) + m\sin 2\vartheta(r,\lambda)\Big)\,dr\Bigg), \qquad (4.1)$$

and hence, to prove Theorem 4.1, it suffices to show that the expression on the right-hand side of (4.1) is positive from some λ_1 onwards.

The integral term in (4.1) was studied in [4] Section 4 (where it was assumed that $k \geq \frac{1}{2}$, but the proof for $k > 0$ is identical). The key idea is to introduce the factor (obtained from the differential equation for the Prüfer angle)

$$1 = \frac{\vartheta'(r) + \frac{k}{r}\sin 2\vartheta(r) - m\cos\vartheta(r)}{\lambda - q(r)}$$

into the integrand and integrate by parts. This brings in an additional factor of order $\frac{1}{\lambda}$ and, upon repetition, higher powers of $\frac{1}{\lambda}$. It can be shown that, after a suitable (depending on the constants a, δ, possibly very considerable) number of such integrations by parts, the λ-derivatives of all resulting integrals and boundary terms are of higher order, as $\lambda \to \infty$, than the leading term which arises as the boundary term at r_0 from the first integration by parts. This gives the following result.

Lemma 4.2. *Let $m > 0$, $k > 0$ and suppose that q satisfies either* (P) *or* (E). *Then, as $\lambda \to \infty$,*

$$\frac{d}{d\lambda}\int_{r_0}^{\infty}\Big(\frac{k}{r}\cos 2\vartheta(r,\lambda) + m\,\sin 2\vartheta(r,\lambda)\Big)\,dr \\ = -\frac{mr_0\sin 2\vartheta(r_0,\lambda) + k\cos 2\vartheta(r_0,\lambda)}{\lambda - q(r_0)} + o\Big(\frac{1}{\lambda}\Big).$$

It remains to find the behaviour, for large λ, of the derivative of $\log|w(r_0,\lambda)|$. In view of the success of the approach of [4] outlined above, it seems a tempting idea to apply a similar process of repeated integrations by parts to the corresponding integral over $[0, r_0]$. However, here the difficulty arises that some terms of the resulting integrals are singular at 0, due to the pole of the angular momentum term, and the very existence of the integral depends on a subtle cancellation of the singularities between terms, based on the asymptotics of the Prüfer angle at 0. While this is more in the character of a technical nuisance, there is the more fundamental problem that apparently some terms of the resulting integral will always remain that do not have a small λ-derivative as $\lambda \to \infty$, so not even a large number of integrations by parts will give a useful asymptotic series.

Therefore a radically different approach to study the first term on the right-hand side of (4.1) is used in the following. We require the assumption that q is constant near 0; it would be interesting to know to what extent the asymptotics for the derivative of the spectral density, which is derived below, carries over to the more general case of non-constant (e.g. continuous) q. As, under our assumption, the differential equation has constant coefficients on $[0, r_0]$, the solution w could be expressed explicitly in terms of Bessel functions. However, this fully explicit form of the solution is not convenient for comparison with the asymptotic found for the integral term; for this purpose it is better to relate this derivative to the Prüfer angle of the solution. As a preliminary step, we consider the differential equation on $(0, r_0]$ without the mass term (the constant potential can be subsumed in the spectral parameter); it has a scaling symmetry which allows for an exact expression of the logarithmic derivative of the Prüfer radius of the solution in term of the Prüfer angle (Lemma 4.3). Subsequently, we include the mass term to obtain an asymptotic form of such a relationship for large spectral parameter (Lemma 4.4), which combines with Lemma 4.2 to complete the proof of Theorem 4.1.

Lemma 4.3. *Let $k > 0$. For any $\lambda > 0$, let $w_0(\cdot, \lambda)$ be the distinguished solution, according to Theorem* 2.1*, of*

$$-i\sigma_3 w_0' + \left(\frac{k}{r}\,\sigma_1 - \lambda\right) w_0 = 0 \tag{4.2}$$

and ϑ_0 the Prüfer angle of w_0. Then

$$\frac{\partial}{\partial\lambda} \log |w_0(r,\lambda)| = -\frac{k}{\lambda} + \frac{k}{\lambda}\,\cos 2\vartheta_0(r,\lambda) \qquad (r > 0, \lambda > 0). \tag{4.3}$$

Proof. We observe that w_0 takes the form $w_0(r,\lambda) = \lambda^{-k} u(\lambda r)$ due to a symmetry of the very simply structured equation (4.2). Indeed, substituting this ansatz in the differential equation, we find

$$\lambda^{-k}\left(-i\sigma_2 \lambda u'(\lambda r) + \left(\frac{k\lambda}{\lambda r} - \lambda\right) u(\lambda r)\right) = 0,$$

which is an identity if we take u to be the distinguished solution of equation (4.2) with $\lambda = 1$.

Therefore the partial derivatives of $w_0(r,\lambda)$ with respect to r and to λ are related, and we obtain

$$\begin{aligned}\frac{\partial}{\partial\lambda} w_0(r,\lambda) &= -\frac{k}{\lambda}\, w_0(r,\lambda) + \frac{r}{\lambda}\frac{\partial}{\partial r} w_0(r,\lambda)\\ &= -\frac{k}{\lambda}\, w_0(r,\lambda) + ri\sigma_2 w_0(r,\lambda) - \frac{k}{\lambda}\,\sigma_3 w_0(r,\lambda),\end{aligned} \tag{4.4}$$

using (4.2) and the identity $i\sigma_2\sigma_1 = \sigma_3$. Consequently,

$$\begin{aligned}\frac{\partial}{\partial\lambda}|w_0(r,\lambda)|^2 &= 2w_0(r,\lambda)^T \frac{\partial}{\partial\lambda} w_0(r,\lambda)\\ &= -\frac{2k}{\lambda}\,|w_0(r,\lambda)|^2 - \frac{2k}{\lambda}\,w_0(r,\lambda)^T\sigma_3 w_0(r,\lambda).\end{aligned}$$

This gives (4.3), using Prüfer variables

$$w_0 = |w_0| \begin{pmatrix}\sin\vartheta_0\\ \cos\vartheta_0\end{pmatrix}. \qquad \square$$

Lemma 4.4. *Let $k > 0$, $m > 0$. For any $\lambda > m$, let $w(\cdot,\lambda)$ be the distinguished solution, according to Theorem* 2.1, *of*

$$-i\sigma_2 w' + \left(m\sigma_3 + \frac{k}{r}\sigma_1 - \lambda\right) w = 0 \tag{4.5}$$

and ϑ the Prüfer angle of w. Then, for any $r > 0$,

$$\frac{\partial}{\partial\lambda}\log|w(r,\lambda)| = -\frac{k}{\lambda} + \frac{k}{\lambda}\cos 2\vartheta(r,\lambda) + \frac{rm}{\lambda}\sin 2\vartheta(r,\lambda) + O\Big(\frac{1}{\lambda^2}\Big)$$

$(\lambda \to \infty)$.

Proof. We begin by observing that the differential equation (4.5) can be rewritten as

$$w'(r,\lambda) = \begin{pmatrix}-\frac{k}{r} & m+\lambda\\ m-\lambda & \frac{k}{r}\end{pmatrix} w(r,\lambda) \tag{4.6}$$

and, as a special case, the differential equation (4.2) will be

$$w_0'(r,\lambda) = \begin{pmatrix}-\frac{k}{r} & \lambda\\ -\lambda & \frac{k}{r}\end{pmatrix} w_0(r,\lambda) \tag{4.7}$$

(the dash denoting the partial derivative w.r.t. r). The solution w can be expressed as

$$w(r,\lambda) = \begin{pmatrix}\tau(\lambda)^{1-k} & 0\\ 0 & \tau(\lambda)^{-k}\end{pmatrix} w_0(\tau(\lambda)r, \lambda - m), \tag{4.8}$$

where $\tau(\lambda) = \sqrt{\frac{\lambda+m}{\lambda-m}}$ and w_0 is the solution of (4.2) considered in Lemma 4.3. Indeed, it is a straightforward calculation to check that w, as defined by this formula (4.8), satisfies (4.6) on the basis that w_0 satisfies (4.7), and has the correct asymptotic

$$w(r,\lambda) = \begin{pmatrix}\tau(\lambda)^{1-k} & 0\\ 0 & \tau(\lambda)^{-k}\end{pmatrix}\begin{pmatrix}o(1)\\ 1+o(1)\end{pmatrix}(\tau(\lambda)r)^k = \begin{pmatrix}\tau(\lambda)\,o(1)\\ 1+o(1)\end{pmatrix} r^k$$

$(r \to 0)$. Differentiation of (4.8) w.r.t. λ gives, denoting by ∂_1 and ∂_2 the partial derivative w.r.t. the first and second argument, respectively,

$$\begin{aligned}\frac{\partial}{\partial\lambda}w(r,\lambda) &= \frac{\tau'(\lambda)}{\tau(\lambda)}\begin{pmatrix}1-k & 0\\ 0 & -k\end{pmatrix}w(r,\lambda)\\ &+ \begin{pmatrix}\tau(\lambda)^{1-k} & 0\\ 0 & \tau(\lambda)^{-k}\end{pmatrix}\Big(r\tau'(\lambda)\partial_1 w_0(\tau(\lambda)r,\lambda-m) + \partial_2 w_0(\tau(\lambda)r,\lambda-m)\Big).\end{aligned}$$

As

$$w'(r,\lambda) = \begin{pmatrix}\tau(\lambda)^{1-k} & 0\\ 0 & \tau(\lambda)^{-k}\end{pmatrix}\tau(\lambda)\partial_1 w_0(\tau(\lambda)r,\lambda-m),$$

we see from the differential equation (4.6) that

$$\begin{aligned}&\begin{pmatrix}\tau(\lambda)^{1-k} & 0\\ 0 & \tau(\lambda)^{-k}\end{pmatrix}r\tau'(\lambda)\partial_1 w_0(\tau(\lambda)r,\lambda-m)\\ &\qquad = \frac{\tau'(\lambda)}{\tau(\lambda)}\begin{pmatrix}-k & r(m+\lambda)\\ r(m-\lambda) & k\end{pmatrix}w(r,\lambda);\end{aligned}$$

moreover, we have from (4.4) the identity

$$\begin{aligned}&\begin{pmatrix}\tau(\lambda)^{1-k} & 0\\ 0 & \tau(\lambda)^{-k}\end{pmatrix}\partial_2 w_0(\tau(\lambda)r,\lambda-m)\\ &\qquad = \left(\frac{-k}{\lambda-m}(1+\sigma_3) + r\begin{pmatrix}0 & \tau(\lambda)^2\\ -1 & 0\end{pmatrix}\right)w(r,\lambda).\end{aligned}$$

Hence we find

$$\frac{\partial}{\partial\lambda}w(r,\lambda) = \frac{1}{\lambda^2-m^2}\begin{pmatrix}-m-2k\lambda & r\lambda\,(\lambda+m)\\ -r\lambda\,(\lambda-m) & 0\end{pmatrix}w(r,\lambda).$$

Therefore, using the Prüfer representation

$$w(r,\lambda) = |w(r,\lambda)|\begin{pmatrix}\sin\vartheta(r,\lambda)\\ \cos\vartheta(r,\lambda)\end{pmatrix},$$

we obtain

$$\begin{aligned}\frac{\partial}{\partial\lambda}\log|w(r,\lambda)|^2 &= \frac{2}{|w(r,\lambda)|^2}\,w(r,\lambda)^T\frac{\partial}{\partial\lambda}w(r,\lambda)^T\\ &= \frac{2}{\lambda^2-m^2}\Big(-(m+2k\lambda)\sin^2\vartheta(r,\lambda) + 2r\lambda m\sin\vartheta(r,\lambda)\,\cos\vartheta(r,\lambda)\Big)\\ &= \frac{2k\lambda}{\lambda^2-m^2}(\cos 2\vartheta(r,\lambda)-1) + \frac{2rm\lambda}{\lambda^2-m^2}\sin 2\vartheta(r,\lambda) + O\Big(\frac{1}{\lambda^2}\Big)\end{aligned}$$

as $\lambda \to \infty$. The statement of Lemma 4.4 now follows in view of

$$\frac{\lambda}{\lambda^2-m^2} = \frac{1}{\lambda} + O\Big(\frac{1}{\lambda^3}\Big) \qquad (\lambda\to\infty).$$

□

Now, combining the statements of Lemma 4.2 and Lemma 4.4 (where we take $r = r_0$ and replace λ with the constant $\lambda - q = \lambda - q(r_0)$ on the interval

$[0, r_0]$) with formula (4.1), we find that

$$\frac{\varrho''(\lambda)}{\varrho'(\lambda)} = \frac{2k}{\lambda - q(r_0)} + o\Big(\frac{1}{\lambda}\Big) = \frac{2k}{\lambda} + o\Big(\frac{1}{\lambda}\Big) \qquad (\lambda \to \infty). \tag{4.9}$$

In particular, there is some $\lambda_1 > 0$ such that $\varrho''(\lambda) > 0$ for all $\lambda > \lambda_1$. This completes the proof of Theorem 4.1.

Remark. Upon integrating the asymptotic (4.9), we see that for any $\varepsilon > 0$, there are constants $c_1, c_2 > 0$ such that the spectral density satisfies

$$c_1\, \lambda^{2k-\varepsilon} \le \varrho'(\lambda) \le c_2\, \lambda^{2k+\varepsilon}$$

for sufficiently large λ. In this context it may be of interest to note the asymptotic of the spectral function itself,

$$|\varrho(\lambda)| \sim \mathrm{const}\, |\lambda|^{2k+1} \qquad (|\lambda| \to \infty),$$

shown (for more general potentials and $k \in \mathbb{R} \setminus (\mathbb{Z} + \frac{1}{2})$) in [5], Theorem 4.2.

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