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# $M$ operators: a generalisation of Weyl–Titchmarsh theory<sup>☆</sup>

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## Abstract

The theory of the Weyl–Titchmarsh  $m$  function for second-order ordinary differential operators is generalized and applied to partial differential operators of the form  $-\Delta + q(x)$  acting in three space dimensions. Weyl operators  $M(z)$  are defined as maps from  $L^2(S_1)$  to  $L^2(S_1)$  ( $S_1 \equiv$  unit sphere in  $\mathbb{R}^3$ ) for exterior and interior boundary value problems, and for the partial differential operator acting in  $L^2(\mathbb{R}^3)$ , with the standard Weyl–Titchmarsh  $m$  function recovered in the special case that  $q$  is spherically symmetric. The analysis is carried out rather explicitly, allowing for the determination of precise norm bounds for  $M$  operators and for the proof of higher dimensional analogues of a number of the fundamental results of standard Weyl–Titchmarsh theory. © 2004 Elsevier B.V. All rights reserved.

## 1. Introduction

The theory of the Weyl–Titchmarsh  $m$  function, with its associated limit point/limit circle analysis [4,7,9,10,12,18,19] has led to important contributions over the years to our understanding of the spectral properties of second-order ordinary differential operators. This paper is devoted to extending this theory so that it applies to partial differential operators in three space dimensions.

For an ordinary differential expression  $\tau = -d^2/dx^2 + q(x)$ , with  $q$  assumed real and integrable over any bounded subinterval of  $[a, \infty)$ , the corresponding Dirichlet  $m$  function may be defined by

$$m(z) = \frac{f'(a, z)}{f(a, z)}, \quad (1.1)$$

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where  $f(\cdot, z)$  is any nontrivial solution in  $L^2((a, \infty))$  of the Schrödinger equation

$$-\frac{d^2 f(x, z)}{dx^2} + q(x)f(x, z) = zf(x, z), \tag{1.2}$$

for complex spectral parameter  $z$ . Here we have assumed limit point case at infinity [10]. We shall also assume  $\text{Im } z > 0$ .

The function  $m$  is a Herglotz function (analytic in the upper half-plane, with positive imaginary part). The (unique) Borel–Stieltjes measure  $\mu$  defined by the Herglotz representation [2] of  $m$  provides a complete description of the spectral properties of the Dirichlet operator  $H = -d^2/dx^2 + q(x)$  in  $L^2((a, \infty))$ , in the sense that  $H$  is unitarily equivalent to a multiplication operator in  $L^2(\mathbb{R}; d\mu)$ .

Algebraically in terms of  $m$ , one may define a one-parameter family of  $m$  functions  $\{m_\alpha\}$  ( $0 \leq \alpha < \pi$ ), with  $\alpha$  labelling a family of real boundary conditions at  $x = a$ ;  $\alpha = 0$  corresponds to the Dirichlet  $m$  function and  $\alpha = \pi/2$  to the Neumann  $m$  function, for which  $m_{\pi/2} = -1/m(z)$ .

One may also define for  $N > a$  an  $m$  function  $m^N(z)$  (or, more generally  $m_\alpha^N(z)$ ) for the finite interval  $a \leq x \leq N$ . The function  $m^N(z)$  is defined in the same way as  $m(z)$ , except that the  $L^2$  condition on  $f$  is replaced by a real boundary condition to be satisfied by  $f$  at the endpoint  $x = N$  of the interval  $[a, N]$ . One of the results of the Weyl theory is that, for arbitrary real boundary condition at  $x = N$  and fixed  $z \in \mathbb{C}^+$ ,  $m^N(z)$  lies on a circle  $\mathcal{C}^N$  in  $\mathbb{C}^+$ , and that as  $N$  increases  $\{\mathcal{C}^N\}$  defines a nesting family of circles which converge in the limit  $N \rightarrow \infty$  (in the limit point case) to the single point  $m(z)$ .

In view of the importance of Weyl theory to the analysis of ordinary differential operators, and the wide range of applications of these ideas (see for example [11] for a recent analysis of the Schrödinger operator for  $q \in L^2(\mathbb{R}^+)$ ), it seems appropriate to look for ways in which an  $m$  function can be defined for partial differential operators. The main purpose of the present paper is to construct an operator-valued Herglotz function  $M(z)$ , together with related families of  $M$  operators corresponding to various boundary conditions on bounded or unbounded subsets of  $\mathbb{R}^3$ , for the differential expression  $\tau = -\Delta + q(x)$ , where  $\Delta$  is the Laplacian operator in three dimensions and  $q$  is a real-valued potential function. A guiding principle of the analysis is that the theoretical framework which we present should as closely as possible reflect the one-dimensional theory of  $m$  functions in the special case that  $q$  is spherically symmetric. Thus for  $q(x) = q(|x|)$  one may verify that the eigenvalues of the Dirichlet  $M$  operator coincide (apart from an additive constant) with the respective values of the Weyl–Titchmarsh  $m$  function for the sequence of one-dimensional problems for potential  $q(x) + \ell(\ell + 1)|x|^{-2}$  ( $\ell = 0, 1, 2, \dots$ ).

In this paper we develop a theoretical framework for the construction and analysis of Weyl  $M(z)$  operators for partial differential expressions  $-\Delta + q(x)$  in three dimensions of space, for a general class of potentials  $q$ , and without assumption of spherical symmetry. The theory which we present is broadly in line with the abstract construction of Weyl operators in terms of a boundary triple (see [14,8] and further references therein), though we differ from this in some respects and our approach is more explicit, allowing precise and detailed estimates of appropriate limits and norms. Given any closed symmetric operator  $T$  in Hilbert space, having equal deficiency indices, one may construct a boundary triple  $\{\mathcal{H}, \Gamma_0, \Gamma_1\}$ , where  $\mathcal{H}$  is an auxiliary Hilbert space and  $\Gamma_0, \Gamma_1$  are operators (called “boundary operators” in the relevant literature) mapping from the domain of  $T^*$  to  $\mathcal{H}$  and satisfying Green’s identity. In this paper, we take for the auxiliary Hilbert space  $\mathcal{H} = L^2(S_1)$ , where  $S_1 = \{x \in \mathbb{R}^3 : |x| = 1\}$  is the unit sphere in  $\mathbb{R}^3$ . In that case we can define  $M(z)$  operators as

mappings from  $L^2(S_1)$  to  $L^2(S_1)$  associated with the operator  $-\Delta + q(x)$ .  $M(z)$  can be defined in terms of solutions of boundary value problems both for the exterior domain  $\Omega = \{x : |x| > 1\}$  and the interior domain  $\Omega_0 = \{x : |x| < 1\}$ .

For the exterior problem a natural choice of  $T$  is the minimal operator  $-\Delta + q(x)$  in  $L^2(\Omega)$  (that is,  $T$  is the closure of  $-\Delta + q(x)$  on  $C_0^\infty(\Omega)$ ), and  $\Gamma$  operators can be defined in terms of traces of functions. Since in that case  $T^*$  is the maximal operator  $-\Delta + q(x)$  in  $L^2(\Omega)$ , these traces are not defined on the whole of the domain  $D(T^*)$  of  $T^*$ , and we have to specify an appropriate function space, a subset of  $D(T^*)$ , on which traces can be evaluated. (Here we differ from the precise definition of the term boundary triple as stated for example in definition (2.1) of [8], while adhering to the basic idea behind the concept.) A possible choice of the function space might be the Sobolev space  $H^2(\Omega)$ , but a better foundation for an  $L^2$  theory of Weyl operators is obtained by taking the space  $\mathcal{D}_1(\Omega)$  considered by Beals and others [6,5,13]. For a precise definition of  $\mathcal{D}_1(\Omega)$  and related spaces, see Section 2 below.

In addition to the  $M$  operator for exterior and interior domains, the  $M$  operator for  $-\Delta + q(x)$  in the whole space  $L^2(\mathbb{R}^3)$  can be defined as a mapping from  $L^2(S_1)$  to  $L^2(S_1)$ , and may be expressed algebraically in terms of the respective exterior and interior operators. All these operators, as well as a related family of  $M$  operators defined subject to a variety of boundary conditions on  $S_1$ , may be regarded as some version of an appropriate Dirichlet to Neumann (or Neumann to Dirichlet) map. This map being nonlocal, we make extensive use of the Beals theory of closed differential operators subject to nonlocal boundary conditions. The analysis may be regarded as the study of a particular analytic family of Steklov–Poincaré operators, modified through the use of nonlocal  $L^2$ -type boundary conditions.

There is a close analogy between the Weyl–Titchmarsh  $m$  function for a differential operator on a bounded interval  $a < x < N$  and the  $M$  operator  $M^A(z)$  for  $-\Delta + q(x)$  for a bounded exterior domain  $\Omega_R = \{x : 1 < |x| < R\}$  in  $\mathbb{R}^3$ . Here  $M^A(z)$  is defined subject to a Neumann condition on the inner surface  $S_1$  and the superfix  $A$  labels a linear operator from  $L^2(S_R)$  to  $L^2(S_R)$  which describes the outer boundary condition on the surface  $S_R = \{x : |x| = R\}$ . Comparison with Weyl theory in one dimension suggests that  $M^A(z)$  will converge to  $M(z)$ , the Weyl operator for the exterior unbounded domain  $\Omega$ , in the limit as  $R \rightarrow \infty$ , and indeed we are able to prove such a result, where the limit is interpreted as a strong limit in the space  $L^2(S_1)$ . We defer to a later paper further discussion of the analogue in  $\mathbb{R}^3$  to the Weyl limiting circles, and of the role of Weyl operators in spectral analysis, for which see [8,17].

The paper is organized as follows. In Section 2, we define the spaces  $\mathcal{D}_1(\Omega)$  and  $\mathcal{D}_1(\Omega_R)$ ; these are spaces of functions  $g$  which are locally of class  $H^2$  and which have  $L^2$  boundary values  $\gamma_1 g, \gamma_1 \partial g / \partial n$  and  $\gamma_R g, \gamma_R \partial g / \partial n$  onto the spherical surfaces  $S_1$  and  $S_R$ , respectively. We construct and estimate various extension maps from  $L^2(S_1)$  and  $L^2(S_R)$  to  $\mathcal{D}_1(\Omega_R)$ . In Section 3, we introduce the Weyl operator  $M^A(z)$  for  $-\Delta + q$  in  $L^2(\Omega_R)$ , subject to Neumann condition on  $S_1$  and nonlocal condition of type  $\gamma_R \partial f / \partial n = A \gamma_R f$  on  $S_R$ .  $M^A(z)$  is bounded (even compact) from  $L^2(S_1)$  to  $L^2(S_1)$ , and analytic in  $z$  for  $z \in \mathbb{C}^+$ , with  $\text{Im} M^A(z) \geq 0$ .  $\|M^A(z)\|$  is bounded uniformly as the operator  $A$  is varied. We prove an identity  $M^A(z) = \gamma_1 (T^A - z)^{-1} \gamma_1^*$ , thus expressing the  $M$  operator in terms of the resolvent of the operator  $T^A = -\Delta + q(x)$ , subject to the given boundary conditions, and of the trace operator  $\gamma_1$  associated to  $S_1$ . We also define Weyl operators  $M_B^A(z)$  for  $-\Delta + q$  in  $L^2(\Omega_R)$ , subject to conditions on both bounding surfaces ( $B$ -type condition on  $S_1$  and  $A$ -type condition on  $S_R$ ), and we prove identities, bounds and basic properties of these operators, including norm continuity in  $A$ .

In Section 4, we define the Weyl operator  $M_B(z)$  for  $-\Delta + q$  in  $L^2(\Omega)$ , where  $\Omega = \{x : |x| > 1\}$ , and prove the strong convergence of  $M_B^A(z)$  to  $M_B(z)$  in the limit as  $R \rightarrow \infty$ . (This is an analogue of the result that  $m^N(z) \rightarrow m(z)$  in the one-dimensional Weyl theory.) We then introduce a Weyl operator  $m_0(z)$  for  $-\Delta + q$  in  $L^2(\Omega)$ , subject to Dirichlet condition on  $S_1$ ;  $m_0(z)$  is the inverse of  $-M_0(z)$  (where  $M_0(z)$  is the operator  $M_B(z)$  for  $B=0$ ) and is the most direct analogue of the Weyl–Titchmarsh function  $m(z)$  for second-order ordinary differential operators on a semi-infinite interval. An identity  $m_0(z) = (\gamma_1 \partial / \partial n)(T_{D_1} - z)^{-1}(\gamma_1 \partial / \partial n)^*$  is proved, expressing  $m_0$  in terms of the resolvent of the operator  $T_{D_1} = -\Delta + q$ , subject to Dirichlet boundary conditions on  $S_1$ ; this identity is a higher dimensional analogue of formulae known to hold in the one-dimensional problem [2]. The Weyl operator  $m_0(z)$  is unbounded from  $L^2(S_1)$  to  $L^2(S_1)$ , but bounded from  $H^1(S_1)$  to  $L^2(S_1)$ . We may refer to  $M_0(z)$  as the Neumann  $M$  operator and  $m_0(z)$  as the Dirichlet  $M$  operator for the exterior problem.

Finally, in Section 5, we define the Weyl operator  $\mathfrak{M}(z)$  for  $T = -\Delta + q$  in  $L^2(\mathbb{R}^3)$ , in terms of a version of the Steklov–Poincaré operator for the surface  $S_1$ . We prove an identity expressing  $\mathfrak{M}$  in terms of the resolvent of  $T$ , and the inverse  $\mathfrak{m}$  of  $\mathfrak{M}$  in terms of the resolvent of the domain decomposed operator  $\mathcal{F} = -\Delta + q$ , with Dirichlet boundary conditions on  $S_1$ . Both  $\mathfrak{M}(z)$  and  $\mathfrak{m}(z)$  can be expressed algebraically in terms of interior and exterior  $M$  operators, in parallel with similar results which can be obtained by domain decomposition methods in the case of ordinary differential operators.

The extension of Weyl theory which we present here provides a theoretical framework for the analysis of Schrödinger operators in  $L^2(\mathbb{R}^3)$ , as well as exterior and interior boundary value problems. A number of authors, including Brasche et al. [8] and Naboko [17] have shown how the study of boundary behaviour in  $z$  of Weyl operators can be used as a tool in spectral analysis. A further result, by the present authors, is the discovery of a higher dimensional analogue of the Weyl family of nesting circles, in which solutions of the Schrödinger equation at complex spectral parameter are characterized as belonging to a nesting family of convex subsets of Hilbert space. These, and other related developments, will be the subject of a forthcoming paper.

## 2. Extension maps

For  $R > 0$  let  $S_R = \{x \in \mathbb{R}^3 : |x| = R\}$  be the sphere of radius  $R$  centred at  $x=0$ , and for  $R \in (1, \infty]$  let  $\Omega_R$  be the region  $\Omega_R = \{x \in \mathbb{R}^3 : 1 < |x| < R\}$ . We shall frequently denote the unbounded region  $\Omega_\infty$  simply by  $\Omega$ . We write  $\|\cdot\|_{S_R}$  for the norm in  $L^2(S_R)$  and  $\|\cdot\|_{\Omega_R}$  for that in  $L^2(\Omega_R)$ .

If  $\Delta$  denotes the Laplacian and  $g$  is a complex function on  $\Omega_R$ , then  $\Delta g$  is well defined as a distribution on  $C_0^\infty(\Omega_R)$ . We also denote by  $\partial g / \partial n$  the radial derivative (in the sense of distributions) of  $g$ , in the direction of increasing radial coordinate. We say that  $g$  has  $L^2$  boundary value on  $S_1$  if  $\lim_{\varepsilon \rightarrow 0^+} g(x + \varepsilon n_x)$  exists as a strong limit in  $L^2(S_1)$ , where  $n_x (\equiv x)$  is the outward normal to  $S_1$  at the point  $x \in S_1$ . Similarly, if  $1 < R < \infty$ ,  $g$  has  $L^2$  boundary value on  $S_R$  if  $\lim_{\varepsilon \rightarrow 0^+} g(x - \varepsilon n_x)$  exists as a strong limit in  $L^2(S_R)$ , with  $x \in S_R$  and  $n_x = x/|x|$ .

Following [5,13], define  $\mathcal{D}_1(\Omega_R)$  to be the set of functions  $g : \Omega_R \rightarrow \mathbb{C}$  such that

- (i)  $g$  and  $\Delta g$  belong to  $L^2(\Omega_R)$ ,
- (ii) both  $g$  and  $\partial g / \partial n$  have  $L^2$  boundary values on  $S_1$  as well as on  $S_R$  if  $R < \infty$ .

We note the inclusions  $H^2(\Omega_R) \subset \mathcal{D}_1(\Omega_R) \subset H^1(\Omega_R)$ . Each of these is a proper inclusion, and in fact one may go further [6] and show that  $\mathcal{D}_1(\Omega_R) \subset H^{3/2}(\Omega_R)$ .

Condition (i) characterizes the domain of the maximal Laplacian operator in  $L^2(\Omega_R)$ , that is the domain of the adjoint of the operator  $\Delta$  defined on  $C_0^\infty(\Omega_R)$ . This domain is much larger than  $\mathcal{D}_1(\Omega_R)$  (functions  $g$  in the domain of the maximal Laplacian need not have  $L^2$  boundary values on the boundary of  $\Omega_R$ , either for  $g$  or for  $\partial g/\partial n$ ). However, if  $g$  satisfies (i), then  $g$  is locally of class  $H^2$ , in the sense that  $g \in H^2(G)$  for every open set  $G$  whose closure lies in  $\Omega_R$ , where  $H^2(G)$  is the Sobolev space  $W^{2,2}(G)$  [1].

Condition (ii) involves the Sobolev trace operators  $\gamma_\rho$  (restriction to the sphere  $S_\rho$  of functions defined on  $\Omega_R$ ,  $1 \leq \rho \leq R < \infty$ ). For any  $s > \frac{1}{2}$ ,  $\gamma_\rho$  is bounded as an operator from  $H^s(\Omega_R)$  to  $H^{s-1/2}(S_\rho)$  and compact from  $H^s(\Omega_R)$  to  $H^{s-1/2-\varepsilon}(S_\rho)$  if  $\varepsilon > 0$ . Since  $\mathcal{D}_1(\Omega_R) \subset H^1(\Omega_R)$ , the  $L^2$ -boundary values on  $S_1$  and  $S_R$  of  $g \in \mathcal{D}_1(\Omega_R)$  are just  $\gamma_1 g$  and  $\gamma_R g$ , respectively. The inclusion  $\mathcal{D}_1(\Omega_R) \subset H^{3/2}(\Omega_R)$  shows that  $\partial g/\partial n \in H^{1/2}(\Omega_R)$  if  $g \in \mathcal{D}_1(\Omega_R)$ . We shall continue to use the notation  $\gamma_1 \partial g/\partial n$  for the  $L^2$ -boundary values of  $\partial g/\partial n$  in this case, even though the Sobolev trace operators  $\gamma_\rho$  are not defined on the whole of  $H^{1/2}(\Omega_R)$ .

If  $\partial g/\partial n$  has an  $L^2$  boundary value on  $S_1$  (or  $S_R$ ), then a simple argument implies the existence of a boundary value for  $g$  as well. Hence it would be sufficient, in (ii) above, to require only that  $\partial g/\partial n$  have  $L^2$  boundary values. One can also show (though we shall not require this result) that  $\partial g/\partial x_i$  ( $i = 1, 2, 3$ ) has  $L^2$ -boundary values for all  $g \in \mathcal{D}_1(\Omega_R)$ .

**Remark 1.** If  $R = \infty$  there is no need to require in (ii) the existence of the  $L^2$  boundary values at infinity. In fact if  $g$  and  $\Delta g$  belong to  $L^2(\Omega)$  (hence  $g \in H^2(\{x : |x| > 2\})$ ), then  $\|\gamma_\rho g\|_{S_\rho}$  and  $\|\gamma_\rho \partial g/\partial n\|_{S_\rho}$  converge to zero as  $\rho \rightarrow \infty$  (this follows from the fact that, for  $h \in H^1(\mathbb{R}^3)$  one has  $\lim_{\rho \rightarrow \infty} \|\gamma_\rho h\|_{S_\rho} = 0$ ; the preceding relation is trivial for  $h \in C_0^\infty(\mathbb{R}^3)$ , and for general  $h$  in  $H^1(\mathbb{R}^3)$  it follows from the density of  $C_0^\infty(\mathbb{R}^3)$  in  $H^1(\mathbb{R}^3)$  and the following bound on  $\gamma_\rho$  as an operator  $H^1(\mathbb{R}^3) \rightarrow L^2(S_\rho)$  (see e.g., Eq. (5) of [3]):

$$\sup_{\rho \geq 1} \|\gamma_\rho\|_{H^1(\mathbb{R}^3) \rightarrow L^2(S_\rho)} \leq 4. \tag{2.1}$$

It will be convenient to use the following norm on  $\mathcal{D}_1(\Omega_R)$ :

$$\|f\|_{\mathcal{D}_1} = \|f\|_{\Omega_R} + \|\Delta f\|_{\Omega_R} + \left\| \gamma_1 \frac{\partial f}{\partial n} \right\|_{S_1} + \left\| \gamma_R \frac{\partial f}{\partial n} \right\|_{S_R}, \tag{2.2}$$

with  $\|\gamma_R \partial f/\partial n\|_{S_R} = 0$  for  $R = \infty$ .

The construction of operators  $M(z)$  in Section 3, as well as subsequent estimates of convergence, are greatly facilitated by the use of *extension maps*. Typically, an extension map on  $L^2(S_1)$  will be a right inverse of the mapping which takes  $g \in \mathcal{D}_1(\Omega_R)$  into  $\gamma_1 \partial g/\partial n \in L^2(S_1)$ . The existence of such extension maps is known (see for example [6]). Here we will need to carry out rather explicit constructions of extension maps appropriate to spherical surfaces, for which in particular precise norm estimates can be determined in terms of the radial parameter  $R$ . An indication of the kind of result that is needed is provided by the following lemma. Further on, in Lemmas 2–4, we present other results on extension maps that will be used in certain later arguments.

**Lemma 1.** *Let  $R \in [2, \infty]$ .*

(a) *For each  $\beta \geq 0$  there exists a bounded linear map  $E_1^{(\beta)} : L^2(S_1) \rightarrow \mathcal{D}_1(\Omega_R)$  such that  $E_1^{(\beta)}v = 0$  in the region  $\{x : |x| \geq 2\}$  and  $\gamma_1 \partial/\partial n E_1^{(\beta)}v = v$  for each  $v \in L^2(S_1)$ , and such that the following norm estimates are satisfied for some constant  $c_1$ :*

$$\|E_1^{(\beta)}\|_{L^2(S_1) \rightarrow \mathcal{D}_1(\Omega_R)} \leq c_1 \sqrt{1 + \beta} \quad \forall R \in [2, \infty], \tag{2.3}$$

$$\|\gamma_1 E_1^{(\beta)}\| \equiv \|\gamma_1 E_1^{(\beta)}\|_{L^2(S_1) \rightarrow L^2(S_1)} \leq \frac{1}{1 + \beta}. \tag{2.4}$$

$E_1^{(\beta)}$  is compact as an operator  $L^2(S_1) \rightarrow L^2(\Omega_R)$ , with

$$\|E_1^{(\beta)}\|_{L^2(S_1) \rightarrow L^2(\Omega_R)} \leq 1. \tag{2.5}$$

(b) *For each  $\beta \geq 0$ ,  $\gamma_1 E_1^{(\beta)}$  maps  $L^2(S_1)$  into  $H^1(S_1)$  and is compact as an operator from  $L^2(S_1)$  to  $H^s(S_1)$  for  $0 \leq s < 1$ .*

(c)  $Q := \gamma_1 E_1^{(0)}$  maps  $L^2(S_1)$  onto  $H^1(S_1)$ .  $Q$  is invertible, and its inverse  $Q^{-1}$  is bounded as an operator from  $H^1(S_1)$  to  $L^2(S_1)$ .

**Proof.** The surface spherical harmonics  $\{Y_{\ell m}\}$ , defined on the sphere  $S_1$ , form an orthonormal basis of  $L^2(S_1)$  (here  $\ell = 0, 1, 2, \dots$  and  $m$  is an integer running from  $-\ell$  to  $+\ell$ ). For  $v \in L^2(S_1)$  we write  $v = \sum_{\ell m} a_{\ell m} Y_{\ell m}$ , so that  $\|v\|_{S_1}^2 = \sum_{\ell m} |a_{\ell m}|^2$ . We take  $E_1^{(\beta)}$  of the form

$$E_1^{(\beta)}v = \sum_{\ell m} a_{\ell m} \psi_{\ell m}^{(\beta)}(x) \tag{2.6}$$

for  $x \in \Omega_R$ , where the functions  $\psi_{\ell m}^{(\beta)}$  are to be defined. The general idea is to make  $\psi_{\ell m}^{(\beta)}$  an approximation to a solution of the Laplace equation in  $\Omega_R$ . Explicitly we take

$$\psi_{\ell m}^{(\beta)}(x) = \frac{\psi_{\ell}^{(\beta)}(|x|)}{|x|} Y_{\ell m}(\omega), \tag{2.7}$$

where now  $\omega = x/|x|$  and  $\psi_{\ell}^{(\beta)}$  is given as a function of  $r = |x|$  for  $1 \leq r \leq R$  by

$$\psi_{\ell}^{(\beta)}(r) = \begin{cases} -\eta(r)r^{-\ell}/(1 + \ell) & \text{for } \ell \geq \beta, \\ \eta(r)(r^{1-\ell} - r^{-\ell}) & \text{for } \ell < \beta. \end{cases} \tag{2.8}$$

Here  $\eta : \mathbb{R} \rightarrow \mathbb{R}$  is a smooth nonincreasing function satisfying  $\eta(t) = 1$  for  $t \leq \frac{5}{4}$  and  $\eta(t) = 0$  for  $t \geq \frac{7}{4}$ , so that the support of  $\psi_{\ell m}^{(\beta)}$  is contained in  $\Omega_2$ .

Noting that  $|\psi_{\ell}^{(\beta)}(r)| \leq r^{-\ell}$ , we have

$$\|\psi_{\ell m}^{(\beta)}\|_{\Omega_R}^2 = \int_1^R |\psi_{\ell}^{(\beta)}(r)|^2 dr \leq \int_1^R r^{-2\ell} dr \leq \frac{1}{|2\ell - 1|} \leq 1. \tag{2.9}$$

Hence

$$\|E_1^{(\beta)}v\|_{\Omega_R}^2 = \sum_{\ell m} |a_{\ell m}|^2 \|\psi_{\ell m}^{(\beta)}\|_{\Omega_R}^2 \leq \|v\|_{S_1}^2 \tag{2.10}$$

which implies (2.5). The compactness of  $E_1^{(\beta)}$  as a mapping from  $L^2(S_1)$  to  $L^2(\Omega_R)$  is a consequence of the fact that  $\|\psi_{\ell m}^{(\beta)}\|_{\Omega_R}^2 = \mathcal{O}(1/2\ell)$  for  $\ell \rightarrow \infty$ .

For  $\ell \geq \beta$  we have

$$\begin{aligned} \|\Delta\psi_{\ell m}^{(\beta)}\|_{\Omega_R}^2 &= \int_1^R \left[ \frac{d^2\psi_{\ell}^{(\beta)}(r)}{dr^2} - \frac{\ell(\ell+1)}{r^2} \psi_{\ell}^{(\beta)}(r) \right]^2 dr \\ &= \int_1^2 \frac{[\eta''(r) - 2\ell\eta'(r)/r]^2}{(1+\ell)^2} r^{-2\ell} dr \leq \text{const} \int_1^2 r^{-2\ell} dr \leq \frac{\text{const}}{|2\ell-1|} \leq \text{const}. \end{aligned}$$

For  $\ell < \beta$  we find

$$\left| \frac{d^2\psi_{\ell}^{(\beta)}(r)}{dr^2} - \frac{\ell(\ell+1)}{r^2} \psi_{\ell}^{(\beta)}(r) \right| = \left| [(r-1)\eta]'' - \frac{2\ell}{r} [(r-1)\eta]' \right| r^{-\ell} \leq \text{const}(\ell+1)r^{-\ell}$$

which leads to the bound

$$\|\Delta\psi_{\ell m}^{(\beta)}\|_{\Omega_R}^2 \leq \text{const} \frac{(\ell+1)^2}{|2\ell-1|} \leq \text{const}(\beta+1).$$

So

$$\|\Delta E_1^{(\beta)}v\|_{\Omega_R}^2 = \sum_{\ell m} |a_{\ell m}|^2 \|\Delta\psi_{\ell m}^{(\beta)}\|_{\Omega_R}^2 \leq \text{const}(\beta+1) \|v\|_{S_1}^2. \tag{2.11}$$

The existence of an  $L^2$  boundary value on  $S_R$  for  $\partial/\partial n E_1^{(\beta)}v$  is trivial, since  $E_1^{(\beta)}v$  vanishes in a neighbourhood of  $S_R$  ( $R \geq 2$ ). To see that  $\partial/\partial n E_1^{(\beta)}v$  has  $v$  as its  $L^2$  boundary value on  $S_1$ , we observe that

$$\left\| \gamma_{\rho} \frac{\partial}{\partial n} E_1^{(\beta)}v - v \right\|_{S_1}^2 = \sum_{\ell m} \left| \frac{(\beta)'(\rho)}{\rho} - \frac{(\beta)(\rho)}{\rho^2} - 1 \right|^2 |a_{\ell m}|^2 \equiv \sum_{\ell m} |\Phi_{\ell}^{(\beta)}(\rho)| |a_{\ell m}|^2. \tag{2.12}$$

The convergence of this quantity to zero, as  $\rho \rightarrow 1+$ , is obtained from the Lebesgue dominated convergence theorem by observing that  $\lim_{\rho \rightarrow 1+} \Phi_{\ell}^{(\beta)} = 0$  for each  $\ell$  and that  $|\Phi_{\ell}^{(\beta)}| \leq 1 + \beta$  for every  $\ell$  and for  $1 < \rho < \frac{5}{4}$ .

The estimates given above lead to bound (2.3), whereas (2.4) is easily obtained by noting that  $|\psi_{\ell}^{(\beta)}(1)| = 1/(\ell+1) \leq 1/(\beta+1)$  for  $\ell \geq \beta$  and that  $\psi_{\ell}^{(\beta)}(1) = 0$  for  $\ell < \beta$ . From the standard characterization of  $H^1(S_1)$  (see for example [15]) and from the fact that  $\psi_{\ell}^{(\beta)}(1) = \mathcal{O}(\ell^{-1})$  for  $\ell \rightarrow \infty$ , one gets that  $\gamma_1 E_1^{(\beta)}$  maps boundedly from  $L^2(S_1)$  to  $H^1(S_1)$ . The compactness of the embedding  $H^1(S_1) \rightarrow H^s(S_1)$  ( $0 \leq s < 1$ ) then implies the second result of (b).

In the case  $\beta = 0$  we have  $\psi_{\ell}^{(0)}(1) = -1/(1+\ell)$  for each  $\ell \geq 0$ , so that

$$\gamma_1 E_1^{(0)}v = - \sum_{\ell m} \frac{a_{\ell m}}{\ell+1} Y_{\ell m}. \tag{2.13}$$

The assertions made in (c) are straightforward consequences of (2.13).  $\square$

**Remark 2.** Lemma 1(a) shows that, given any  $v \in L^2(S_1)$ , there exists  $g \in \mathcal{D}_1(\Omega_R)$  for which  $\gamma_1 \partial g / \partial n = v$ . From Lemma 1(c) one sees that, given any  $w \in H^1(S_1)$ , there exists  $g \in \mathcal{D}_1(\Omega_R)$  for which  $\gamma_1 g = w$ .

The map  $F$  from  $w$  to  $g$  is given by  $F = E_1^{(0)}Q^{-1}$ , where  $Q = \gamma_1 E_1^{(0)}$ .  $F$  is bounded from  $H^1(S_1)$  to  $\mathcal{D}_1(\Omega_R)$ .

In the case  $\beta \neq 0$ ,  $\gamma_1 E_1^{(\beta)}$  maps boundedly into, but not onto,  $H^1(S_1)$ . The main purpose of the construction of the one-parameter family  $\{E_1^{(\beta)}\}$  of extension maps is to show that a bounded extension map  $E_1^{(\beta)}$  can be found for which  $\gamma_1 E_1^{(\beta)}$  has arbitrarily small norm as an operator from  $L^2(S_1)$  to  $L^2(S_1)$ . This consequence of Lemma 1 will be needed in Lemma 2.

In later developments we shall need a generalization of the extension operators obtained in Lemma 1, more precisely bounded mappings:  $F_1 : L^2(S_1) \rightarrow \mathcal{D}_1(\Omega_R)$  satisfying  $(\gamma_1 \partial/\partial n - B\gamma_1)F_1 v = v$  for all  $v \in L^2(S_1)$ , where  $B$  is a fixed bounded operator in  $L^2(S_1)$ . The operators given in Lemma 1 correspond to the special case  $B = 0$ .

**Lemma 2.** *Let  $B$  be a bounded operator in  $L^2(S_1)$  and  $R \in [2, \infty]$ . There exists a bounded linear map  $F_1 : L^2(S_1) \rightarrow \mathcal{D}_1(\Omega_R)$  such that  $F_1 v = 0$  in the region  $\{x : |x| \geq 2\}$  and  $(\gamma_1 \partial/\partial n - B\gamma_1)F_1 v = v$  for each  $v \in L^2(S_1)$ .  $F_1$  is compact as an operator  $L^2(S_1) \rightarrow L^2(\Omega_R)$ , and  $\gamma_1 F_1$  is compact as an operator  $L^2(S_1) \rightarrow H^s(S_1)$  for  $0 \leq s < 1$ . Furthermore, the following norm estimates are satisfied, for some constant  $c$  independent of  $R$  and of  $B$ :*

$$\|F_1\|_{L^2(S_1) \rightarrow \mathcal{D}_1(\Omega_R)} \leq c\sqrt{1 + \|B\|} \quad \forall R \in [2, \infty], \tag{2.14}$$

$$\|F_1\|_{L^2(S_1) \rightarrow L^2(\Omega_R)} \leq 2, \tag{2.15}$$

$$\|\gamma_1 F_1\|_{L^2(S_1) \rightarrow L^2(S_1)} \leq 2. \tag{2.16}$$

**Proof.** Let  $Q_1 = \gamma_1 E_1^{(\beta)}$  with  $\beta = 2\|B\|$  and with  $E_1^{(\beta)}$  as in Lemma 1. By (2.4) we have  $\|BQ_1\|_{L^2(S_1) \rightarrow L^2(S_1)} \leq \|B\|(1 + 2\|B\|)^{-1} \leq \frac{1}{2}$ , so that  $I - BQ_1$  is invertible (here  $I$  denotes the identity operator in  $L^2(S_1)$ ). We set  $F_1 = E_1^{(\beta)}(I - BQ_1)^{-1}$ , with again the choice  $\beta = 2\|B\|$ . Since  $\gamma_1 \partial/\partial n E_1^{(\beta)} u = u$  for arbitrary  $u \in L^2(S_1)$ , we have, for arbitrary  $v \in L^2(S_1)$ :

$$\gamma_1 \frac{\partial}{\partial n} F_1 v = \gamma_1 \frac{\partial}{\partial n} E_1^{(\beta)} (I - BQ_1)^{-1} v = (I - BQ_1)^{-1} v,$$

whereas  $B\gamma_1 F_1 v = BQ_1(I - BQ_1)^{-1} v$ . These two equations imply that  $(\gamma_1 \partial/\partial n - B\gamma_1)F_1 v = v$ . The remaining statements of the lemma are straightforward consequences of the results of Lemma 1.  $\square$

Analogous results to those of Lemmas 1 and 2 may be obtained in the case of extension operators from  $L^2(S_R)$  to  $\mathcal{D}_1(\Omega_R)$ . Here it will be important to derive operator norm bounds which are independent of  $R$ . We summarize the main conclusions of this analysis in the following two lemmas.

**Lemma 3.** *For each  $R \in [2, \infty)$  there exists a bounded extension map  $E_R : L^2(S_R) \rightarrow \mathcal{D}_1(\Omega_R)$  satisfying  $E_R v = 0$  near  $S_1$  and  $\gamma_R \partial/\partial n E_R v = v$  for all  $v \in L^2(S_R)$ , and such that the norms of  $E_R : L^2(S_R) \rightarrow \mathcal{D}_1(\Omega_R)$  and of  $\gamma_R E_R : L^2(S_R) \rightarrow L^2(S_R)$  are bounded by a constant which is independent of  $R$ .*

**Proof.** We proceed along similar lines to the proof of Lemma 1. For  $v \in L^2(S_R)$  we write  $v = \sum_{\ell m} a_{\ell m} Y_{\ell m}$ , where  $\|v\|_{S_R}^2 = \int_{S_R} |v(x)|^2 R^2 d\omega = R^2 \sum_{\ell m} |a_{\ell m}|^2$ . Now define  $E_R$  by

$$(E_R v)(x) = \sum_{\ell m} a_{\ell m} \Psi_{\ell m}(x)$$

for  $x \in \Omega_R$ . We take

$$\Psi_{\ell m}(x) = \frac{\psi_\ell^R(|x|)}{|x|} Y_{\ell m}(\omega),$$

where  $\omega = x/|x|$  and  $\psi_\ell^R$  is given as a function of  $r = |x|$ , for  $1 \leq r \leq R$  and  $R \geq 2$ , by

$$\psi_\ell^R(r) = \begin{cases} \eta(r) \frac{R^2}{\ell} \left(\frac{r}{R}\right)^{\ell+1} & \text{for } \ell > R, \\ R(r-R)\phi(R-r) & \text{for } \ell \leq R. \end{cases} \tag{2.17}$$

Here  $\eta : \mathbb{R} \rightarrow \mathbb{R}$  is a smooth nondecreasing function satisfying  $\eta(y) = 0$  for  $y \leq \frac{5}{4}$  and  $\eta(y) = 1$  for  $y \geq \frac{7}{4}$ , and  $\phi(y) = \eta(2-y)$ .

In the case  $\ell > R$ , the  $L^2(\Omega_R)$  norm of  $\Psi_{\ell m}$  is given by

$$\begin{aligned} \|\Psi_{\ell m}\|_{\Omega_R}^2 &= \int_1^R |\Psi_\ell^R(r)|^2 dr \leq \frac{R^4}{\ell^2} \int_1^R \left(\frac{r}{R}\right)^{2\ell+2} dr \\ &\leq \frac{R^5}{\ell^2(2\ell+3)} < \frac{R^2}{2}. \end{aligned}$$

For  $\ell \leq R$  the support of  $\Psi_{\ell m}$  is contained in the region  $\{x : R-1 \leq |x| \leq R\}$ , and again one finds  $\|\Psi_{\ell m}\|_{\Omega_R}^2 < R^2/2$ .

For  $\ell > R$ , noting that the support of  $\eta'$  is contained in interval  $(1,2)$ , we have

$$\begin{aligned} \|\Delta \Psi_{\ell m}\|_{\Omega_R}^2 &= \int_1^2 \frac{R^2}{\ell^2} \left(\frac{r}{R}\right)^{2\ell} [r\eta''(r) + 2(\ell+1)\eta'(r)]^2 dr \\ &\leq \text{const} \frac{R^3}{2\ell+1} \leq \text{const} R^2. \end{aligned}$$

In the case  $\ell \leq R$  one obtains

$$\begin{aligned} \|\Delta \Psi_{\ell m}\|_{\Omega_R}^2 &= R^2 \int_{R-1}^R \left[ (r-R)\phi''(R-r) - 2\phi'(R-r) - \frac{\ell(\ell+1)}{r^2}(r-R)\phi(R-r) \right]^2 dr \\ &\leq \text{const} R^2. \end{aligned}$$

The extension property  $\gamma_R \hat{\partial} / \partial n E_R v = v$  follows from the fact that  $d/dr[\psi_\ell^R(r)/r] = 1$  at  $r=R$ , and  $E_R v$  vanishes in a neighbourhood of  $S_1$ . Hence, using expression (2.2) for the norm on  $\mathcal{D}_1(\Omega_R)$ , we can estimate the norm of  $E_R$  as a mapping from  $L^2(S_R)$  to  $\mathcal{D}_1(\Omega_R)$  and deduce that indeed this norm is bounded by a constant independent of  $R$ .

The bound on the norm of  $\gamma_R E_R : L^2(S_R) \rightarrow L^2(S_R)$  follows on using  $|\psi_\ell^R(r)/r| \leq 1$  at  $r=R$ .  $\square$

Just as in the case of Lemma 1, the norm of  $\gamma_R E_R$  may be taken to be arbitrarily small, as shown by the following result.

**Corollary.** For each  $R \in [2, \infty)$  there exists a one-parameter family  $\{E_R^{(\beta)}\}$ ,  $\beta \geq 1$ , of bounded extension maps from  $L^2(S_R)$  to  $\mathcal{D}_1(\Omega_R)$  satisfying  $E_R^{(\beta)}v = 0$  near  $S_1$  and  $\gamma_R \partial/\partial n E_R v = v$  for each  $v \in L^2(S_R)$  as well as the following norm estimates (with  $c$  independent of  $R$ ):

$$\|E_R^{(\beta)}\|_{L^2(S_R) \rightarrow \mathcal{D}_1(\Omega_R)} \leq c\beta^2, \tag{2.18}$$

$$\|E_R^{(\beta)}\|_{L^2(S_R) \rightarrow L^2(\Omega_R)} \leq 1, \tag{2.19}$$

$$\|\gamma_R E_R^{(\beta)}\| = \|\gamma_R E_R^{(\beta)}\|_{L^2(S_R) \rightarrow L^2(S_R)} \leq \frac{1}{\beta}. \tag{2.20}$$

The proof proceeds as in the proof of Lemma 2, except that, in definition (2.17) of  $\psi_\ell^R$ , we replace the criteria  $\ell > R$  and  $\ell \leq R$  by  $\ell > \beta R$  and  $\ell \leq \beta R$ , respectively.

**Lemma 4.** Let  $R \in [2, \infty)$  and  $A$  a bounded operator in  $L^2(S_R)$ . There exists a bounded linear map  $F_R : L^2(S_R) \rightarrow \mathcal{D}_1(\Omega_R)$  such that  $F_R v = 0$  near  $S_1$  and  $(\gamma_R \partial/\partial n - A\gamma_R)F_R v = v$  for all  $v \in L^2(S_R)$  and such that, for some constant  $c$  independent both of  $A$  and of  $R$ :

$$\|F_R\|_{L^2(S_R) \rightarrow \mathcal{D}_1(\Omega_R)} \leq c(1 + \|A\|^2), \tag{2.21}$$

$$\|F_R\|_{L^2(S_R) \rightarrow L^2(\Omega_R)} \leq 2, \tag{2.22}$$

$$\|\gamma_R F_R\|_{L^2(S_R) \rightarrow L^2(S_R)} \leq 2. \tag{2.23}$$

**Proof.** Let  $Q_R = \gamma_R E_R^{(\beta)}$  with  $\beta = 1 + 2\|A\|$  and  $E_R^{(\beta)}$  as in the corollary to Lemma 3. Then, by (2.20):

$$\|AQ_R\|_{L^2(S_R) \rightarrow L^2(S_R)} \leq \|A\| \frac{1}{1 + 2\|A\|} < \frac{1}{2}.$$

By proceeding in analogy with the proof of Lemma 2, one finds that  $F_R := E_R^{(\beta)}(I - AQ_R)^{-1}$  has the required properties.  $\square$

### 3. $M$ operators for exterior bounded regions

To define  $M(z)$  for the region  $\Omega_R = \{x : 1 < |x| < R\}$ , with  $2 \leq R < \infty$ , we impose a boundary condition on the outer boundary surface  $S_R$ . Let  $A$  be a bounded operator on  $L^2(S_R)$ , having positive imaginary part in the sense that  $(2i)^{-1}(A - A^*) \equiv \text{Im } A \geq 0$ , where  $A^*$  is the adjoint of  $A$ .

A function  $g \in \mathcal{D}_1(\Omega_R)$  is said to satisfy the  $A$  boundary condition on  $S_R$  if  $\gamma_R \partial g/\partial n = A\gamma_R g$ . As in the case of the function  $m(z)$  in one dimension, the operator  $M(z)$  will be defined in terms of the boundary behaviour of appropriate solutions of the Schrödinger equation with complex spectral parameter  $z$ . Here we rely on the following lemma, where we suppose for simplicity that  $q$  is bounded on  $\Omega_R$ , and real.

**Lemma 5.** Suppose  $\text{Im } z > 0$ , and let  $A$  be bounded on  $L^2(S_R)$ , with positive imaginary part. Then given arbitrary  $v \in L^2(S_1)$ , there exists a unique function  $f \in \mathcal{D}_1(\Omega_R)$  satisfying

$$-\Delta f + qf - zf = 0 \tag{3.1}$$

together with the boundary conditions

$$\gamma_R \frac{\partial f}{\partial n} = A\gamma_R f, \tag{3.2}$$

$$\gamma_1 \frac{\partial f}{\partial n} = v. \tag{3.3}$$

**Proof.** Note that, for  $f \in \mathcal{D}_1(\Omega_R)$ , the fact that  $f$  is locally  $H^2$  implies that one can interpret (3.1) in the sense of distributions. However, in general the solution of (3.1)–(3.3) need not belong to  $H^2(\Omega_R)$ . We shall construct explicitly the solution  $f$  of the Schrödinger equation, in terms of a Schrödinger operator  $T^A$  acting in  $L^2(S_R)$ .

(i) We define  $T^A = -\Delta + q$ , with domain in  $L^2(\Omega_R)$  given by  $D(T^A) = \{g \in \mathcal{D}_1(\Omega_R) : \gamma_1 \partial g / \partial n = 0, \gamma_R \partial g / \partial n = A\gamma_R g\}$ . Thus  $T^A$  is defined subject to Neumann boundary condition on  $S_1$  and  $A$  boundary condition on  $S_R$ . The results of Beals and others, [6,5,13], which allow  $A$ -type boundary conditions, imply that  $T^A$  is a closed operator in  $L^2(S_R)$ , with adjoint given by  $(T^A)^* = T^{A^*}$ , where  $T^{A^*}$  is defined as for  $T^A$ , but with  $A^*$  boundary condition  $\gamma_R \partial g / \partial n = A^* \gamma_R g$ .

Now with  $h \in D(T^A)$ , integrate over  $\Omega_R$  the identity

$$\nabla \cdot (\bar{h} \nabla h - h \nabla \bar{h}) = \bar{h} \Delta h - h \Delta \bar{h},$$

and apply the divergence theorem. (Since  $h \in H^2_{\text{loc}}(\Omega_R)$ , we can apply the divergence theorem first of all for the region  $1 + \varepsilon < |x| < R - \varepsilon$ , and then take the limit  $\varepsilon \rightarrow +0$ .) Noting that  $h$  and  $\partial h / \partial n$  have  $L^2$  boundary values on  $S_1$  and  $S_R$ , and using the boundary conditions for  $h$  on these two surfaces, this leads to

$$\begin{aligned} \text{Im} \langle (T^A - z)h, h \rangle_{\Omega_R} &= \text{Im } z \|h\|_{\Omega_R}^2 + \frac{1}{2i} \int_{S_R} \left( \bar{h} \frac{\partial h}{\partial n} - h \frac{\partial \bar{h}}{\partial n} \right) dS - \frac{1}{2i} \int_{S_1} \left( \bar{h} \frac{\partial h}{\partial n} - h \frac{\partial \bar{h}}{\partial n} \right) dS \\ &= \text{Im } z \|h\|_{\Omega_R}^2 + \frac{1}{2i} \langle \gamma_R h, (A - A^*) \gamma_R h \rangle_{S_R} \geq \text{Im } z \|h\|_{\Omega_R}^2. \end{aligned} \tag{3.4}$$

In particular  $T^A$  has no eigenvalue in the upper half-plane.

A similar argument shows that  $T^{A^*}$  has no eigenvalue in the lower half-plane. Hence the null space of  $(T^A)^* - \bar{z}$  is  $\{0\}$ , so that the range of  $T^A - z$  is dense in  $L^2(\Omega_R)$ . Since  $T^A$  is closed, the resolvent operator  $(T^A - z)^{-1}$  is defined on the whole space  $L^2(\Omega_R)$  and satisfies  $\|(T^A - z)^{-1}\| \leq 1/\text{Im } z$  as a consequence of (3.4) (here the norm of the resolvent is an operator norm on  $L^2(\Omega_R)$ ).

(ii) Given any  $v \in L^2(S_1)$ , let  $g = E_1^{(0)} v \in \mathcal{D}_1(\Omega_R)$ , where  $E_1^{(0)}$  is as in Lemma 1. Then  $\Delta g, qg \in L^2(\Omega_R)$ , and  $\gamma_1 \partial g / \partial n = v, \gamma_R g = \gamma_R \partial g / \partial n = 0$  (since  $g$  vanishes in a neighbourhood of  $S_R$ ). We define

$$f = -(T^A - z)^{-1}(-\Delta g + qg - zg) + g. \tag{3.5}$$

Then

$$(-\Delta + q - z)f = -(T^A - z)(T^A - z)^{-1}(-\Delta g + qg - zg) + (-\Delta g + qg - zg) = 0.$$

For any  $h \in L^2(\Omega_R)$ , both  $(T^A - z)^{-1}h$  and  $g$  (trivially) satisfy the  $A$  boundary condition on  $S_R$ ; hence so too does  $f$ . Since  $(T^A - z)^{-1}h$  will satisfy the Neumann condition on  $S_1$ , we have  $\gamma_1 \partial f / \partial n = \gamma_1 \partial g / \partial n = v$ .

Thus  $f$  satisfies (3.1)–(3.3). It remains to show that  $f \in \mathcal{D}_1(\Omega_R)$  satisfying these three equations is unique. But the difference between any two solutions of (3.1)–(3.3) will belong to  $\mathcal{D}_1(\Omega_R)$  and satisfy (3.1), together with the  $A$  boundary condition on  $S_R$  and Neumann condition on  $S_1$ . This difference must be the zero function, otherwise  $T^A$  would have eigenvalue  $z$  in the upper half-plane.  $\square$

We now make the following definition.

**Definition 1.** Given any  $R \in [2, \infty)$  and any bounded linear operator  $A : L^2(S_R) \rightarrow L^2(S_R)$  with  $\text{Im } A \geq 0$ , the operator  $M^A(z)$  ( $M$  operator in the region  $\Omega_R$  subject to Neumann boundary condition on  $S_1$  and  $A$  boundary condition on  $S_R$ ) is defined as an operator from  $L^2(S_1)$  to  $L^2(S_1)$ , for any  $z \in \mathbb{C}^+$ , by

$$M^A(z)v = -w, \tag{3.6}$$

where  $w = \gamma_1 f$  and  $f$  is the unique solution, in  $\mathcal{D}_1(\Omega_R)$ , of

$$-\Delta f + qf - zf = 0, \gamma_R \frac{\partial f}{\partial n} = A\gamma_R f, \quad \gamma_1 \frac{\partial f}{\partial n} = v. \tag{3.7}$$

Thus  $M^A(z)$ , acting in  $L^2(S_1)$ , maps the boundary value on  $S_1$  of  $\partial f / \partial n$  to minus the boundary value of  $f$ , for solutions of (3.1) subject to  $A$  boundary condition on  $S_R$ .

**Remark 3.** In the same manner, if  $\mathcal{A}$  is a bounded linear operator in  $L^2(S_R)$  with  $\text{Im } \mathcal{A} \leq 0$ , one can associate to each  $\xi \in \mathbb{C}^-$  ( $\text{Im } \xi < 0$ ) an operator  $M^{\mathcal{A}}(\xi) : L^2(S_1) \rightarrow L^2(S_1)$  defined as follows:  $M^{\mathcal{A}}(\xi)$  maps the boundary value (on  $S_1$ ) of  $\partial \tilde{f} / \partial n$  to minus the boundary value of  $\tilde{f}$ , for solutions  $\tilde{f}$  of  $-\Delta \tilde{f} + q\tilde{f} - \bar{z}\tilde{f} = 0$  subject to  $\mathcal{A}$  boundary condition on  $S_R$ . We shall use this on various occasions, with  $\xi = \bar{z}$  ( $\text{Im } z > 0$ ) and  $\mathcal{A} = A^*$  ( $\text{Im } A \geq 0$ ), i.e., for  $z$  and  $A$  as in Definition 1. So, for  $\tilde{v} \in L^2(S_1)$ , we have  $M^{A^*}(\bar{z})\tilde{v} = -\gamma_1 \tilde{f}$ , where  $\tilde{f}$  is the unique solution, in  $\mathcal{D}_1(\Omega_R)$ , of

$$-\Delta \tilde{f} + q\tilde{f} - \bar{z}\tilde{f} = 0, \gamma_R \frac{\partial \tilde{f}}{\partial n} = A^* \gamma_R \tilde{f}, \quad \gamma_1 \frac{\partial \tilde{f}}{\partial n} = \tilde{v}. \tag{3.8}$$

Now let  $f$  and  $\tilde{f}$  be as in (3.7) and (3.8), respectively. Then

$$\nabla \cdot (\tilde{f} \nabla f - f \nabla \tilde{f}) = 0. \tag{3.9}$$

We can integrate this identity over  $\Omega_R$  to obtain

$$\left\langle \gamma_R \tilde{f}, \gamma_R \frac{\partial f}{\partial n} \right\rangle_{S_R} - \left\langle \gamma_R \frac{\partial \tilde{f}}{\partial n}, \gamma_R f \right\rangle_{S_R} = \left\langle \gamma_1 \tilde{f}, \gamma_1 \frac{\partial f}{\partial n} \right\rangle_{S_1} - \left\langle \gamma_1 \frac{\partial \tilde{f}}{\partial n}, \gamma_1 f \right\rangle_{S_1}.$$

Using the boundary conditions for  $f$  and  $\tilde{f}$ , the left-hand side of this equation becomes  $\langle \gamma_R \tilde{f}, A \gamma_R f \rangle_{S_R} - \langle A^* \gamma_R \tilde{f}, \gamma_R f \rangle_{S_R} = 0$ , and the right-hand side is  $\langle \tilde{v}, M^A(z)v \rangle - \langle M^{A^*}(\bar{z})\tilde{v}, v \rangle$ .

We may deduce that  $M^{A^*}(\bar{z}) = [M^A(z)]^*$  (adjoint of  $M^A(z)$  as an operator on  $L^2(S_1)$ ). Since both  $M^A(z)$  and  $M^{A^*}(\bar{z})$  are defined on the whole of  $L^2(S_1)$ , it follows from the closed graph theorem that these two operators are bounded. In fact, much more can be shown. The following theorem implies that the bounds on their norms are independent both of  $R$  and of the boundary operator  $A$ .

**Theorem 1.** *Suppose  $q$  is bounded on  $\Omega_R$ . Then the operator  $M^A(z)$  is norm bounded from  $L^2(S_1)$  to  $L^2(S_1)$ , with bound  $\|M^A(z)\| \leq c$ , where  $c = c(z, q)$  depends on  $z$  and  $q$  but is independent of both  $R$  and the boundary operator  $A$ . More precisely:*

$$\|M^A(z)\| = 1 + (1 + \kappa) c_1^2 \left\{ \frac{1 + \kappa}{\text{Im } z} + 1 \right\} \tag{3.10}$$

with  $c_1$  as in Lemma 1 and  $\kappa = \sup_{x \in \Omega_R} |q(x) - z|$ .

**Proof.** We follow the notation of the proof of Lemma 5. For  $v \in L^2(S_1)$ , let  $g = E_1^{(0)}v$ ,  $h = -\Delta g + qg - zg$  and  $f = -(T^A - z)^{-1}h + g$ . Since  $\|\gamma_1 E_1^{(0)}\|_{L^2(S_1) \rightarrow L^2(S_1)} \leq 1$  and  $\|E_1^{(0)}\|_{L^2(S_1) \rightarrow \mathcal{D}_1(\Omega_R)} \leq c_1$  by Lemma 1, one has the following bounds (with  $\kappa$  as in (3.10)):

$$\|\gamma_1 g\|_{S_1} \leq \|v\|_{S_1}, \quad \|h\|_{\Omega_R} \leq c_1 (1 + \kappa) \|v\|_{S_1}, \tag{3.11}$$

$$\|f\|_{\Omega_R} \leq c_1 \left( \frac{1 + \kappa}{\text{Im } z} + 1 \right) \|v\|_{S_1}. \tag{3.12}$$

Now, for arbitrary  $\mathfrak{h} \in L^2(\Omega_R)$ , set  $\mathfrak{k} = (T^{A^*} - \bar{z})^{-1}\mathfrak{h}$ , so that  $\mathfrak{k}$  satisfies Neumann boundary condition on  $S_1$  and  $A^*$  boundary condition on  $S_R$ . Then  $f$  and  $\mathfrak{k}$  satisfy, respectively, the equations  $\Delta f = (q - z)f$  and  $\Delta \mathfrak{k} = (q - z)\mathfrak{k} - \bar{\mathfrak{h}}$ , from which follows the identity

$$\nabla \cdot (\bar{\mathfrak{k}} \nabla f - f \nabla \bar{\mathfrak{k}}) = \bar{\mathfrak{k}} \Delta f - f \Delta \bar{\mathfrak{k}} = f \bar{\mathfrak{h}}.$$

Integrating over  $\Omega_R$  (i.e., over the region  $1 + \varepsilon < |x| < R - \varepsilon$ , followed by the limit  $\varepsilon \rightarrow +0$ ) and using the divergence theorem, we have

$$\langle \mathfrak{h}, f \rangle_{\Omega_R} = \left\langle \gamma_R \mathfrak{k}, \gamma_R \frac{\partial f}{\partial n} \right\rangle_{S_R} - \left\langle \gamma_R \frac{\partial \mathfrak{k}}{\partial n}, \gamma_R f \right\rangle_{S_R} - \left\langle \gamma_1 \mathfrak{k}, \gamma_1 \frac{\partial f}{\partial n} \right\rangle_{S_1}.$$

Here the first two inner products on the right-hand side cancel, because of the  $A$  boundary condition for  $f$  and the  $A^*$  boundary condition for  $\mathfrak{k}$ , and we are left with

$$\langle \mathfrak{h}, f \rangle_{\Omega_R} = -\langle \gamma_1 (T^{A^*} - \bar{z})^{-1} \mathfrak{h}, v \rangle_{S_1}, \tag{3.13}$$

where we have substituted the  $L^2$  boundary value for  $\partial f / \partial n$  on  $S_1$ . So, by taking into account (3.12), we have

$$\begin{aligned} \|\gamma_1(T^{A^*} - \bar{z})^{-1} \mathfrak{h}\|_{S_1} &= \sup_{\|v\|_{S_1}=1} |\langle \gamma_1(T^{A^*} - \bar{z})^{-1} \mathfrak{h}, v \rangle_{S_1}| \\ &\leq \sup_{\|v\|_{S_1}=1} \|\mathfrak{h}\|_{\Omega_R} \|f\|_{\Omega_R} \\ &\leq \|\mathfrak{h}\|_{\Omega_R} c_1 \left\{ \frac{1 + \kappa}{\text{Im } z} + 1 \right\}. \end{aligned}$$

This implies that

$$\|\gamma_1(T^{A^*} - \bar{z})^{-1}\|_{L^2(\Omega_R) \rightarrow L^2(S_1)} \leq c_1 \left\{ \frac{1 + \kappa}{\text{Im } z} + 1 \right\}. \tag{3.14}$$

A similar argument, starting from the identity for  $\nabla \cdot (\bar{\mathfrak{k}} \nabla \tilde{f} - \tilde{f} \nabla \bar{\mathfrak{k}})$ , with  $\mathfrak{k} = (T^A - z)^{-1} \mathfrak{h}$  and with  $\tilde{f}$  as in (3.8), leads to the bound

$$\|\gamma_1(T^A - z)^{-1}\|_{L^2(\Omega_R) \rightarrow L^2(S_1)} \leq c_1 \left\{ \frac{1 + \kappa}{\text{Im } z} + 1 \right\}. \tag{3.15}$$

Now, from the definition of  $M^A(z)$ , we have

$$M^A(z)v = -\gamma_1 f = \gamma_1(T^A - z)^{-1} h - \gamma_1 g \tag{3.16}$$

which leads to bound (3.10) by using (3.11) and (3.15).  $\square$

From (3.13) we see that the mapping from  $v$  to  $f$  is just the adjoint of the map  $-\gamma_1(T^{A^*} - \bar{z})^{-1}$ , which is bounded from  $L^2(\Omega_R)$  to  $L^2(S_1)$ . Thus

$$f = -[\gamma_1(T^{A^*} - \bar{z})^{-1}]^* v. \tag{3.17}$$

Since  $M^A(z)v = -\gamma_1 f$ , we have for  $M^A(z)$  the closed expression

$$M^A(z) = \gamma_1[\gamma_1(T^{A^*} - \bar{z})^{-1}]^*, \tag{3.18}$$

which we may write formally as

$$M^A(z) = \gamma_1(T^A - z)^{-1} \gamma_1^*. \tag{3.19}$$

It is clear that the norm of the operator  $M^{A^*}(\bar{z})$ , defined in Remark 3, also satisfies bound (3.10), and that the mapping from  $\tilde{v}$  to  $\tilde{f}$  determined by (3.8) is as follows

$$\tilde{f} = -[\gamma_1(T^A - z)^{-1}]^* \tilde{v}. \tag{3.20}$$

**Corollary.**

- (a)  $M^A(z)$  maps  $L^2(S_1)$  into  $H^1(S_1)$ .
- (b)  $M^A(z)$  is compact as an operator  $L^2(S_1) \rightarrow L^2(S_1)$ .

**Proof.** (a) If  $f$  is as in the preceding proof, we have  $f \in \mathcal{D}_1(\Omega_R) \subseteq H^{3/2}(\Omega_R)$ . Since  $\gamma_1$  maps  $H^{3/2}(\Omega_R)$  into  $H^1(S_1)$ , the result follows. (See Section 4 for an alternative proof applicable to the  $M$  operator for unbounded regions.)

(b) The operator  $M^A(z)$ , being bounded, is closed from  $L^2(S_1)$  to  $L^2(S_1)$ , hence also from  $L^2(S_1)$  to  $H^1(S_1)$ . It follows (closed graph theorem) that  $M^A(z)$  is bounded as a map from  $L^2(S_1)$  to  $H^1(S_1)$ . Since  $H^1(S_1)$  is compactly embedded in  $L^2(S_1)$ , we see that  $M^A(z) : L^2(S_1) \rightarrow L^2(S_1)$  is compact.  $\square$

**Remark.** It will be shown later that in fact  $M^A(z)$  maps  $L^2(S_1)$  onto  $H^1(S_1)$ .

The following proposition confirms for  $M^A(z)$  the two basic properties of positivity of imaginary part, and analyticity in  $z$ .

**Proposition 1.** Let  $z \in \mathbb{C}^+$ .

(a)  $M^A(z)$  has strictly positive imaginary part:

$$\text{Im} \langle v, M^A(z)v \rangle_{S_1} > 0 \quad \forall v \neq 0 \text{ in } L^2(S_1). \tag{3.21}$$

(b)  $dM^A(z)/dz$  exists as  $\lim_{z' \rightarrow z} [M^A(z') - M^A(z)]/(z' - z)$  (limit in operator norm) and thus defines a bounded operator in  $L^2(S_1)$ .

**Proof.** (a) Let  $v \in L^2(S_1)$  be arbitrary. Define  $f$  as before (e.g., in the proof of Lemma 5), so that  $\gamma_1 \partial f / \partial n = v$  and  $-\gamma_1 f = M^A(z)v$ . From the divergence theorem, we have

$$(z - \bar{z}) \int_{\Omega_R} f \bar{f} \, dx = \int_{S_R} \left( f \frac{\partial \bar{f}}{\partial n} - \bar{f} \frac{\partial f}{\partial n} \right) \, dS - \int_{S_1} \left( f \frac{\partial \bar{f}}{\partial n} - \bar{f} \frac{\partial f}{\partial n} \right) \, dS.$$

Hence

$$\begin{aligned} \text{Im} \langle v, M^A(z)v \rangle_{S_1} &= \text{Im} \left\langle \gamma_1 f, \gamma_1 \frac{\partial f}{\partial n} \right\rangle_{S_1} \\ &= \text{Im} z \|f\|_{\Omega_R}^2 + \langle \gamma_R f, (\text{Im } A) \gamma_R f \rangle_{S_R} \geq \text{Im} z \|f\|_{\Omega_R}^2 \geq 0. \end{aligned}$$

If  $\text{Im} \langle v, M^A(z)v \rangle_{S_1} = 0$ , then  $\|f\|_{\Omega_R} = 0$ , hence  $f = 0$  and thus  $v = \gamma_1 \partial f / \partial n = 0$ .

(b) It is straightforward to use (3.18) to evaluate the derivative  $dM^A(z)/dz$  through a limiting argument, and we have

$$\frac{dM^A(z)}{dz} = [\gamma_1(T^A - z)^{-1}][\gamma_1(T^{A*} - \bar{z})^{-1}]^*. \tag{3.22}$$

We have seen that both factors on the right-hand side have finite norm, implying that  $dM^A(z)/dz$  is bounded from  $L^2(S_1)$  to  $L^2(S_1)$ . (The dependence of the norm on  $z$  is such that  $\|dM^A(z)/dz\|$  has a bound of order  $1/\text{Im } z$  in the limit as  $z$  approaches the real axis.)  $\square$

We note the following identity which is obtained by using (3.17) and (3.20):

$$\left\langle \tilde{v}, \frac{dM^A(z)}{dz} v \right\rangle_{S_1} = \langle \tilde{f}, f \rangle_{\Omega_R}. \tag{3.23}$$

Part (a) of Proposition 1 implies that the operator  $M^A(z)$  is invertible. We write  $m^A(z)$  for minus its inverse :  $m^A(z) = -[M^A(z)]^{-1}$ . The operator  $m^A(z)$  is unbounded in  $L^2(S_1)$ , with domain contained in  $H^1(S_1)$ . A more specific description will be given at the end of Section 4.

We now consider the definition and properties of  $M$  operators with respect to a pair  $A, B$  of boundary operators, with  $A$  acting on  $L^2$  of the outer surface  $S_R$  as before, and  $B$  acting on  $L^2$  of the inner surface  $S_1$ .

**Definition 2.** Given any  $R \in [2, \infty)$  and bounded linear operators  $A : L^2(S_R) \rightarrow L^2(S_R)$ ,  $B : L^2(S_1) \rightarrow L^2(S_1)$  with  $\text{Im} A \geq 0$ ,  $\text{Im} B \leq 0$ , the operator  $M_B^A(z)$  is defined as an operator from  $L^2(S_1)$  to  $L^2(S_1)$ , for any  $z \in \mathbb{C}^+$ , by

$$M_B^A(z)v = -w, \tag{3.24}$$

where  $w = \gamma_1 f$  and  $f$  is the unique solution, in  $\mathcal{D}_1(\Omega_R)$ , of

$$-\Delta f + qf - zf = 0 \tag{3.25}$$

subject to the boundary conditions  $\gamma_R \partial f / \partial n = A \gamma_R f$  ( $A$  boundary condition on  $S_R$ ) and

$$\gamma_1 \frac{\partial f}{\partial n} - B \gamma_1 f = v. \tag{3.26}$$

Thus  $M_B^A(z)$  maps  $\gamma_1 \partial f / \partial n - B \gamma_1 f$  to the boundary value (on  $S_1$ ) of  $f$ , for solutions of (3.25) subject to  $A$  boundary condition on  $S_R$ . The special case  $B = 0$  corresponds to  $M^A(z)$  previously defined.

The proof of the existence and uniqueness of  $M_B^A(z)$  and of its properties when  $B \neq 0$  involves arguments similar to those of the first part of this section. We define the operator  $T_B^A$  in  $L^2(\Omega_R)$  as  $-\Delta + q$  subject to  $A$  boundary condition on  $S_R$  and  $B$  boundary condition on  $S_1$  :  $T_B^A = -\Delta + q$  with domain  $D(T_B^A) = \{g \in \mathcal{D}_1(\Omega_R) : \gamma_R \partial g / \partial n = A \gamma_R g, \gamma_1 \partial g / \partial n = B \gamma_1 g\}$ .  $T_B^A$  is a closed operator with adjoint  $(T_B^A)^* = T_{B^*}^A$ . We use the extension operator  $F_1$  from Lemma 2 and set, for given  $v \in L^2(S_1)$ :

$$g = F_1 v, \quad h = -\Delta g + qg - zg, \quad f = -(T_B^A - z)^{-1} h + g. \tag{3.27}$$

Recalling that  $g$  vanishes in a neighbourhood of  $S_R$ , we may conclude that  $f$  satisfies the conditions of Definition 2. Uniqueness of  $f$  follows from the observation that  $T_B^A$  can have no eigenvalues in the upper half-plane.

In view of Definition 2, we now have

$$M_B^A(z)v = \gamma_1 (T_B^A - z)^{-1} h - \gamma_1 g. \tag{3.28}$$

For later use we observe that, with  $c$  as in Lemma 2 and  $\kappa$  as in Theorem 1:

$$\|h\|_{\Omega_R} \leq [c(1 + \|B\|)]^{1/2} + 2\kappa \|v\|_{S_1}. \tag{3.29}$$

**Theorem 2.** Suppose  $q$  is bounded on  $\Omega_R$ . Then the operator  $M_B^A(z)$  given in Definition 2 is norm bounded from  $L^2(S_1)$  to  $L^2(S_1)$ , with bound  $\|M_B^A(z)\| \leq c(1 + \|B\|)$ , where  $c = c(z, q)$  is independent of  $R$  and of the boundary operators  $A$  and  $B$ .

**Proof.** The proof follows closely the arguments of that of Theorem 1, with  $F_1$  instead of  $E_1^{(0)}$  (hence with  $c(1 + \|B\|)^{1/2}$  instead of the constant  $c_1$ ); the function  $\tilde{f} \in \mathcal{D}_1(\Omega_R)$  is here defined, for given

$\tilde{v} \in L^2(S_1)$ , to be the solution of  $(-\Delta + q - \bar{z})\tilde{f} = 0$  subject to  $A^*$  boundary condition on  $S_R$  and the condition  $\gamma_1 \partial \tilde{f} / \partial n - B^* \gamma_1 \tilde{f} = \tilde{v}$  on  $S_1$ . One obtains in particular that

$$M_B^A(z) = \gamma_1 [\gamma_1 (T_{B^*}^{A^*} - \bar{z})^{-1}]^*, \tag{3.30}$$

written formally as  $M_B^A(z) = \gamma_1 (T_B^A - z)^{-1} \gamma_1^*$ .  $\square$

We mention that the estimate of  $\|M_B^A(z)\|$  is optimal in the sense that with zero potential and fixed  $z$  and  $R$ , a sequence  $\{B_n\}$  of boundary operators can be found for which the norm of  $M_{B_n}^A(z)$  increases linearly with  $\|B_n\|$ , as  $n$  is increased.

For arbitrary bounded  $B$ , one can express the operator  $M_B^A(z)$  in terms of  $M^A(z)$ . To do this, note that, with  $f$  given as in Definition 2,  $\gamma_1 f = -M^A(z) \gamma_1 \partial f / \partial n$  is in the range of  $M^A(z)$ , and we have

$$[(M^A(z))^{-1} + B]M_B^A(z)v = -[(M^A(z))^{-1} + B]\gamma_1 f = \gamma_1 \frac{\partial f}{\partial n} - B\gamma_1 f = v.$$

Here  $v \in L^2(S_1)$  is arbitrary and we may deduce that the range of  $(M^A(z))^{-1} + B$  is the whole of  $L^2(S_1)$ . Moreover the operator  $(M^A(z))^{-1} + B$  is invertible since, if  $[(M^A(z))^{-1} + B]u = 0$  for some  $u \in L^2(S_1)$ , then

$$\langle M^A(z)^* Bu, (M^A(z))^{-1} u + Bu \rangle_{S_1} = \langle u, B^* u \rangle_{S_1} + \langle Bu, M^A(z) Bu \rangle_{S_1} = 0.$$

Since  $\text{Im } B^* \geq 0$  and  $\text{Im } M^A(z) > 0$ , this implies that  $u = 0$ . So we have the following result for the  $M$  operator with boundary operators on both  $S_1$  and  $S_R$ .

**Proposition 2.** *The operator  $M_B^A(z)$ , given by Definition 2, is related to  $M^A(z)$  by*

$$M_B^A(z) = [(M^A(z))^{-1} + B]^{-1} = [-m^A(z) + B]^{-1}. \tag{3.31}$$

We derive a result on continuity of  $M_B^A(z)$  as a function of the boundary operator  $A$  (Lemma 6). We first show that there is a constant  $c = c(z, q)$  independent of  $R$  and of the boundary operators  $A, B$  such that

$$\|\gamma_R (T_{B^*}^{A^*} - \bar{z})^{-1}\|_{L^2(\Omega_R) \rightarrow L^2(S_R)} \leq c(1 + \|A\|^2). \tag{3.32}$$

For the proof, let  $v \in L^2(S_R)$  and define  $f_R$  in  $\mathcal{D}_1(\Omega_R)$  by

$$f_R = -(T_B^A - z)^{-1} h_R + g_R,$$

where  $g_R = F_R v$  and  $h_R = -\Delta g_R + q g_R - z g_R$ , with  $F_R$  given by Lemma 4. Note that  $g_R$  vanishes in a neighbourhood of  $S_1$ . Then  $f_R$  satisfies  $-\Delta f_R + q f_R - z f_R = 0$ , subject to the  $B$  boundary condition on  $S_1$  and the condition  $(\gamma_R \partial / \partial n - A \gamma_R) f_R = v$  on  $S_R$ . By proceeding as in the derivation of (3.13), one obtains the following identity, for each  $\mathfrak{h} \in L^2(S_R)$ :

$$\langle \mathfrak{h}, f_R \rangle_{\Omega_R} = \langle \gamma_R (T_{B^*}^{A^*} - \bar{z})^{-1} \mathfrak{h}, v \rangle_{S_R}.$$

Estimate (3.32) now follows since, by (2.21), we have  $\|f_R\|_{\Omega_R} \leq \text{const}(1 + \|A\|^2) \|v\|_{S_R}$ .

By a similar argument one also finds that

$$\|\gamma_R (T_B^A - z)^{-1}\|_{L^2(\Omega_R) \rightarrow L^2(S_R)} \leq c(1 + \|A\|^2). \tag{3.33}$$

**Lemma 6.** *The operators  $M_B^A(z)$  are norm continuous with respect to the boundary operator on the outer surface:*

$$\|M_B^A(z) - M_B^{A'}(z)\| \leq c(1 + \|A\|^2)(1 + \|A'\|^2)(1 + \|B\|)\|A - A'\|, \tag{3.34}$$

where the constant  $c = c(z, q)$  depends on  $z$  and  $q$ , but is independent of  $R$  and of the boundary operators  $A, A'$  and  $B$ .

**Proof.** (i) For arbitrary  $\mathfrak{h}, \mathfrak{h}'$  in  $L^2(\Omega_R)$ , set  $\mathfrak{k} = (T_{B^*}^{A^*} - \bar{z})^{-1}\mathfrak{h}$ ,  $\mathfrak{k}' = (T_B^{A'} - z)^{-1}\mathfrak{h}'$ , and observe the identity

$$\nabla \cdot (\mathfrak{k}' \nabla \bar{\mathfrak{k}} - \bar{\mathfrak{k}} \nabla \mathfrak{k}') = \bar{\mathfrak{k}} \mathfrak{h}' - \mathfrak{k}' \bar{\mathfrak{h}}.$$

On integration over  $\Omega_R$  and applying the divergence theorem, one then obtains

$$\begin{aligned} & \langle \mathfrak{h}, (T_B^A - z)^{-1}\mathfrak{h}' - (T_B^{A'} - z)^{-1}\mathfrak{h}' \rangle_{\Omega_R} \\ &= \left\langle \gamma_R \frac{\partial}{\partial n} (T_{B^*}^{A^*} - \bar{z})^{-1}\mathfrak{h}, \gamma_R (T_B^{A'} - z)^{-1}\mathfrak{h}' \right\rangle_{S_R} \\ & \quad - \langle \gamma_R (T_{B^*}^{A^*} - \bar{z})^{-1}\mathfrak{h}, \gamma_R \frac{\partial}{\partial n} (T_B^{A'} - z)^{-1}\mathfrak{h}' \rangle_{S_R} \\ &= \langle \gamma_R (T_{B^*}^{A^*} - \bar{z})^{-1}\mathfrak{h}, (A - A')\gamma_R (T_B^{A'} - z)^{-1}\mathfrak{h}' \rangle_{S_R}. \end{aligned}$$

By virtue of (3.32) and (3.33), this leads to

$$\|(T_B^A - z)^{-1} - (T_B^{A'} - z)^{-1}\|_{L^2(\Omega_R) \rightarrow L^2(\Omega_R)} \leq c(z, q)(1 + \|A\|^2)(1 + \|A'\|^2)\|A - A'\|. \tag{3.35}$$

(ii) Now, for each  $A$ , consider the operator  $S^A = -[\gamma_1(T_{B^*}^{A^*} - \bar{z})^{-1}]^* : L^2(S_1) \rightarrow L^2(\Omega_R)$  associating to  $v \in L^2(S_1)$  the function  $f^A = -(T_B^A - z)^{-1}h + g$  introduced in (3.27). Then

$$\begin{aligned} \|(S^A - S^{A'})v\|_{\Omega_R} &= \|(T_B^A - z)^{-1}h - (T_B^{A'} - z)^{-1}h\|_{\Omega_R} \\ &\leq \|(T_B^A - z)^{-1} - (T_B^{A'} - z)^{-1}\|_{L^2(\Omega_R) \rightarrow L^2(\Omega_R)} \|h\|_{\Omega_R}. \end{aligned}$$

By using (3.35) and (3.29), we now get

$$\begin{aligned} \|(S^A)^* - (S^{A'})^*\| &= \|\gamma_1(T_{B^*}^{A^*} - \bar{z})^{-1} - \gamma_1(T_{B^*}^{A'^*} - \bar{z})^{-1}\|_{L^2(\Omega_R) \rightarrow L^2(S_1)} \\ &\leq c(z, q)(1 + \|A\|^2)(1 + \|A'\|^2)(1 + \|B\|)^{1/2}\|A - A'\|. \end{aligned}$$

Since  $M_{B^*}^{A^*}(\bar{z})v = \gamma_1(T_{B^*}^{A^*} - \bar{z})^{-1}\tilde{h} + g$  with  $g = F_1v$  and  $\tilde{h} = (-\Delta + q - \bar{z})g$  (so that  $\|\tilde{h}\|_{\Omega_R}$  satisfies (3.29)), we see that  $\|M_{B^*}^{A^*}(\bar{z}) - M_{B^*}^{A'^*}(\bar{z})\|$  is bounded by the r.h.s. of (3.34). To complete the proof, it suffices to observe that  $M_B^A(z) = [M_{B^*}^{A^*}(\bar{z})]^*$ .  $\square$

Lemma 6 shows that  $M_B^A(z)$  is norm continuous in  $A$ , for fixed  $B$  and  $z$ . If we consider a sequence  $\{A_n\}$  of boundary operators on  $S_R$ , such that  $\|A_n\| \rightarrow \infty$  as  $n \rightarrow \infty$ , it might be expected that the corresponding  $M$  operators converge to the operator  $M_B^{D^R}(z)$  subject to Dirichlet boundary condition on  $S_R$  (defined by a minor modification of Definition 2, in which the  $A$  boundary condition is replaced on  $S_R$  by the Dirichlet boundary condition  $\gamma_R f = 0$ ). The following lemma, the proof of

which will be given elsewhere, presents a modified version of this result, in which the condition  $A_n \rightarrow \infty$  is interpreted in a special way.

**Lemma 7.** *Let  $R \in [2, \infty)$  and let  $\{A_n\}$  be a sequence of bounded boundary operators from  $L^2(S_R)$  to  $L^2(S_R)$ , with  $\text{Im} A_n \geq 0$ . Let  $d(A_n)$  be the distance, in the complex plane, between  $\mathbb{R}^+$  and the numerical range of  $A_n$  (defined as the set  $\langle v, A_n v \rangle / \|v\|^2$  as  $v$  is varied over  $L^2(S_R)$ ), and suppose that  $d(A_n) \rightarrow \infty$  as  $n \rightarrow \infty$ . Then  $M_B^{A_n}(z)$  converges in norm to  $M_B^{D_R}(z)$  in the limit  $n \rightarrow \infty$ , for each  $z \in \mathbb{C}^+$ .*

#### 4. $M$ operators for exterior unbounded region

It is now straightforward to extend our definition of  $M(z)$  operators to cover the case of an  $M$  operator for the exterior region  $\Omega = \{x : |x| > 1\}$ , subject to a boundary condition at the inner surface  $S_1$ . For simplicity, we assume the potential function  $q(x)$  is bounded for  $x \in \Omega$ .

**Definition 3.** Given any bounded linear operator  $B : L^2(S_1) \rightarrow L^2(S_1)$  with  $\text{Im} B \leq 0$ , the operator  $M_B(z) : L^2(S_1) \rightarrow L^2(S_1)$  is defined for any  $z \in \mathbb{C}^+$  by

$$M_B(z)v = -w, \tag{4.1}$$

where  $w = \gamma_1 f$  and  $f$  is the unique solution, in  $\mathcal{D}_1(\Omega)$ , of  $-\Delta f + qf - zf = 0$ , subject to the boundary condition  $\gamma_1 \partial f / \partial n - B\gamma_1 f = v$ .

Thus the definition of  $M_B(z)$  is similar to that of  $M_B^A(z)$ , except that there is now no outer boundary and the solution  $f$  of the Schrödinger equation is defined for  $x$  in the infinite region  $\Omega$ .

To verify the existence of  $f$  in the above definition, we use the extension operator  $F_1 : L^2(S_1) \rightarrow \mathcal{D}_1(\Omega)$  constructed in Lemma 2 (with  $R = \infty$ ). The solution  $f$  demanded by Definition 3 is given by

$$f = -(T_B - z)^{-1}h + g, \tag{4.2}$$

where  $g = F_1 v$ ,  $h = -\Delta g + qg - zg$  and  $T_B$  is the Schrödinger operator  $-\Delta + q$  in  $L^2(\Omega)$ , with domain consisting of all functions in  $\mathcal{D}_1(\Omega)$  satisfying  $B$  boundary condition on  $S_1$ . Again uniqueness of  $f$  follows from the fact that  $T_B$  has no eigenvalues in the upper half-plane.

For  $z \in \mathbb{C}^+$ ,  $M_B(z)$  is analytic with strictly positive imaginary part. As an operator from  $L^2(S_1)$  to  $L^2(S_1)$ ,  $M_B(z)$  is compact and norm bounded, with

$$\|M_B(z)\| \leq c(z, q)(1 + \|B\|). \tag{4.3}$$

Proofs of these results follow the same arguments as before, and are actually simpler since we do not need to take into account a boundary condition at the outer surface.

We now consider a family  $\{A(R)\}_{2 \leq R < \infty}$  of boundary operators. Each  $A(R)$  is bounded from  $L^2(S_R)$  to  $L^2(S_R)$  and has  $\text{Im} A(R) \geq 0$ . We take  $B$  to be bounded from  $L^2(S_1)$  to  $L^2(S_1)$ , with  $\text{Im} B \leq 0$ . Then for each  $R \geq 2$  and  $z \in \mathbb{C}^+$ , the operators  $M_B^{A(R)}(z)$  and  $M_B(z)$  are defined and

bounded from  $L^2(S_1)$  to  $L^2(S_1)$ , and we consider the question: in what sense (if any) does  $M_B^{A(R)}(z)$  converge to  $M_B(z)$  as  $R \rightarrow \infty$ ? To answer this question, we shall need the following lemma.

**Lemma 8.** *Assume that  $\|A(R)\|_{L^2(S_R) \rightarrow L^2(S_R)}$  is bounded by a constant independent of  $R$ . Then*

$$s - \lim_{R \rightarrow \infty} \gamma_1(T_B^{A(R)} - z)^{-1} = \gamma_1(T_B - z)^{-1}. \tag{4.4}$$

Eq. (4.4) requires some clarification, since the operators  $T_B^{A(R)}$  and  $T_B$  do not act in the same space. Let  $\mathfrak{h} \in L^2(\Omega)$  be of bounded support and suppose that the support of  $\mathfrak{h}$  is contained in the region  $\{x : |x| \leq R_0\}$ . Then for any  $R > R_0$ , we interpret  $\mathfrak{h}$  (more correctly the restriction of  $\mathfrak{h}$  to  $\Omega_R$ ) as an element of  $L^2(\Omega_R)$ . In that case we can make sense of both  $\gamma_1(T_B^{A(R)} - z)^{-1}\mathfrak{h}$  and  $\gamma_1(T_B - z)^{-1}\mathfrak{h}$  as elements of  $L^2(S_1)$ , and (4.4) should be taken to mean that

$$s - \lim_{R \rightarrow \infty} \gamma_1(T_B^{A(R)} - z)^{-1}\mathfrak{h} = \gamma_1(T_B - z)^{-1}\mathfrak{h} \tag{4.5}$$

for all  $\mathfrak{h}$  of bounded support which are square integrable over  $\Omega$ .

By a continuity argument, using estimates for  $\|\gamma_1(T_B^{A(R)} - z)^{-1}\|$  and  $\|\gamma_1(T_B - z)^{-1}\|$ , one could deduce that

$$s - \lim_{R \rightarrow \infty} \gamma_1(T_B^{A(R)} - z)^{-1}\chi_R g = \gamma_1(T_B - z)^{-1}g$$

for all  $g \in L^2(\Omega)$ , where  $\chi_R$  denotes the orthogonal projection in  $L^2(\Omega)$  with range  $L^2(\Omega_R)$ .

**Proof.** We denote by  $\tilde{F}_1 : L^2(S_1) \rightarrow \mathcal{D}_1(\Omega_R)$  the extension operator associated, as in Lemma 2, to the boundary operator  $B^*$ , i.e., satisfying  $(\gamma_1 \partial / \partial n - B^* \gamma_1) \tilde{F}_1 \tilde{v} = \tilde{v}$  for all  $\tilde{v} \in L^2(S_1)$ .  $\tilde{F}_1 \tilde{v}$  vanishes outside the ball  $\{x : |x| \leq 2\}$ , and  $\tilde{F}_1$  satisfies the norm bounds (2.14)–(2.16).

For given  $\tilde{v} \in L^2(S_1)$ , we set  $\tilde{g} = \tilde{F}_1 \tilde{v}$ ,  $\tilde{\mathfrak{h}} = -\Delta \tilde{g} + q \tilde{g} - z \tilde{g}$  and  $\tilde{f} = -(T_B^{A(R)*} - \bar{z})^{-1} \tilde{\mathfrak{h}} + \tilde{g}$ . Then  $\tilde{f}$  satisfies  $-\Delta \tilde{f} + q \tilde{f} - \bar{z} \tilde{f} = 0$ , with  $(\gamma_1 \partial / \partial n - B^* \gamma_1) \tilde{f} = \tilde{v}$  and  $A(R)^*$  boundary condition on  $S_R$ .

Using the norm bound (3.32) on  $\gamma_R (T_B^{A(R)*} - \bar{z})^{-1}$ , and noting that  $R \mapsto \|A(R)\|$  is assumed bounded, we may deduce that  $\|\gamma_R \tilde{f}\|_{S_R}$  is bounded uniformly in  $R$  by  $\text{const} \|\tilde{v}\|_{S_1}$ , for  $R > 2$ , and we have an identical bound for  $\|\gamma_R \partial / \partial n \tilde{f}\|_{S_R}$ , due to the  $A(R)^*$  boundary condition of  $\tilde{f}$ .

Now take  $\mathfrak{h} \in L^2(\Omega)$ , such that the support of  $\mathfrak{h}$  is contained in  $\Omega_R$  for all  $R$  sufficiently large. Setting  $\mathfrak{k} = (T_B^{A(R)} - z)^{-1} \mathfrak{h}$  and integrating over  $\Omega_R$  the identity  $\nabla \cdot (\tilde{\mathfrak{k}} \nabla \tilde{f} - \tilde{f} \nabla \tilde{\mathfrak{k}}) = \tilde{\mathfrak{h}} \tilde{f}$ , we find, on using the boundary conditions for  $\mathfrak{k}$  and  $\tilde{f}$ :

$$\langle \mathfrak{h}, \tilde{f} \rangle_{\Omega_R} = -\langle \gamma_1 \mathfrak{k}, \tilde{v} \rangle_{S_1} = -\langle \gamma_1 (T_B^{A(R)} - z)^{-1} \mathfrak{h}, \tilde{v} \rangle_{S_1}. \tag{4.6}$$

We can integrate over  $\Omega_R$  the same identity, with this time  $\mathfrak{k} = (T_B - z)^{-1} \mathfrak{h}$ , to obtain in this case

$$\begin{aligned} \langle \mathfrak{h}, \tilde{f} \rangle_{\Omega_R} = & -\langle \gamma_1 (T_B - z)^{-1} \mathfrak{h}, \tilde{v} \rangle_{S_1} + \left\langle \gamma_R (T_B - z)^{-1} \mathfrak{h}, \gamma_R \frac{\partial \tilde{f}}{\partial n} \right\rangle_{S_R} \\ & - \left\langle \gamma_R \frac{\partial}{\partial n} (T_B - z)^{-1} \mathfrak{h}, \gamma_R \tilde{f} \right\rangle_{S_R}. \end{aligned} \tag{4.7}$$

Subtracting (4.7) from (4.6) now leads to

$$\langle \gamma_1(T_B^{A(R)} - z)^{-1}\mathfrak{h} - \gamma_1(T_B - z)^{-1}\mathfrak{h}, \tilde{v} \rangle_{S_1} = \langle \gamma_R \frac{\partial}{\partial n}(T_B - z)^{-1}\mathfrak{h}, \gamma_R \tilde{f} \rangle_{S_R} - \left\langle \gamma_R(T_B - z)^{-1}\mathfrak{h}, \gamma_R \frac{\partial \tilde{f}}{\partial n} \right\rangle_{S_R}.$$

We have seen that  $\|\gamma_R \tilde{f}\|_{S_R} \leq \text{const} \|\tilde{v}\|_{S_1}$ ,  $\|\gamma_R \partial \tilde{f} / \partial n\|_{S_R} \leq \text{const} \|\tilde{v}\|_{S_1}$ . Moreover, by Remark 1 in Section 2, both  $\|\gamma_R \partial / \partial n (T_B - z)^{-1} \mathfrak{h}\|_{S_R}$  and  $\|\gamma_R (T_B - z)^{-1} \mathfrak{h}\|_{S_R}$  converge to zero in the limit as  $R \rightarrow \infty$ . Hence it follows that  $\lim_{R \rightarrow \infty} \|\gamma_1(T_B^{A(R)} - z)^{-1} \mathfrak{h} - \gamma_1(T_B - z)^{-1} \mathfrak{h}\|_{S_1} = 0$ .  $\square$

Lemma 8 is the principal ingredient in the proof of convergence of  $M$  operators for the region  $\Omega_R$ , in the limit  $R \rightarrow \infty$ , to  $M$  operators for the exterior unbounded region.

**Theorem 3.** *Suppose that  $q$  is bounded on  $\Omega_R$ . Let  $B$  be fixed ( $\text{Im } B \leq 0$ ) and suppose that  $\sup_{R \geq 0} \|A(R)\| < \infty$ . Then  $M_B^{A(R)}(z)$  converges strongly to  $M_B(z)$  in the limit as  $R \rightarrow \infty$ , for each  $z \in \mathbb{C}^+$ .*

**Proof.** Let  $v \in L^2(S_1)$  be arbitrary. We use the extension operator  $F_1$  from Lemma 2 to construct the solution  $f_R$  in  $\mathcal{D}_1(\Omega_R)$  of  $-\Delta f_R + q f_R - z f_R = 0$  subject to  $\gamma_1 \partial / \partial n f_R - B \gamma_1 f_R = v$  and the  $A(R)$  boundary condition on  $S_R$ . Explicitly we have  $f_R = -(T_B^{A(R)} - z)^{-1} h + g$ , where  $g = F_1 v$  and  $h = -\Delta g + qg - zg$ .

We keep the extension operator  $F_1$  fixed and regard  $g$ , with  $g(x) = 0$  for  $|x| \geq 2$ , as an element of  $\mathcal{D}_1(\Omega)$ . Then we can use the same functions  $g$  and  $h$  to construct the solution  $f$  in  $\mathcal{D}_1(\Omega)$  of  $-\Delta f + qf - zf = 0$ , subject to  $\gamma_1 \partial f / \partial n - B \gamma_1 f = v$ . Explicitly this gives  $f = -(T_B - z)^{-1} h + g$ . Hence

$$M_B^{A(R)}(z)v = \gamma_1(T_B^{A(R)} - z)^{-1}h - \gamma_1g,$$

$$M_B(z)v = \gamma_1(T_B - z)^{-1}h - \gamma_1g.$$

The conclusion of the theorem now follows from Lemma 8.  $\square$

By using estimates required for the proof of Lemma 8, one may also show that  $M_B^{D_R}(z)$  (Dirichlet boundary conditions on  $S_R$ ) converges strongly to  $M_B(z)$  in the limit as  $R \rightarrow \infty$ .

In what follows, we shall be particularly interested in the operator  $M_0(z)$ , i.e., the operator  $M_B(z)$  in the case  $B = 0$ . Thus  $M_0(z)$  is the  $M$  operator for the exterior region  $\Omega$ , with Neumann boundary condition at the surface  $S_1$ .

Since the range of  $\gamma_1 E_1^{(0)}$  is  $H^1(S_1)$  and the resolvent of the Neumann Schrödinger operator maps into  $H^2(\Omega)$ , it follows that  $M_0(z)$  maps into  $H_1(S_1)$ . We shall find that in fact  $M_0(z)$  maps onto  $H^1(S_1)$ , so that its inverse (denoted by  $-m_0(z)$ ) will be an operator from  $H^1(S_1)$  to  $L^2(S_1)$ . Below we introduce  $m_0(z)$  by an alternative method and then relate it to  $M_0(z)$ .

**Definition 4.** The operator  $m_0(z): H^1(S_1) \rightarrow L^2(S_1)$  is defined for any  $z \in \mathbb{C}^+$  by

$$m_0(z)w = v, \tag{4.8}$$

where  $v = \gamma_1 \partial f / \partial n$  and  $f$  is the unique solution, in  $\mathcal{D}_1(\Omega_R)$ , of  $-\Delta f + qf - zf = 0$ , subject to the boundary condition  $\gamma_1 f = w$ .

As previously, one may construct the solution  $f$  explicitly, through the use of an appropriate extension operator  $F : H^1(S_1) \rightarrow \mathcal{D}_1(\Omega)$ . Let  $Q = \gamma_1 E_1^{(0)}$  and  $F = E_1^{(0)} Q^{-1}$  as in Remark 2 of Section 2.  $F$  is bounded from  $H^1(S_1)$  to  $\mathcal{D}_1(\Omega)$  and satisfies  $\gamma_1 F w = w$  for all  $w \in H^1(S_1)$ . For fixed  $w \in H^1(S_1)$  we set  $g = Fw$ ,  $h = -\Delta g + qg - zg$  and  $f = -(T_{D_1} - z)^{-1} h + g$ , where  $T_{D_1} = -\Delta + q$  in  $L^2(\Omega)$ , with Dirichlet boundary condition on  $S_1$ .

Noting that  $\gamma_1 \partial / \partial n (T_{D_1} - z)^{-1}$  is bounded from  $L^2(\Omega)$  to  $L^2(S_1)$  and that  $\gamma_1 \partial / \partial n F = \gamma_1 \partial / \partial n E_1^{(0)} Q^{-1} = Q^{-1}$  is bounded from  $H^1(S_1)$  to  $L^2(S_1)$  (see Lemma 1), we find that  $m_0(z)$  is bounded from  $H^1(S_1)$  to  $L^2(S_1)$  (though unbounded as an operator in  $L^2(S_1)$ ). Similar estimates for other versions of the Steklov–Poincaré operator as a mapping from  $H^1$  to  $L^2$  spaces can be found in the literature; see for example [16, Chapter 4]. Also, setting  $v = \gamma_1 \partial / \partial n f$ , we see, by comparing with Definition 3, that  $M_0(z)v = w$ . Hence  $m_0(z) = -[M_0(z)]^{-1}$ , and the range of  $M_0(z)$  is the entire space  $H^1(S_1)$ .

To derive an identity for  $m_0(z)$ , we can follow the proof of Theorem 1 up to Eq. (3.13), with  $T^{A^*}$  replaced by  $T_{D_1}$  and  $\Omega_R$  replaced by  $\Omega$ , to obtain

$$\langle \mathfrak{h}, f \rangle_\Omega = \left\langle \gamma_1 \frac{\partial}{\partial n} (T_{D_1} - \bar{z})^{-1} \mathfrak{h}, w \right\rangle_{S_1} \tag{4.9}$$

for arbitrary  $w \in L^2(S_1)$ . So the mapping from  $w$  to  $f$  is the adjoint of the map  $\gamma_1 \partial / \partial n (T_{D_1} - \bar{z})^{-1}$ , which is bounded from  $L^2(\Omega)$  to  $L^2(S_1)$ . Since  $m_0(z)w = \gamma_1 \partial f / \partial n$ , we now have

$$m_0(z) = \gamma_1 \frac{\partial}{\partial n} \left[ \gamma_1 \frac{\partial}{\partial n} (T_{D_1} - \bar{z})^{-1} \right]^*, \tag{4.10}$$

which we write formally as

$$m_0(z) = \left( \gamma_1 \frac{\partial}{\partial n} \right) (T_{D_1} - z)^{-1} \left( \gamma_1 \frac{\partial}{\partial n} \right)^*.$$

### 5. $\mathfrak{M}(z)$ operator associated to a Schrödinger operator in $L^2(\mathbb{R}^3)$

In Section 4, we considered the definition and some of the main properties of  $M(z)$  operators for the exterior unbounded region  $\Omega$ . In particular we have defined, for  $z \in \mathbb{C}^+$ , the operator  $M_0(z) : L^2(S_1) \rightarrow L^2(S_1)$  with Neumann boundary condition at the surface  $S_1$ .

The same ideas and methods can be applied to the theory of  $M$  operators for the interior bounded region  $\Omega_0 = \{x : |x| < 1\}$ . Here we define  $\mathcal{D}_1(\Omega_0)$  to be the set of functions  $g : \Omega_0 \rightarrow \mathbb{C}$  such that  $g, \Delta g$  belong to  $L^2(\Omega_0)$ , with  $\Delta g$  defined in the sense of distributions, and both  $g$  and  $\partial g / \partial n$  have  $L^2$  boundary values on  $S_1$ . We shall denote by  $\mathcal{D}_1(\mathbb{R}^3 \setminus S_1)$  the set of functions  $g : \mathbb{R}^3 \setminus S_1 \rightarrow \mathbb{C}$ , such that the restriction of  $g$  to  $\Omega_0$  belongs to  $\mathcal{D}_1(\Omega_0)$  and the restriction of  $g$  to  $\Omega$  belongs to  $\mathcal{D}_1(\Omega)$ . For functions  $g \in \mathcal{D}_1(\mathbb{R}^3 \setminus S_1)$  we distinguish between the boundary values  $\gamma_1^+ g, \gamma_1^+ \partial g / \partial n$  with  $g$  considered as an element of  $\mathcal{D}_1(\Omega)$  and the boundary values  $\gamma_1^- g, \gamma_1^- \partial g / \partial n$  with  $g$  considered as an element of  $\mathcal{D}_1(\Omega_0)$ . Note that  $\partial g / \partial n$  is always a derivative in the direction of increasing radial coordinate. We suppose that  $q(x)$  is bounded for  $x \in \Omega_0$ .

The operator  $M_0^{\text{int}}(z)$  ( $M$  operator for the interior region  $\Omega_0$  with Neumann condition on  $S_1$ ) is defined for  $z \in \mathbb{C}^+$  as the mapping from  $\gamma_1 \partial f / \partial n$  to  $\gamma_1 f$  for solutions  $f$  in  $\mathcal{D}_1(\Omega_0)$  of  $-\Delta f + qf - zf = 0$ . (Note that in contrast to the definition of  $M_0(z)$ , we map  $\gamma_1 \partial f / \partial n$  to  $\gamma_1 f$  rather than  $-\gamma_1 f$ ; this ensures that  $M_0^{\text{int}}(z)$  will have strictly positive imaginary part.) Previous arguments can easily be adapted to show that  $M_0^{\text{int}}(z)$  is a compact operator from  $L^2(S_1)$  to  $L^2(S_1)$ , with range equal to  $H^1(S_1)$ .

We seek to combine algebraically the operators  $M_0^{\text{int}}(z)$  and  $M_0(z)$  to construct an  $M$  operator for the entire space  $\mathbb{R}^3$ . To do so, we make use of the following lemmas.

**Lemma 9.** *Suppose  $g \in \mathcal{D}_1(\mathbb{R}^3 \setminus S_1)$  is such that  $\gamma_1^+ g = \gamma_1^- g$  and  $\gamma_1^+ \partial g / \partial n = \gamma_1^- \partial g / \partial n$ . Then  $g \in \mathcal{D}_1(\mathbb{R}^3) \equiv H^2(\mathbb{R}^3)$ .*

**Proof.** We must show that  $\Delta g \in L^2(\mathbb{R}^3)$ , where  $\Delta g$  is interpreted as a distributional derivative, with test functions from  $C_0^\infty(\mathbb{R}^3)$ . For  $0 < \varepsilon < 1$ , we denote by  $\mathcal{S}_\varepsilon$  the region  $\mathcal{S}_\varepsilon = \{x : |x| < 1 - \varepsilon\} \cup \{x : |x| > 1 + \varepsilon\}$ . For arbitrary  $\phi \in C_0^\infty(\mathbb{R}^3)$ , integrate over  $\mathcal{S}_\varepsilon$  the identity  $\nabla \cdot (\bar{\phi} \nabla g - g \nabla \bar{\phi}) = \bar{\phi} \Delta g - g \Delta \bar{\phi}$ , and apply the divergence theorem to give

$$\langle \Delta \phi, g \rangle_{\mathcal{S}_\varepsilon} = \langle \phi, \Delta g \rangle_{\mathcal{S}_\varepsilon} + \int_{S_{1+\varepsilon}} \left( \bar{\phi} \frac{\partial g}{\partial n} - g \frac{\partial \bar{\phi}}{\partial n} \right) dS - \int_{S_{1-\varepsilon}} \left( \bar{\phi} \frac{\partial g}{\partial n} - g \frac{\partial \bar{\phi}}{\partial n} \right) dS.$$

From the assumptions regarding the  $L^2$  boundary values of  $g$  and  $\partial g / \partial n$  and the fact that  $\phi$  is a  $C^\infty$  function, it follows that the two boundary integrals, over spheres of radius  $1 + \varepsilon$  and  $1 - \varepsilon$ , respectively, cancel in the limit  $\varepsilon \rightarrow +0$ . Hence, on taking this limit, we have  $|\langle \Delta \phi, g \rangle| \leq \text{const} \|\phi\|$ , where now both inner product and norm are in  $L^2(\mathbb{R}^3)$ . This shows that  $\Delta g \in L^2(\mathbb{R}^3)$ .  $\square$

**Lemma 10.** *Suppose  $q(x)$  is bounded for  $x \in \mathbb{R}^3$ , and let  $z \in \mathbb{C}^+$ . Then, given arbitrary  $v \in L^2(S_1)$ , there exists a unique function  $f$  in  $\mathcal{D}_1(\mathbb{R}^3 \setminus S_1)$  satisfying*

$$-\Delta f + qf - zf = 0 \quad \text{in } \Omega_0 \cup \Omega \tag{5.1}$$

together with the conditions  $\gamma_1^+ f = \gamma_1^- f$  and  $\gamma_1^+ \partial f / \partial n - \gamma_1^- \partial f / \partial n = v$ .

**Proof.** Let  $T$  be the self-adjoint Schrödinger operator  $-\Delta + q$  in  $L^2(\mathbb{R}^3)$ . Recall that  $D(T) = H^2(\mathbb{R}^3)$ .

The uniqueness of the function  $f$  in the Lemma is easily verified, since by Lemma 9 the difference between any two distinct solutions for  $f$  would belong to  $H^2(\mathbb{R}^3)$  and hence would be an eigenfunction of  $T$  with complex eigenvalue.

To prove the existence of a solution for  $f$ , we construct an extension operator  $E : L^2(S_1) \rightarrow \mathcal{D}_1(\mathbb{R}^3 \setminus S_1)$  having the properties that, for arbitrary  $v \in L^2(S_1)$ ,

$$\gamma_1^+ E v = \gamma_1^- E v, \left( \gamma_1^+ \frac{\partial}{\partial n} - \gamma_1^- \frac{\partial}{\partial n} \right) E v = v. \tag{5.2}$$

Explicitly, we can take  $E$  as in the definition of  $E_1^{(0)}$  (see Lemma 1 and Eqs. (2.6), (2.7)), with Eq. (2.8) now replaced by

$$\psi_\ell^{(0)}(r) = \begin{cases} -\frac{\eta(r)r^{\ell+1}}{2\ell+1} & \text{for } r < 1, \\ -\frac{\eta(r)r^{-\ell}}{2\ell+1} & \text{for } r > 1 \end{cases} \tag{5.3}$$

and where  $\eta: \mathbb{R} \rightarrow \mathbb{R}$  is a function of class  $C_0^\infty$  satisfying  $\eta(y) = 0$  in a neighbourhood of  $y = 0$  and  $\eta(y) = 1$  in a neighbourhood of  $y = 1$ .

Note that  $E$  is bounded from  $L^2(S_1)$  to  $\mathcal{D}_1(\mathbb{R}^3 \setminus S_1)$ , where in the image space we use the norm  $\|g\| = \|g\|_{\mathcal{D}_1(\Omega_0)} + \|g\|_{\mathcal{D}_1(\Omega)}$ . Moreover  $Q_1 \equiv \gamma_1^\pm E$  is bounded from  $L^2(S_1)$  to  $H^1(S_1)$ , and hence compact as mapping from  $L^2(S_1)$  to  $L^2(S_1)$ .

The function  $f$  to satisfy Lemma 10 is now given by  $f = -(T - z)^{-1}h + g$ , with  $g = Ev$  and  $h = -\Delta g + qg - zg$ .  $\square$

**Definition 5.** For  $z \in \mathbb{C}^+$ , the operator  $\mathfrak{M}(z): L^2(S_1) \rightarrow L^2(S_1)$  is defined by

$$\mathfrak{M}(z)v = -w, \tag{5.4}$$

where  $w = \gamma_1^\pm f$  and  $f$  is the unique solution, in  $\mathcal{D}_1(\mathbb{R}^3 \setminus S_1)$ , of  $-\Delta f + qf - zf = 0$  subject to the conditions

$$\gamma_1^+ f = \gamma_1^- f, \quad \gamma_1^+ \frac{\partial f}{\partial n} - \gamma_1^- \frac{\partial f}{\partial n} = v. \tag{5.5}$$

The following theorem provides an explicit expression for  $\mathfrak{M}(z)$ .

**Theorem 4.** Suppose  $q(x)$  is bounded for  $x \in \mathbb{R}^3$ , and take  $z \in \mathbb{C}^+$ . Then

$$\mathfrak{M}(z) = \gamma_1[\gamma_1(T - \bar{z})^{-1}]^* \quad (= \gamma_1(T - z)^{-1}\gamma_1^*). \tag{5.6}$$

$\mathfrak{M}(z)$  is bounded for fixed  $z \in \mathbb{C}^+$ , with strictly positive imaginary part, and is analytic in  $z$  (in operator norm).  $\mathfrak{M}(z)$  is given, in terms of the interior and exterior  $M$  operators, by

$$\mathfrak{M}(z) = [(M_0(z))^{-1} + (M_0^{\text{int}}(z))^{-1}]^{-1} \equiv -[m_0(z) + m_0^{\text{int}}(z)]^{-1}. \tag{5.7}$$

**Proof.** Let  $\mathcal{S}_\varepsilon$  be as in the proof of Lemma 9. Take  $\mathfrak{h} \in L^2(\mathbb{R}^3)$  arbitrary, and let  $f$  be as prescribed by Definition 5. With  $\mathfrak{k} = (T - \bar{z})^{-1}\mathfrak{h}$ , we may integrate over  $\mathcal{S}_\varepsilon$  the identity  $\nabla \cdot (\bar{\mathfrak{k}}\nabla f - f\nabla\bar{\mathfrak{k}}) = f\bar{\mathfrak{h}}$  and take the limit  $\varepsilon \rightarrow +0$ . On using the boundary conditions for  $f$  at the surface  $S_1$ , this leads to the result

$$\begin{aligned} \langle \mathfrak{h}, f \rangle_{\mathbb{R}^3} &= \left\langle \gamma_1 \frac{\partial \bar{\mathfrak{k}}}{\partial n}, \gamma_1^+ f \right\rangle_{S_1} - \left\langle \gamma_1 \frac{\partial \bar{\mathfrak{k}}}{\partial n}, \gamma_1^- f \right\rangle_{S_1} - \left\langle \gamma_1 \bar{\mathfrak{k}}, \gamma_1^+ \frac{\partial f}{\partial n} \right\rangle_{S_1} + \left\langle \gamma_1 \bar{\mathfrak{k}}, \gamma_1^- \frac{\partial f}{\partial n} \right\rangle_{S_1} \\ &= -\langle \gamma_1(T - \bar{z})^{-1}\mathfrak{h}, v \rangle_{S_1}. \end{aligned}$$

Hence the mapping from  $v$  to  $-f$  is the adjoint of  $\gamma_1(T - \bar{z})^{-1}$ . Since  $\mathfrak{M}(z)$  maps from  $v$  to  $-\gamma_1^\pm f$ , Eq. (5.6) follows. The remaining properties of  $\mathfrak{M}(z)$  are proved as in previous sections.

Note that a function  $w \in L^2(S_1)$  will belong to the range of  $\mathfrak{M}(z)$  if and only if  $w$  is in the intersection of the respective ranges of  $M_0^{\text{int}}(z)$  and  $M_0(z)$ . Hence  $\text{range } \mathfrak{M}(z) = H^1(S_1)$ , which is also the domain of  $(M_0(z))^{-1} + (M_0^{\text{int}}(z))^{-1}$ .

With  $f$  as above we have

$$(M_0(z))^{-1}\mathfrak{M}(z)v = -(M_0(z))^{-1}\gamma_1^+ f = \gamma_1^+ \frac{\partial f}{\partial n},$$

$$(M_0^{\text{int}}(z))^{-1}\mathfrak{M}(z)v = -(M_0^{\text{int}}(z))^{-1}\gamma_1^- f = -\gamma_1^- \frac{\partial f}{\partial n}.$$

Hence

$$[(M_0(z))^{-1} + (M_0^{\text{int}}(z))^{-1}]\mathfrak{M}(z)v = (\gamma_1^+ - \gamma_1^-) \frac{\partial f}{\partial n} = v$$

and we have verified Eq. (5.7).  $\square$

**Corollary.** For each  $z \in \mathbb{C}^+$ ,  $\mathfrak{M}(z)$  maps  $L^2(S_1)$  onto  $H^1(S_1)$ , and is a compact map from  $L^2(S_1)$  into  $L^2(S_1)$ .

**Proof.** Define an operator  $m(z)$ , the inverse of  $\mathfrak{M}(z)$ , which sends  $\gamma_1^\pm f$  to  $\gamma_1^- \partial f / \partial n - \gamma_1^+ \partial f / \partial n$  for solutions in  $\mathcal{D}_1(\mathbb{R}^3 \setminus S_1)$  of  $-\Delta f + qf - zf = 0$  satisfying  $\gamma_1^+ f = \gamma_1^- f$ . We can then follow similar arguments as for  $m_0(z)$ , using an extension operator  $EQ_1^{-1}$  instead of  $E_1^{(0)}Q^{-1}$  and replacing the Dirichlet resolvent for the exterior region by a direct sum  $(\mathcal{T} - z)^{-1}$  of Dirichlet resolvents for the interior and exterior regions, respectively. As for  $m_0(z)$ , one can prove that  $m(z)$  maps from  $H^1(S_1)$  onto  $L^2(S_1)$ , and the results of the corollary follow as before.  $\square$

The operator  $m(z)$  is given formally by the expression

$$m(z) = (\gamma_1^+ - \gamma_1^-) \frac{\partial}{\partial n} (\mathcal{T} - z)^{-1} \left[ (\gamma_1^+ - \gamma_1^-) \frac{\partial}{\partial n} \right]^* . \tag{5.8}$$

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