

Home Search Collections Journals About Contact us My IOPscience

On the optimization of the principal eigenvalue for single-centre point-interaction operators in a bounded region

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 2008 J. Phys. A: Math. Theor. 41 065305 (http://iopscience.iop.org/1751-8121/41/6/065305) View the table of contents for this issue, or go to the journal homepage for more

Download details: IP Address: 171.66.16.152 The article was downloaded on 03/06/2010 at 07:25

Please note that terms and conditions apply.

J. Phys. A: Math. Theor. 41 (2008) 065305 (15pp)

doi:10.1088/1751-8113/41/6/065305

# On the optimization of the principal eigenvalue for single-centre point-interaction operators in a bounded region

# Pavel Exner<sup>1,2</sup> and Andrea Mantile<sup>2,3</sup>

<sup>1</sup> Department of Theoretical Physics, NPI, Academy of Sciences, 25068 Řež near Prague, Prague, Czech Republic

<sup>2</sup> Doppler Institute, Czech Technical University, Břehová 7, 11519 Prague, Czechia

<sup>3</sup> IRMAR, Université Rennes 1, Campus de Beaulieu, 35042, Rennes Cedex, France

Received 28 November 2007, in final form 18 December 2007 Published 29 January 2008 Online at stacks.iop.org/JPhysA/41/065305

## Abstract

We investigate relations between spectral properties of a single-centre pointinteraction Hamiltonian describing a particle confined to a bounded domain  $\Omega \subset \mathbb{R}^d$ , d = 2, 3, with a Dirichlet boundary, and the geometry of  $\Omega$ . For this class of operators, Krein's formula yields an explicit representation of the resolvent in terms of the integral kernel of the unperturbed one,  $(-\Delta_{\Omega}^D + z)^{-1}$ . We use a moving plane analysis to characterize the behaviour of the groundstate energy of the Hamiltonian with respect to the point-interaction position and the shape of  $\Omega$ , in particular, we establish some conditions showing how to place the interaction to optimize the principal eigenvalue.

PACS numbers: 03.65.Ge, 03.65.Db

## 1. Introduction

Relations between the geometry of a domain and spectral properties of corresponding operators belong to the most traditional question in mathematical physics; one can recall, e.g., the Faber–Krahn inequality [Fa23, Kr25] or the Payne–Pólya-Weinberger conjecture [PPW55] proved by Ashbaugh and Benguria [AB92a, AB92b]. A particular example concerns the situation where the domain in question is not simply connected. For instance, one may ask how to place a hard wall obstacle in a given domain so as to optimize the fundamental energy of the corresponding Dirichlet Laplacian. This question was first posed by Hersch [He63] who found that a doubly connected fixed membrane, bounded by two circles of given radii, has a maximal ground-state energy when the two circles are concentric. More recently, some rather explicit minimizing conditions have been obtained in the analogous problem for the Dirichlet Laplacian on multiply connected *n*-dimensional domains of a general shape [HKK01]; for the

particular case of a circular hard wall obstacle in a disc, it appears that the minimum is reached when the obstacle touches the boundary.

In connection with the last-mentioned problem one can also ask what happens if such a 'hard' obstacle is replaced by another object, say, by a potential barrier or well. In this paper we are going to address this question in the particular case when such a potential is singular, in other words, a point interaction. Recalling basic results about these interactions [AGHH05] we see that the problem makes sense in dimension  $d \leq 3$ . Furthermore, a simple perturbative argument shows that in the one-dimensional situation the answer may depend on the sign of the  $\delta$  potential; we restrict here our attention to the more singular case of dimension d = 2, 3.

Problems of this type were to our knowledge solved so far only in cases where the domain has a simple geometry such as a straight strip in  $\mathbb{R}^2$ , see [EGŠT96], or a planar layer in  $\mathbb{R}^3$ , see [EN02], where the eigenvalue problem can be solved more or less explicitly. Here we consider that the domain  $\Omega$ , to which the particle is confined, is bounded and otherwise quite general, see below. The operator of interest will be the corresponding Dirichlet Laplacian perturbed by a single-point interaction of a fixed coupling constant; we will ask about the dependence of its principal eigenvalue on the perturbation position. Using a figurative expression, to be made precise below, we are going to show that the ground-state energy *increases* as the point moves towards the boundary of  $\Omega$ , in contrast to the case of a Dirichlet obstacle mentioned above.

Our method is based on the fact that one is able to express the resolvent of the operator in question by means of Krein's formula. The resulting spectral condition allows us to characterize the principal eigenvalue as a function of the interaction position in a non-perturbative setting. Then we exploit the maximum principle and a domain reflection technique, analogous to that used in [HKK01], to demonstrate our main result, theorem 4.3, expressing strict monotonicity of the principal eigenvalue with respect to certain directions. Using this conclusion, we formulate then some conditions under which the eigenvalue reaches its minimum value for a fixed  $\Omega$ .

#### 2. Confined point interactions in two and three dimensions

The definition domain and the spectral properties of point interaction Hamiltonians in dimensions two and three are usually expressed in terms of the free Green function, i.e. the integral kernel of the operator  $(-\Delta + z)^{-1}$ , cf [AGHH05]. This is true both if the configuration space is the whole  $\mathbb{R}^d$  or if the particle is confined to a subset  $\Omega$  of it by a hard wall corresponding to the Dirichlet boundary condition. In the latter case Green's function is defined by the equation

$$\begin{cases} (-\Delta + z)\mathcal{G}_0^z(\underline{x}, \underline{x}') = \delta(\underline{x} - \underline{x}') \\ \mathcal{G}_0^z(\underline{x}, \underline{x}')\big|_{x \in \partial\Omega} = 0 \end{cases}; \qquad \underline{x}' \in \Omega,$$
(2.1)

which admits a solution in  $L^2(\Omega)$  whenever -z does not belong to the spectrum of the Dirichlet Laplacian  $-\Delta_{\Omega}^{D}$  defined in the standard way through the associated quadratic form [RS78]. Throughout this paper,  $\Omega$  is supposed to be an open regular set in  $\mathbb{R}^d$ , d = 2, 3, bounded and connected, not necessarily simply; we assume that  $\partial \Omega$  is piecewise  $C^1$ .

Under these hypotheses  $-\Delta_{\Omega}^{D}$  has a purely discrete spectrum; we denote by  $\{\lambda_{n}\}_{n \in \mathbb{N}_{0}}$ , where  $\mathbb{N}_{0} := \mathbb{N} \cup \{0\}$ , its eigenvalues, and by  $\{\psi_{n,k}\}|k = 1, \ldots, N_{n}, n \in \mathbb{N}_{0}$  the corresponding system of eigenfunctions,  $N_{n}$  being the multiplicity of the *n*th eigenvalue. Projecting (2.1) on the vectors  $\psi_{n,k}$ , it is easy to check the validity of the following standard Fourier expansion of  $\mathcal{G}_0^z$ ,

$$\mathcal{G}_0^z(\underline{x}, \underline{x}') = \sum_{\substack{n \in \mathbb{N}_0 \\ k \leqslant N_n}} \frac{\psi_{n,k}(\underline{x}')\psi_{n,k}(\underline{x})}{\lambda_n + z}.$$
(2.2)

An alternative representation of the kernel, which will be extensively used in this paper, can be given in terms of the 'free' Green's function  $\mathcal{G}^{z}(\underline{x}, \underline{x}')$ , in other words, the integral kernel of  $(-\Delta + z)^{-1}$  in the whole space<sup>4</sup>,

$$\mathcal{G}^{z}(\underline{x}, \underline{x}') = \frac{1}{2\pi} K_{0}(\sqrt{z}|\underline{x} - \underline{x}'|) \qquad \text{in} \quad \mathbb{R}^{2}$$
(2.3)

$$\mathcal{G}^{z}(\underline{x}, \underline{x}') = \frac{e^{-\sqrt{z}|\underline{x}-\underline{x}'|}}{4\pi|\underline{x}-\underline{x}'|} \qquad \text{in} \quad \mathbb{R}^{3}.$$
(2.4)

Here  $K_0$  denotes the Macdonald (or modified Hankel) function. Using the boundary conditions in (2.1), we can express the kernel of interest as

$$\mathcal{G}_0^z(\underline{x}, \underline{x}') = \mathcal{G}^z(\underline{x}, \underline{x}') - h(\underline{x}, \underline{x}', \sqrt{z}), \qquad (2.5)$$

where  $\mathcal{G}^z$  is defined by (2.3) and (2.4) and  $h(\underline{x}, \underline{x}', \sqrt{z})$  solves the boundary value problem

$$\begin{cases} (-\Delta+z)h(\underline{x},\underline{x}',\sqrt{z}) = 0\\ h(\underline{x},\underline{x}',\sqrt{z})\Big|_{\underline{x}\in\partial\Omega} = \mathcal{G}^{z}(\underline{x},\underline{x}')\Big|_{\underline{x}\in\partial\Omega} & \text{for any } \underline{x}'\in\Omega. \end{cases}$$
(2.6)

In the next step we construct the operator which will be our main object perturbing  $-\Delta_{\Omega}^{D}$  by a single point interaction with the support at a point  $\underline{x}_{0} \in \Omega$ . Such Hamiltonians are defined by the self-adjoint extensions of the symmetric operator

$$\begin{cases} D(H_0) = \left\{ \psi \in H^2 \cap H_0^1(\Omega) \middle| \psi(\underline{x}_0) = 0 \right\} \\ H_0 \psi = -\Delta \psi. \end{cases}$$
(2.7)

Following the von Neumann theory [AG63, RS75], we observe that the restriction (2.7) has deficiency indices (1, 1); consequently, we arrive at a one-parameter family of self-adjoint operators  $H_{\alpha}$ . For fixed  $\alpha \in \mathbb{R}, \lambda \in \mathbb{C} \setminus \mathbb{R}$  and a domain  $\Omega \subset \mathbb{R}^2$  we have

$$D(H_{\alpha}) = \left\{ \psi \in L^{2}(\Omega) \middle| \psi = \phi^{\lambda} + q \mathcal{G}_{0}^{\lambda}(\cdot, \underline{x}_{0}), \phi^{\lambda} \in H^{2} \cap H_{0}^{1}(\Omega), \\ \phi^{\lambda}(\underline{x}_{0}) = \frac{q}{2\pi} (\alpha - \ln \sqrt{\lambda} - 2\pi h(\underline{x}_{0}, \underline{x}_{0}, \sqrt{\lambda})) \right\}$$
(2.8)

while for  $\Omega \subset \mathbb{R}^3$  the operator domain is

$$D(H_{\alpha}) = \left\{ \psi \in L^{2}(\Omega) \middle| : \psi = \phi^{\lambda} + q \mathcal{G}_{0}^{\lambda}(\cdot, \underline{x}_{0}), \phi^{\lambda} \in H^{2} \cap H_{0}^{1}(\Omega), \\ \phi^{\lambda}(\underline{x}_{0}) = q \left( \alpha + \frac{\sqrt{\lambda}}{4\pi} + h(\underline{x}_{0}, \underline{x}_{0}, \sqrt{\lambda}) \right) \right\}.$$

$$(2.9)$$

In both cases the parameter  $\lambda$  determines a representation of the operator domain, roughly speaking, a split between the regular and singular part; for a fixed choice of  $\lambda$  the action of  $H_{\alpha}$  is the following:

$$H_{\alpha}\psi = -\Delta\phi^{\lambda} - \lambda q \mathcal{G}_{0}^{\lambda}(\cdot, \underline{x}_{0}).$$
(2.10)

<sup>4</sup> Here and in the following we use the convention in which the negative real axis represents the cut of the square root  $\sqrt{z}$  in the complex plane.

It is convenient to include into this description also infinite values of the parameter  $\alpha$ , in which case the coefficient q of the singular part—sometimes referred to as the *charge* of the state—vanishes. It is equivalent to the absence of the point interaction: the domain reduces in this case to  $H^2 \cap H_0^1(\Omega)$  and the self-adjoint extensions corresponding to  $\alpha = \pm \infty$  are identified with the unperturbed operator  $-\Delta_{\Omega}^{D}$ .

Making use of Krein's formula [AG63] the action of the resolvent,  $R_z^{\alpha} = (H_{\alpha} + z)^{-1}$ on  $L^2(\Omega)$ , can be expressed as a rank-1 perturbation of its 'free' counterpart  $(-\Delta + z)^{-1}$ , specifically

$$R_z^{\alpha}\varphi = (-\Delta + z)^{-1}\varphi + q_z((-\Delta + z)^{-1}\varphi)(\underline{x}_0)\mathcal{G}_0^z(\cdot, \underline{x}_0).$$
(2.11)

In this formula, of course, the first term is the regular part of the function  $R_z^{\alpha}\varphi \in D(H_{\alpha})$ while the value  $q_z((-\Delta + z)^{-1}\varphi)(\underline{x}_0)$  denotes the corresponding charge. Using the boundary conditions in (2.8) and (2.9) we can identify the coefficient  $q_z$  with

$$q_z = (\alpha - \ln \sqrt{z} - 2\pi h(\underline{x}_0, \underline{x}_0, \sqrt{z}))^{-1}, \qquad \Omega \subset \mathbb{R}^2$$
(2.12)

$$q_z = \left(\alpha + \frac{\sqrt{z}}{4\pi} + h(\underline{x}_0, \underline{x}_0, \sqrt{z})\right)^{-1}, \qquad \Omega \subset \mathbb{R}^3.$$
(2.13)

Furthermore, the Fourier expansion

$$(-\Delta+z)^{-1}\varphi = \sum_{\substack{n \in \mathbb{N}_0 \\ k \leqslant N_n}} \frac{(\varphi, \psi_{n,k})}{\lambda_n + z} \psi_{n,k}$$
(2.14)

yields the following explicit expression

$$R_{z}^{\alpha}\varphi = \sum_{\substack{n \in \mathbb{N}_{0} \\ k \leqslant N_{n}}} \frac{(\varphi, \psi_{n,k})}{\lambda_{n} + z} \psi_{n,k} + 2\pi \sum_{\substack{n \in \mathbb{N}_{0} \\ k \leqslant N_{n}}} \frac{(\varphi, \psi_{n,k})}{\lambda_{n} + z} \frac{\psi_{n,k}(\underline{x}_{0})}{\alpha - \ln\sqrt{z} - 2\pi h(\underline{x}_{0}, \underline{x}_{0}, \sqrt{z})} \mathcal{G}_{0}^{z}(\cdot, \underline{x}_{0})$$

$$(2.15)$$

for  $\Omega \subset \mathbb{R}^2,$  and its counterpart

$$R_{z}^{\alpha}\varphi = \sum_{\substack{n \in \mathbb{N}_{0} \\ k \leqslant N_{n}}} \frac{(\varphi, \psi_{n,k})}{\lambda_{n} + z} \psi_{n,k} + \sum_{\substack{n \in \mathbb{N}_{0} \\ k \leqslant N_{n}}} \frac{(\varphi, \psi_{n,k})}{\lambda_{n} + z} \frac{\psi_{n,k}(\underline{x}_{0})}{\alpha + \frac{\sqrt{z}}{4\pi} + h(\underline{x}_{0}, \underline{x}_{0}, \sqrt{z})} \mathcal{G}_{0}^{z}(\cdot, \underline{x}_{0})$$
(2.16)

for  $\Omega \subset \mathbb{R}^3$ .

# 3. The principal eigenvalue of $H_{\alpha}$

As usual, the Krein formula allows us to determine the spectrum through the denominator of the perturbation term. In particular, it follows from resolvent equations (2.15) and (2.16) that the spectrum of  $H_{\alpha}$  is formed by the solutions of the equations

$$\alpha - \ln \sqrt{-\xi} - 2\pi h(\underline{x}_0, \underline{x}_0, \sqrt{-\xi}) = 0, \qquad \Omega \subset \mathbb{R}^2$$
  
$$\alpha + \frac{\sqrt{-\xi}}{4\pi} + h(\underline{x}_0, \underline{x}_0, \sqrt{-\xi}) = 0, \qquad \Omega \subset \mathbb{R}^3$$
  
(3.1)

to which one has to add eigenvalues of  $-\Delta_{\Omega}^{D}$ , the degenerate ones in any case and the nondegenerate ones,  $\lambda_{\bar{n}}$ , provided that the corresponding eigenfunction  $\psi_{\bar{n}}$  satisfies the condition (see, e.g. in [BFM07])

$$\psi_{\bar{n}}(\underline{x}_0) = 0. \tag{3.2}$$

This does not concern, however, the bottom of the spectrum which we are interested in here, because the ground state of  $-\Delta_D^{\Omega}$  is non-degenerate and can be represented by a positive function.

The subject of this section is the principal eigenvalue of the point-interaction operator  $H_{\alpha}$ . We are going to show, in particular, that for any  $\alpha \in \mathbb{R}$  there exists a unique simple eigenvalue of  $H_{\alpha}$  below the spectral threshold of  $-\Delta_{\Omega}^{D}$ . As a preliminary, we need to characterize the derivatives of  $h(\underline{x}_{0}, \underline{x}_{0}, \sqrt{z})$  with respect to the variable  $\sqrt{z}$ .

**Lemma 3.1.** Let z be a positive real number; the function  $y \mapsto h(\underline{x}, \underline{x}', y)$ , defined by (2.6) with  $y := \sqrt{z}$ , satisfies the conditions

$$\frac{1}{y} \left( \frac{1}{y} + 2\pi \partial_y h(\underline{x}', \underline{x}', y) \right) > 0, \qquad \Omega \subset \mathbb{R}^2$$

$$\frac{1}{y} \left( \frac{1}{4\pi} + \partial_y h(\underline{x}', \underline{x}', y) \right) > 0, \qquad \Omega \subset \mathbb{R}^3.$$
(3.3)

Furthermore, for any z < 0 and  $h(\underline{x}, \underline{x}', iy)$ , defined by (2.6) with  $y := \sqrt{|z|}$ , we have

$$\frac{\pi}{2} + 2\pi \operatorname{Im} h(\underline{x}', \underline{x}', \mathrm{i}y) = 0, \qquad \Omega \subset \mathbb{R}^2$$

$$\frac{y}{4\pi} + \operatorname{Im} h(\underline{x}', \underline{x}', \mathrm{i}y) = 0, \qquad \Omega \subset \mathbb{R}^3$$
(3.4)

and

$$\frac{1}{y} + 2\pi \partial_y \operatorname{Re} h(\underline{x}', \underline{x}', \mathrm{i}y) < 0, \qquad \Omega \subset \mathbb{R}^2$$
  
$$\partial_y \operatorname{Re} h(\underline{x}', \underline{x}', \mathrm{i}y) < 0, \qquad \Omega \subset \mathbb{R}^3.$$
(3.5)

**Proof.** We start with the 3D case. Let  $z_j$ , j = 1, 2, be a pair of positive values; setting  $y_j := \sqrt{z_j}$  we obtain from equation (2.5) in combination with the first resolvent formula the relation

$$(y_1^2 - y_2^2) (\mathcal{G}_0^{y_1^2}, \mathcal{G}_0^{y_2^2})_{L^2(\Omega)} = \lim_{\underline{x} \to \underline{x'}} \left[ \mathcal{G}^{y_2^2}(\underline{x}, \underline{x'}) - \mathcal{G}^{y_1^2}(\underline{x}, \underline{x'}) \right] + h(\underline{x'}, \underline{x'}, y_1) - h(\underline{x'}, \underline{x'}, y_2),$$

$$(3.6)$$

where  $(\cdot, \cdot)_{L^2(\Omega)}$  denotes the scalar product in  $L^2(\Omega)$ . The limit on the rhs is easily seen to be

$$\lim_{\underline{x}\to\underline{x}'} [\mathcal{G}^{y_2^2}(\underline{x},\underline{x}') - \mathcal{G}^{y_1^2}(\underline{x},\underline{x}')] = \frac{1}{4\pi} (y_1 - y_2).$$
(3.7)

Substituting this expression into (3.6) we obtain

$$(y_1 + y_2) \left( \mathcal{G}_0^{y_1^2}, \mathcal{G}_0^{y_2^2} \right)_{L^2(\Omega)} = \frac{1}{4\pi} + \frac{h(\underline{x}', \underline{x}', y_1) - h(\underline{x}', \underline{x}', y_2)}{y_1 - y_2},$$
(3.8)

and consequently, in the limit  $y_1 \rightarrow y_2$  we arrive at

$$\frac{1}{4\pi} + \partial_y h(\underline{x}', \underline{x}', y_2) = 2y_2 \left\| \mathcal{G}_0^{y_2^2} \right\|_{L^2(\Omega)}^2 > 0.$$
(3.9)

On the other hand, for negative values of z a similar argument yields

$$(y_1^2 - y_2^2) (\mathcal{G}_0^{-y_1^2}, \mathcal{G}_0^{-y_2^2})_{L^2(\Omega)} = \lim_{\underline{x} \to \underline{x}'} [\mathcal{G}^{-y_1^2}(\underline{x}, \underline{x}') - (\mathcal{G}^{-y_2^2})^*(\underline{x}, \underline{x}')] - h(\underline{x}', \underline{x}', \mathrm{i}y_1) + h^*(\underline{x}', \underline{x}', \mathrm{i}y_2)$$
(3.10)

with the asterisk denoting complex conjugation and  $y_j := \sqrt{|z_j|}$ . The limit on the rhs is

$$\lim_{\underline{x}\to\underline{x}'} [\mathcal{G}^{-y_1^2}(\underline{x},\underline{x}') - (\mathcal{G}^{-y_2^2})^*(\underline{x},\underline{x}')] = -\frac{1}{4\pi}(y_1 + y_2)$$
(3.11)

from which we obtain a relation replacing (3.8), namely

$$\left(y_1^2 - y_2^2\right) \left(\mathcal{G}_0^{-y_1^2}, \mathcal{G}_0^{-y_2^2}\right)_{L^2(\Omega)} = -\frac{\mathrm{i}}{4\pi} \left(y_1 + y_2\right) - h(\underline{x}', \underline{x}', \mathrm{i}y_1) + h^*(\underline{x}', \underline{x}', \mathrm{i}y_2).$$
(3.12)

The second one of the relations (3.4) then follows from here by setting  $y_1 = y_2$ . As for the real part of (3.10) given by

$$\frac{1}{2} \left( y_1^2 - y_2^2 \right) \left[ \left( \mathcal{G}_0^{-y_1^2}, \mathcal{G}_0^{-y_2^2} \right)_{L^2(\Omega)} + \left( \mathcal{G}_0^{-y_2^2}, \mathcal{G}_0^{-y_1^2} \right)_{L^2(\Omega)} \right] \\ = \lim_{\underline{x} \to \underline{x}'} [\operatorname{Re} \mathcal{G}^{-y_1^2}(\underline{x}, \underline{x}') - \operatorname{Re} \mathcal{G}^{-y_2^2}(\underline{x}, \underline{x}')] - \operatorname{Re} h(\underline{x}', \underline{x}', \mathrm{i}y_1) + \operatorname{Re} h(\underline{x}', \underline{x}', \mathrm{i}y_2)$$
(3.13)

we note that the first term on the rhs is in fact zero; dividing the remaining ones by  $y_1 - y_2$ and taking the limit as  $y_1 \rightarrow y_2$ , we arrive at

$$-\partial_{y} \operatorname{Re} h(\underline{x}', \underline{x}', \mathrm{i}y_{2}) = 2y_{2} \left\| \mathcal{G}_{0}^{-y_{2}^{2}} \right\|_{L^{2}(\Omega)}^{2} > 0.$$
(3.14)

In the 2D case the validity of relations (3.3), (3.4) and (3.5) can be checked following the same idea. Taking into account the logarithmic singularity of  $\mathcal{G}^{z}(\underline{x}, \underline{x}')$  as  $\underline{x} \to \underline{x}'$ —see, e.g., [AS72]—we find for z > 0

$$\lim_{\underline{x} \to \underline{x}'} \left[ \mathcal{G}^{y_2^2}(\underline{x}, \underline{x}') - \mathcal{G}^{y_1^2}(\underline{x}, \underline{x}') \right] = \frac{1}{2\pi} (\ln y_1 - \ln y_2),$$
(3.15)

while for z < 0 we have

$$\lim_{\underline{x}\to\underline{x}'} \left[ \mathcal{G}^{-y_1^2}(\underline{x},\underline{x}') - (\mathcal{G}^{-y_2^2})^*(\underline{x},\underline{x}') \right] = \frac{1}{2\pi} (-i\pi + \ln y_1 - \ln y_2); \quad (3.16)$$

this concludes the proof.

In the next two lemmata, we deal with the solutions of equations (3.1) below the spectrum of  $-\Delta_{\Omega}^{D}$ . We are going to show that for a fixed real  $\alpha$  there is a unique such solution. It is convenient to treat the 2D and 3D cases separately.

**Lemma 3.2.** Let  $\lambda_0$  denote the first eigenvalue of  $-\Delta_{\Omega}^D$  corresponding to the domain  $\Omega \subset \mathbb{R}^3$ . For any  $\alpha \in \mathbb{R}$ , the equation

$$\alpha + \frac{\sqrt{-\xi}}{4\pi} + h(\underline{x}_0, \underline{x}_0, \sqrt{-\xi}) = 0, \qquad \xi \in (-\infty, \lambda_0)$$
(3.17)

admits a unique solution, denoted  $\xi(\alpha)$ , such that

$$\lim_{\alpha \to -\infty} \xi(\alpha) = -\infty, \qquad \xi(-h(\underline{x}_0, \underline{x}_0, 0)) = 0, \tag{3.18}$$

and

$$\lim_{\alpha \to +\infty} \xi(\alpha) = \lambda_0. \tag{3.19}$$

**Proof.** In order to study solutions of (3.17), we need to find the dependence of  $h(\underline{x}_0, \underline{x}_0, \sqrt{-\xi})$  on the variable  $\sqrt{-\xi}$ . We start by considering the case  $\xi \leq 0$ . Setting  $y = \sqrt{|\xi|}$ , equation (3.17) assumes the form

$$\frac{y}{4\pi} = -\alpha - h(\underline{x}_0, \underline{x}_0, y) = 0, \qquad y \ge 0$$
(3.20)

and its solutions can be geometrically interpreted as the abscissas of the intersection points between the curves at the left- and the right-hand side of (3.20). We will show that for any fixed

choice of  $\underline{x}_0 \in \Omega$ ,  $h(\underline{x}_0, \underline{x}_0, y)$  is a positive and strictly decreasing function of the variable y, such that

$$\lim_{y \to +\infty} h(\underline{x}_0, \underline{x}_0, y) = 0.$$
(3.21)

Let us consider the boundary value problem

$$\begin{cases} (-\Delta + y^2)h(\underline{x}, \underline{x}_0, y) = 0\\ h(\underline{x}, \underline{x}_0, y)\Big|_{\underline{x} \in \partial \Omega} = \frac{e^{-y|\underline{x} - \underline{x}_0|}}{4\pi |\underline{x} - \underline{x}_0|}\Big|_{\underline{x} \in \partial \Omega}; \qquad (3.22) \end{cases}$$

The solution of (3.22) is infinitely smooth in the open set  $\Omega$ , continuous and positive on its boundary. The strong maximum principle—cf [Ev98]—in this case allows us to claim that *h* is strictly positive in  $\Omega$  reaching its maximum on the boundary,

$$0 < h(\underline{x}, \underline{x}_0, y) < \sup_{\underline{x'} \in \partial\Omega} \frac{e^{-y|\underline{x'} - \underline{x}_0|}}{4\pi |\underline{x'} - \underline{x}_0|} \qquad \text{for} \quad \forall \underline{x} \in \Omega, \, y \ge 0.$$
(3.23)

Furthermore. the derivative  $\partial_{y}h$  satisfies the equation

$$\begin{cases} (-\Delta + y^2)\partial_y h(\underline{x}, \underline{x}_0, y) = -2yh(\underline{x}, \underline{x}_0, y) \\ \partial_y h(\underline{x}, \underline{x}_0, y)\Big|_{\underline{x} \in \partial\Omega} = -\frac{e^{-y|\underline{x}-\underline{x}_0|}}{4\pi}\Big|_{\underline{x} \in \partial\Omega} \qquad (3.24) \end{cases}$$

the solution of which belongs to  $C^2(\Omega) \cap C(\overline{\Omega})$  in view of the regularity of the source term and the boundary value. The maximum principle—see the version given in [Br83, Thm IX.27]—in this case implies

$$\partial_y h(\underline{x}, \underline{x}_0, y) < 0 \quad \text{for} \quad \forall \underline{x} \in \Omega, y > 0.$$
 (3.25)

In particular, the solution of (3.24) for y = 0 is  $\partial_y h(\underline{x}, \underline{x}_0, 0) = -\frac{1}{4\pi}$ . This characterization of  $h(\underline{x}_0, \underline{x}_0, y)$  allows us to claim that the equation (3.20) admits at least one solution for any  $\alpha \in (-\infty, -h(\underline{x}_0, \underline{x}_0, 0)]$  and that the conditions (3.18) hold. Moreover, the second one of the relations (3.3) in lemma 3.1 implies the monotonicity of the function  $\alpha \mapsto y(\alpha)$  implicitly defined by (3.20); this grants the uniqueness of the solution.

Next we turn to (3.17) for  $\xi \in (0, \lambda_0)$ . In this case, setting  $y := \sqrt{\xi}$ , the equation reads as

$$\alpha + \frac{1y}{4\pi} + h(\underline{x}_0, \underline{x}_0, iy) = 0.$$
(3.26)

According to the second one of the relations (3.4), this is equivalent to

$$\alpha + \operatorname{Re} h(\underline{x}_0, \underline{x}_0, \mathrm{i}y) = 0, \qquad (3.27)$$

where  $\operatorname{Re} h$  satisfies the boundary value problem

$$\begin{cases} (-\Delta - y^2) \operatorname{Re} h(\underline{x}, \underline{x}_0, iy) = 0\\ \operatorname{Re} h(\underline{x}, \underline{x}_0, y)|_{\underline{x} \in \partial \Omega} = \frac{\cos y |\underline{x} - \underline{x}_0|}{4\pi |\underline{x} - \underline{x}_0|} \Big|_{\underline{x} \in \partial \Omega}; & (3.28) \end{cases}$$

It is worthwhile to note that  $h(\underline{x}, \underline{x}_0, y)$  is not defined for  $y = \sqrt{\lambda_0}$ . In particular, one can show that<sup>5</sup>

$$\lim_{|\varepsilon|\to 0} \|\varepsilon h(\cdot, \underline{x}_0, i\sqrt{\lambda_0 - \varepsilon}) + \psi_0(\underline{x}_0)\psi_0(\cdot)\|_{L^2(U)} = 0,$$
(3.29)

<sup>5</sup> Relation (3.29) easily follows, e.g., from lemma 2 in [BFM07].

where  $\psi_0$  is the principal eigenstate of the Dirichlet Laplacian and U is any subset of  $\Omega$ . In view of the boundedness of  $\psi_0$  and the arbitrariness of U, this relation also implies

$$\lim_{y \to \sqrt{\lambda_0}} |h(\underline{x}_0, \underline{x}_0, \mathbf{i}y)| = +\infty.$$
(3.30)

Using this result together with the conditions (3.4) and (3.5) of lemma 3.1, we conclude that Re  $h(\underline{x}_0, \underline{x}_0, iy)$  is a strictly decreasing function of  $y \in (0, \sqrt{\lambda_0})$  whose behaviour for  $y \to \sqrt{\lambda_0}$  is given by

$$\lim_{y \to \sqrt{\lambda_0}} \operatorname{Re} h(\underline{x}_0, \underline{x}_0, \mathrm{i}y) = -\infty.$$
(3.31)

Summing up this discussion, equation (3.27) has a unique positive solution  $y = y(\alpha)$  for any  $\alpha \in (-h(\underline{x}_0, \underline{x}_0, 0), +\infty)$ , and this solution asymptotically approaches the value  $\lambda_0$  as  $\alpha \to +\infty$ ; in combination with the first part this concludes the proof of the lemma.

Next we deal with the eigenvalue equation in the two-dimensional case. Recall that the free Green's function related to this problem is the modified Bessel function  $K_0$ , which is strictly positive and convex in  $\mathbb{R}^+$  and admits the following representation [AS72]

$$K_0(x) = -\left\{\ln\frac{x}{2} + \gamma\right\} I_0(x) + \sum_{n=1}^{+\infty} c_n \frac{x^{2n}}{(2n!)^{2n}},$$
(3.32)

where  $\gamma \approx 0.577$  is the Euler–Mascheroni constant,  $c_n = \sum_{k=1}^{n} \frac{1}{k}$ , and  $I_0(x)$  is the other modified Bessel function given by the series

$$I_0(x) = \sum_{n=0}^{+\infty} \frac{x^{2n}}{(2n!)^{2n}}.$$
(3.33)

In the following proof we will make use of the asymptotic properties of  $K_0$ ,

$$\lim_{x \to 0^+} K_0(x) = +\infty, \qquad \lim_{x \to +\infty} K_0(x) = 0.$$
(3.34)

**Lemma 3.3.** Let  $\lambda_0$  denote the first eigenvalue of  $-\Delta_{\Omega}^D$  corresponding to the domain  $\Omega \subset \mathbb{R}^2$ . For any  $\alpha \in \mathbb{R}$ , the equation

$$\alpha - \ln \sqrt{-\xi} - 2\pi h(\underline{x}_0, \underline{x}_0, \sqrt{-\xi}) = 0, \qquad \xi \in (-\infty, \lambda_0), \qquad (3.35)$$

admits an unique solution, denoted  $\xi(\alpha)$ , such that

$$\lim_{\alpha \to +\infty} \xi(\alpha) = -\infty, \qquad \xi(f(\underline{x}_0, \underline{x}_0, 0)) = 0, \tag{3.36}$$

and

$$\lim_{\alpha \to -\infty} \xi(\alpha) = \lambda_0, \tag{3.37}$$

where  $f(\underline{x}, \underline{x}_0, \sqrt{-\xi})$  in the second one of the relations (3.36) is a  $C^{+\infty}(\Omega) \cap C(\overline{\Omega})$ -regular function of both the spatial variables defined by

$$f(\underline{x}, \underline{x}_0, \sqrt{-\xi}) = 2\pi h(\underline{x}, \underline{x}_0, \sqrt{-\xi}) + \ln \sqrt{-\xi} I_0(\sqrt{-\xi} |\underline{x} - \underline{x}_0|), \qquad \xi < \lambda_0.$$
(3.38)

**Proof.** The argument follows the same line as in lemma 3.2, the main difference coming from the specific form of the Green functions in two dimensions. For  $\xi \leq 0$  and  $y := \sqrt{|\xi|}$ , equation (3.35) reads

$$\alpha = \ln y + 2\pi h(\underline{x}_0, \underline{x}_0, y), \tag{3.39}$$

where  $h(\underline{x}, \underline{x}_0, \sqrt{y})$ , the solution of the boundary value problem

$$\begin{cases} (-\Delta + y^2)h(\underline{x}, \underline{x}_0, y) = 0\\ h(\underline{x}, \underline{x}_0, y)\Big|_{\underline{x} \in \partial \Omega} = \frac{1}{2\pi} K_0(y|\underline{x} - \underline{x}_0|)\Big|_{\underline{x} \in \partial \Omega}; \qquad (3.40) \end{cases}$$

is strictly positive in  $\Omega$ , as it follows from the maximum principle and the positivity of the boundary values. Consequently, the rhs of (3.39) diverges as  $y \to +\infty$ . Moreover, from (3.3) we know that  $\ln y + 2\pi h(\underline{x}_0, \underline{x}_0, y)$  is strictly increasing as a function of y in the whole  $\mathbb{R}^+$ . In order to study the behaviour for  $y \to 0$ , we introduce the auxiliary function  $f(\underline{x}, \underline{x}_0, y)$ , defined in (3.38) which solves the boundary value problem

$$\begin{cases} (-\Delta + y^2) f(\underline{x}, \underline{x}_0, y) = 0\\ h(\underline{x}, \underline{x}_0, y) \Big|_{\underline{x} \in \partial \Omega} = \frac{1}{2\pi} K_0(y |\underline{x} - \underline{x}_0|) + \ln y I_0(\sqrt{-\xi} |\underline{x} - \underline{x}_0|) \Big|_{\underline{x} \in \partial \Omega} ; \qquad \underline{x}_0 \in \Omega. \end{cases}$$

$$(3.41)$$

Using the definition (3.33), it is easy to verify that the quantity  $\ln y + 2\pi h(\underline{x}_0, \underline{x}_0, y)$  coincides with the value of f in  $\underline{x}_0$ , thus for  $y \to 0^+$  we have

$$\lim_{y \to 0^+} (\ln y + 2\pi h(\underline{x}_0, \underline{x}_0, y)) = \lim_{y^+ \to 0} f(\underline{x}_0, \underline{x}_0, y).$$

In this limit, the problem (3.41) simplifies to

$$\begin{cases} -\Delta f(\underline{x}, \underline{x}_0, 0) = 0\\ h(\underline{x}, \underline{x}_0, 0) \Big|_{\underline{x} \in \partial \Omega} = -\frac{1}{2\pi} \left\{ \ln \frac{|\underline{x} - \underline{x}_0|}{2} + \gamma \right\} \Big|_{\underline{x} \in \partial \Omega}; \quad \underline{x}_0 \in \Omega, \quad (3.42) \end{cases}$$

where the representation (3.32) has been considered; the regularity of the boundary condition in (3.42) implies  $f(\underline{x}, \underline{x}_0, 0) \in C^{+\infty}(\Omega) \cap C(\overline{\Omega})$ . So far we have shown that  $(\ln y + 2\pi h(\underline{x}_0, \underline{x}_0, y))$  is a strictly increasing function of  $y \in \mathbb{R}^+$  such that

$$\lim_{y \to +\infty} (\ln y + 2\pi h(\underline{x}_0, \underline{x}_0, y)) = +\infty$$
(3.43)

and

$$\lim_{y \to 0^+} (\ln y + 2\pi h(\underline{x}_0, \underline{x}_0, y)) = f(\underline{x}_0, \underline{x}_0, 0).$$
(3.44)

From here we can conclude that equation (3.35) admits an unique solution,  $\xi(\alpha) \leq 0$ , for any  $\alpha \in [f(\underline{x}_0, \underline{x}_0, 0), +\infty)$ , which satisfies the conditions (3.36).

In the case of a positive eigenvalue  $\xi \in (0, \lambda_0)$ , setting  $y = \sqrt{\xi}$  we rewrite equation (3.35) as

$$\alpha = \ln iy + 2\pi h(\underline{x}_0, \underline{x}_0, iy) \tag{3.45}$$

which due to (3.4) is equivalent to

$$\alpha = \ln y + 2\pi \operatorname{Re} h(\underline{x}_0, \underline{x}_0, \mathrm{i}y). \tag{3.46}$$

As in the 3D case, we note that the rhs of (3.46) is a strictly decreasing function, cf (3.5), diverging as  $y \to \sqrt{\lambda_0}$ ; the sought conclusion easily follows.

Since the spectrum of  $H_{\alpha}$  is determined by the solutions of the equations (3.1), the above lemmata have the following implication which means that in a sense point interactions in dimension two and three can be always regarded as 'attractive'.

**Corollary 3.4.** For any real  $\alpha$ , the operator  $H_{\alpha}$  defined by (2.8)–(2.10) has a unique spectral point below the spectral threshold of  $-\Delta_{\Omega}^{D}$ .

## 4. Dependence of the principal eigenvalue on the position of the interaction

Now we pass to our main topic. We will characterize the behaviour of the principal eigenvalue of the point-interaction Hamiltonians  $H_{\alpha}$  for a fixed bounded domain  $\Omega \subset \mathbb{R}^d$ , d = 2, 3, as the interaction site moves towards the boundary of  $\Omega$ . We will restrict our attention to domains having an interior reflection property with respect to a suitable hyperplane, in the following sense:

**Definition 4.1.** Consider a hyperplane P of dimension d - 1 in  $\mathbb{R}^d$  and denote by  $S^P$  the mirror image of a set  $S \subset \mathbb{R}^d$  with respect to P provided  $S \cap P = \emptyset$ . The domain  $\Omega$  is said to have the interior reflection property with respect to P if  $P \cap \Omega \neq \emptyset$  and there is an open connected component  $\Omega_s \subset \Omega \setminus P$  such that  $\Omega_s^P$  is a proper subset of  $\Omega \setminus \overline{\Omega}_s$ . We call  $\Omega_s$  the smaller side of  $\Omega$  and P an interior reflection hyperplane.

To prove our main result, we need following auxiliary statement.

**Lemma 4.2.** Let  $\mathcal{G}_0^z(\underline{x}, \underline{x}')$  be defined by (2.5) and (2.6) and  $z \in \mathbb{R}$ . For values of z above  $-\lambda_0$ , the following implications hold,

$$z \in [0, +\infty) \implies \mathcal{G}_0^z(\underline{x}, \underline{x}') > 0 \quad \text{in } \Omega$$

$$(4.1)$$

and

$$z \in (-\lambda_0, 0) :\Longrightarrow: \operatorname{Re} \mathcal{G}_0^z(\underline{x}, \underline{x}') > 0 \qquad \text{in} \quad \Omega.$$

$$(4.2)$$

**Proof.** For  $\Omega \subset \mathbb{R}^3$  and  $z \in [0, +\infty)$ , the Green function

$$\mathcal{G}_0^z(\underline{x}, \underline{x}') = \frac{\mathrm{e}^{-\sqrt{z}|\underline{x}-\underline{x}'|}}{4\pi |\underline{x}-\underline{x}'|} - h(\underline{x}, \underline{x}', \sqrt{z}) \tag{4.3}$$

is certainly positive in a small enough open neighbourhood  $B_{\underline{x}'}$  of the point  $\underline{x}'$  due to the boundedness of  $h(\underline{x}, \underline{x}', \sqrt{z})$ . Moreover, it solves the boundary value problem

$$\begin{cases} (-\Delta + z)\mathcal{G}_0^z(\underline{x}, \underline{x}') = 0 & \text{in } \Omega \setminus B_{\underline{x}'} \\ \mathcal{G}_0^z\big|_{\partial\Omega} = 0, \qquad \mathcal{G}_0\big|_{\partial B_{\underline{x}'}} > 0 \end{cases}; \qquad \underline{x}' \in \Omega.$$

$$(4.4)$$

It follows from the maximum principle that  $\mathcal{G}_0^z$  is strictly positive in the whole  $\Omega$ .

To prove the other implication in the 3D case, note that for  $z \in (-\lambda_0, 0)$  we have

$$\operatorname{Re}\mathcal{G}_{0}^{z}(\underline{x},\underline{x}') = \frac{\cos\sqrt{|z||\underline{x}-\underline{x}'|}}{4\pi|\underline{x}-\underline{x}'|} - \operatorname{Re}h(\underline{x},\underline{x}',i\sqrt{|z|}).$$
(4.5)

Once more we can find a suitable open neighbourhood of the point  $\underline{x}'$ , which we call  $B_{\underline{x}'}$ , where this function is positive. In  $\Omega \setminus B_{x'} \operatorname{Re} \mathcal{G}_0^z(\underline{x}, \underline{x}')$  solves the boundary value problem

$$\begin{cases} (-\Delta+z)\operatorname{Re}\mathcal{G}_{0}^{z}(\underline{x},\underline{x}')=0 & \text{in } \Omega \setminus B_{\underline{x}'} \\ \mathcal{G}_{0}|_{\partial\Omega}=0, & \mathcal{G}_{0}|_{\partial B_{x'}}>0 \end{cases} \quad (4.6)$$

Under the condition  $z > -\lambda_0$  we can still apply the maximum principle obtaining in this way Re  $\mathcal{G}_0^z(\underline{x}, \underline{x}') > 0$  in  $\Omega$ . Finally, in the 2D case the proof follows the same line with the replacement (4.3) and (4.5) by the corresponding 2D Green's function

$$\mathcal{G}_0^z(\underline{x}, \underline{x}') = K_0(\sqrt{z}|\underline{x} - \underline{x}'|) - h(\underline{x}, \underline{x}', \sqrt{z})$$

$$(4.7)$$

and taking into account the asymptotic properties of  $K_0(x)$  as  $x \to 0$ .

Now we are in position to prove our main result. The next theorem shows that, under the interior reflection conditions imposed on the domain  $\Omega$ , the principal eigenvalue of  $H_{\alpha}$ increases as the interaction site moves towards the boundary of the smaller side  $\Omega_s$  of  $\Omega$ .

**Theorem 4.3.** Let P be an interior reflection hyperplane for the domain  $\Omega$  and denote by <u>n</u> the normal vector to P pointing towards  $\Omega_s$ . Assume that  $\underline{x}_0 \in \Omega \cap (\partial \Omega_s \cap P)$ ; then the principal eigenvalue  $\xi$  of the point-interaction  $H_{\alpha}$  with the perturbation placed at  $\underline{x}_0$  satisfies the condition

$$\underline{n} \cdot \nabla_{x_0} \xi > 0. \tag{4.8}$$

**Proof.** Consider first the 3D case. To analyse the dependence of  $\xi$  on the interaction position  $\underline{x}_0$ , we have to distinguish between the negative and positive spectral points. If  $\alpha \in (-\infty, -h(\underline{x}_0, \underline{x}_0, 0)]$ , then  $\xi = \xi(\underline{x}_0)$  is by lemma 3.2 a negative solution of (3.20). Replacing  $\sqrt{|\xi|}$  with  $y(\underline{x}_0)$  and taking the gradient with respect to  $\underline{x}_0$  in (3.20) we find

$$\nabla_{\underline{x}_0} y(\underline{x}_0) \left( \frac{1}{4\pi} + \partial_y h \right) = -\nabla_{\underline{x}_0} h(\underline{x}_0, \underline{x}_0, y).$$
(4.9)

Next we consider the term  $\nabla_{\underline{x}_0} h(\underline{x}_0, \underline{x}_0, y)$  on the rhs of the last equation; under our interior reflection assumptions we will show that this vector is oriented towards the smaller side of  $\Omega$ . To this aim we note that, in view of the relations (2.2)–(2.4),  $h(\underline{x}, \underline{x}', y)$  can be written as

$$h(\underline{x}, \underline{x}', y) = \frac{e^{-y|\underline{x}-\underline{x}'|}}{4\pi |\underline{x}-\underline{x}'|} - \sum_{\substack{n \in \mathbb{N}_0 \\ k \le N_n}} \frac{\psi_{n,k}(\underline{x}')\psi_{n,k}(\underline{x})}{\lambda_n + y^2}$$
(4.10)

for any  $\underline{x} \neq \underline{x}'$ . From the symmetry of this expression and the regularity  $h(\underline{x}, \underline{x}', y)$  it follows that

$$\nabla_{\underline{x}'}h(\underline{x},\underline{x}',y)|_{\underline{x}=\underline{x}'=\underline{x}_0} = \nabla_{\underline{x}}h(\underline{x},\underline{x}',y)|_{\underline{x}=\underline{x}'=\underline{x}_0}$$
(4.11)

and

$$\nabla_{\underline{x}_0} h(\underline{x}_0, \underline{x}_0, y) = 2\nabla_{\underline{x}} h(\underline{x}, \underline{x}', y)|_{\underline{x} = \underline{x}' = \underline{x}_0}.$$
(4.12)

To analyse the orientation of this vector, we introduce the function u defined on the smaller part of  $\Omega$  by

$$u(\underline{x}, \underline{x}_0, y) = h(\underline{x}, \underline{x}_0, y) - h(\underline{x}^P, \underline{x}_0, y), \qquad \underline{x} \in \Omega_s,$$
(4.13)

where  $\underline{x}^{P}$  denotes the mirror image of  $\underline{x} \in \Omega_{s}$  through the plane *P*. The following equation holds

$$\begin{cases} (-\Delta + y^2)u = 0 & \text{in } \Omega_s \\ u|_{P\cap\Omega} = 0, & u|_{\partial\Omega_s\cap\partial\Omega} = \frac{e^{-y|\underline{x}-\underline{x}_0|}}{4\pi |\underline{x}-\underline{x}_0|} - h(\underline{x}^P, \underline{x}_0, y) \Big|_{\underline{x}\in\partial\Omega_s\cap\partial\Omega} & \vdots \end{cases}; \qquad \underline{x}_0 \in \Omega \cap P$$

$$(4.14)$$

It is worthwhile to note that the boundary value on  $\partial \Omega_s \cap \partial \Omega$  can be identified with the value of  $\mathcal{G}_0^{\gamma^2}(\underline{x}, \underline{x}_0)$  on the set  $(\partial \Omega s \cap \partial \Omega)^P$ , indeed we have

$$\mathcal{G}_{0}^{y^{2}}(\underline{x}, \underline{x}_{0})\Big|_{(\partial\Omega s \cap \partial\Omega)^{P}} = \frac{e^{-y|\underline{x}-\underline{x}_{0}|}}{4\pi |\underline{x}-\underline{x}_{0}|} - h(\underline{x}, \underline{x}_{0}, y)\Big|_{(\partial\Omega s \cap \partial\Omega)^{P}}$$
$$= \frac{e^{-y|\underline{x}-\underline{x}_{0}|}}{4\pi |\underline{x}-\underline{x}_{0}|} - h(\underline{x}^{P}, \underline{x}_{0}, y)\Big|_{\partial\Omega s \cap \partial\Omega}$$
(4.15)

Then it follows from (4.1) that u is positive on  $\partial \Omega s \cap \partial \Omega$  and by the maximum principle, u > 0 holds in  $\Omega_s$ . In particular, u reaches its minimum on the points of the open surface  $P \cap \Omega$ ; the Hopf boundary-point lemma in this case implies

$$\underline{n} \cdot \nabla_{\underline{x}} u > 0 \qquad \text{for} \quad \forall \, \underline{x} \in P \cap \Omega.$$
(4.16)

Due to the definition (4.13), in combination with the relation

$$\underline{n} \cdot \nabla_{\underline{x}} h(\underline{x}^P, \underline{x}_0, y) = -\underline{n} \cdot \nabla_{\underline{x}^P} h(\underline{x}^P, \underline{x}_0, y) \quad \text{in} \quad \Omega_s \cup (P \cap \Omega),$$
(4.17)

the last inequality also implies

$$2\underline{n} \cdot \nabla_{\underline{x}} h(\underline{x}, \underline{x}_0, y) > 0 \qquad \text{for} \quad \forall \underline{x} \in P \cap \Omega.$$
(4.18)

Substituting (4.12) and (4.18) into the rhs of (4.9) and taking the projection in the direction of the vector <u>n</u> we obtain

$$\underline{n} \cdot \nabla_{\underline{x}_0} y(\underline{x}_0) \left( \frac{1}{4\pi} + \partial_y h \right) = -\underline{n} \cdot \nabla_{\underline{x}_0} h(\underline{x}_0, \underline{x}_0, y) < 0.$$
(4.19)

The term  $\nabla_{\underline{x}_0} y(\underline{x}_0)$  at the lhs of (4.19) is related to  $\nabla_{\underline{x}_0} \xi$  by

$$\nabla_{\underline{x}_0} y = -\frac{1}{y} \nabla_{\underline{x}_0} \xi \tag{4.20}$$

from which it follows that

$$\frac{1}{y}\left(\frac{1}{4\pi} + \partial_y h\right) \nabla_{\underline{x}_0} \xi > 0.$$
(4.21)

The sought inequality (4.8) follows easily from (4.21) taking into account the condition (3.3).

In the opposite case,  $\alpha > -h(\underline{x}_0, \underline{x}_0, 0)$ , the first spectral point of  $H_{\alpha}$  is a strictly positive solution of the equation

$$\alpha + \operatorname{Re} h(\underline{x}_0, \underline{x}_0, \mathbf{i}\sqrt{\xi}) = 0 \tag{4.22}$$

with  $\xi < \lambda_0$ —cf (3.27) in lemma 3.2. Replacing  $\sqrt{\xi}$  with  $y(\underline{x}_0)$  and taking the gradient with respect to  $\underline{x}_0$  in (4.22), we obtain

$$\nabla_{\underline{x}_0} y \partial_y \operatorname{Re} h(\underline{x}_0, \underline{x}_0, \mathrm{i}y) = -\nabla_{\underline{x}_0} \operatorname{Re} h(\underline{x}_0, \underline{x}_0, \mathrm{i}y).$$
(4.23)

In order to check the orientation of the vector at the rhs of this expression, we note again that due to the symmetry of the function

$$\operatorname{Re} h(\underline{x}, \underline{x}', \mathrm{i}y) = \frac{\cos y |\underline{x} - \underline{x}'|}{4\pi |\underline{x} - \underline{x}'|} - \sum_{\substack{n \in \mathbb{N}_0 \\ k \leqslant N_n}} \frac{\psi_{n,k}(\underline{x}')\psi_{n,k}(\underline{x})}{\lambda_n - y^2}$$
(4.24)

the gradient  $\nabla_{\underline{x}_0} \operatorname{Re} h(\underline{x}_0, \underline{x}_0, iy)$  can be expressed as

$$\nabla_{\underline{x}_0} \operatorname{Re} h(\underline{x}_0, \underline{x}_0, \mathrm{i}y) = 2\nabla_{\underline{x}} \operatorname{Re} h(\underline{x}, \underline{x}', y) \Big|_{\underline{x} = \underline{x}' = \underline{x}_0}.$$
(4.25)

Then we follow the line of the first part of the proof introducing the function u,

$$u(\underline{x}, \underline{x}_0, y) = \operatorname{Re} h(\underline{x}, \underline{x}_0, iy) - \operatorname{Re} h(\underline{x}^P, \underline{x}_0, iy), \qquad \underline{x} \in \Omega_s.$$
(4.26)

Proceeding as before and taking into account the implication (4.2) we find easily

$$\underline{n} \cdot \nabla_{\underline{x}} u > 0 \tag{4.27}$$

and

$$2\underline{n} \cdot \nabla_{\underline{x}} \operatorname{Re} h(\underline{x}, \underline{x}_0, y) > 0 \quad \text{for} \quad \forall \underline{x} \in P \cap \Omega;$$

$$(4.28)$$

substituting (4.25) and (4.28) into the rhs of (4.23), we conclude that

$$\underline{n} \cdot \nabla_{\underline{x}_0} y \partial_y \operatorname{Re} h(\underline{x}_0, \underline{x}_0, \mathrm{i}y) < 0.$$
(4.29)

The claim (4.8) is then obtained from (4.29) by taking into account the relation

$$\nabla_{\underline{x}_0} y = \frac{1}{y} \nabla_{\underline{x}_0} \xi \tag{4.30}$$

and the inequality (3.5) from lemma 3.1. This concludes the argument in the three-dimensional case; the two-dimensional one can be dealt with in the same way, step by step. П

## 5. Optimization of $\xi(\mathbf{x}_0)$

By theorem 4.3 the spectral threshold of the operator  $H_{\alpha}$  increases as the interaction position  $\underline{x}_0$  moves towards the boundary of the domain  $\Omega$ . This result provides us with some insights on how to place the point-interaction centre to minimize the principal eigenvalue of the Hamiltonian  $H_{\alpha}$ . For the sake of simplicity, we begin with the case of a convex  $\Omega$ . Let  $\Pi$  be the set of all the hyperplanes P of interior reflection for  $\Omega$ ; we denote by  $\Omega_{s,P}$  the smaller part related to  $P \in \Pi$ , provided it exists, and by  $\Sigma$  the union

$$\Sigma = \bigcup_{P \in \Pi} \Omega_{s,P}.$$
(5.1)

The following claim is a straightforward consequence of theorem 1.

**Corollary 5.1.** Let  $\Omega$  be an open convex domain in  $\mathbb{R}^d$ , d = 2, 3, and let  $H_\alpha$  be a pointinteraction operator in  $\Omega$  with the perturbation placed at  $\underline{x}_{\Omega}$ . The principal eigenvalue of  $H_{\alpha}$ , considered as a function of the interaction centre, takes its minimum value when  $\underline{x}_0$  belongs to the open set  $\Omega \setminus \Sigma$ .

**Proof.** Note first that the continuity of  $h(\underline{x}, \underline{x}_0, y)$  implies the continuity of solutions of the eigenvalue equations (3.1), thus the principal eigenvalue  $\xi(\underline{x}_0)$  has at least one minimum point  $\underline{x}_0^m \in \overline{\Omega}$ . We use reduction ad absurdum: assume  $\underline{x}_0^m \in \Omega_{s,P}$  for a suitable hyperplane  $P \in \Pi$ . Due to the convexity of the domain, there exists another hyperplane  $P' \in \Pi$  parallel to P and such that

$$\underline{x}_0^m \in \partial \Omega_{s,P'} \cap P', \tag{5.2}$$

however, under this assumption theorem 4.3 implies the inequality

$$\underline{n} \cdot \underline{v}_{\underline{x}_0} \xi > 0 \tag{5.3}$$

from which a contradiction follows easily.

In the case of highly symmetric domains such as the interior of a circle or an ellipse in the plane, and similarly a ball and an interior of an ellipsoid in three dimensions, it is easy to identify the set  $\Sigma$  with the centre of such a domain. More generally, the convexity of  $\Omega$ ensures the validity of the interior reflection property needed in theorem 4.3 with respect to some hyperplane passing through a point sufficiently close to the boundary. In this situation the above result can be used to localize the optimal position of  $\underline{x}_0$  in a 'central' subset of the domain  $\Omega$ .

A slight generalization of the above argument leads us to an analogous rule to localize the minimum points of the principal eigenvalue for a point interaction within non-convex domains. Let  $P \in \Pi$  and consider the one-parameter family of hyperplanes  $P_t$ ,

$$\begin{cases} P_t = \{ \underline{x} + \underline{n}t : \underline{x} \in P, t \in [0, T] \} \\ T = \max\{ t \in \mathbb{R}^+ : P_t \cap \Omega \neq \emptyset \}, \end{cases}$$
(5.4)

where <u>n</u> denotes the unit normal to P directed towards the smaller part  $\Omega_s$  of  $\Omega$ . We denote as  $\Pi'$  the subset formed by all those hyperplanes  $P \in \Pi$  such that

$$P_t \in \Pi \qquad \text{for} \qquad \forall t \in [0, T]. \tag{5.5}$$

It is important to note that in the non-convex case, to any hyperplane of interior reflection there may correspond more than one smaller part. Next we denote by  $\Theta_{s,P}$  the union of all the smaller parts related to P, and by  $\Sigma'$  the set

$$\Sigma' = \bigcup_{P \in \Pi'} \Theta_{s,P}.$$
(5.6)

**Corollary 5.2.** Assume that  $\Omega$  is an open domain in  $\mathbb{R}^d$ , d = 2, 3, and  $H_\alpha$  is a point-interaction operator in  $\Omega$  with the perturbation placed at  $\underline{x}_{\Omega}$ . The principal eigenvalue of  $H_{\alpha}$ , regarded as a function of  $\underline{x}_0$ , takes its minimum value when  $\underline{x}_0$  belongs to the open set  $\Omega \setminus \Sigma'$ .

**Proof.** The argument is an easy modification of the proof of corollary 5.1.

.

Non-convex domains with a reasonably simple boundary such as, for instance, the union of two intersecting discs or a dog-bone profile in two dimensions, can be easily analysed using corollary 5.2. It is also worthwhile to stress that the results of this section do not depend on the parameter  $\alpha$ , hence the optimal placement of the point interaction with respect to the minimum of the principal eigenvalues can be the same irrespective of the interaction 'strength'.

Let us finally comment on the relation to the work [HKK01] mentioned in the introduction. We have said that for a hard-wall obstacle the principal eigenvalue decreases as it moves towards the boundary. The difference of the two effects can be traced back to the different boundary conditions which characterize the operator domains in the two cases. While the hard obstacle is characterized by the Dirichlet boundary condition, the point-interaction operator  $H_{\alpha}$ considered here can be obtained as the norm-resolvent limit of a family of sphere interactions Hamiltonians  $H_{\alpha}(r)$  with the boundary condition of a *mixed type* as the radius  $r \to 0$ . In the three-dimensional case, for instance, the operator  $H_{\alpha}(r)$  is explicitly given by

$$\begin{cases} H_{\alpha}(r) = -\Delta & \text{on} \quad \Omega \backslash S_r \\ D(H_{\alpha}(r)) = \left\{ \psi \in H^1(\mathbb{R}^3) \, \middle| \, (\partial_n \psi)_+ - (\partial_n \psi)_- = \frac{1}{4\pi \alpha r^2 + r} \psi \right\}, \end{cases}$$

where  $S_r$  denotes the sphere of radius r centred at  $\underline{x}_0$  and  $(\partial_n \psi)_+ - (\partial_n \psi)_-$  is the jump of the normal derivative of  $\psi$  on the interaction surface [FT93, Sh03]. Another insight into the difference of the two situations can be obtained from [E\$96].

#### Acknowledgments

We wish to thank Rodolfo Figari and Francesco Chiacchio, as well as to the referee, for their useful remarks. This research was partially supported by GAAS and MEYS of the Czech Republic under projects A100480501 and LC06002.

## References

- [AS72] Abramowitz M and Stegun I A (ed) 1972 Handbook of Mathematical Functions (New York: Dover)
- [AG63] Akhiezer N I and Glazman I M 1963 Theory of Linear Operators in Hilbert Space vol II (New York: Frederick Ungar Publishing Co.)
- [AGHH05] Albeverio S, Gesztesy F, Högh-Krohn R and Holden H 2005 Solvable Models in Quantum Mechanics 2nd edn, with an appendix by P Exner (Providence, RI: American Mathematical Society)

- [AB92a] Ashbaugh M S and Benguria R D 1992 A sharp bound for the ratio of the first two eigenvalues of Dirichlet Laplacians and extensions Ann. Math. 135 601–28
- [AB92b] Ashbaugh M S and Benguria R D 1992 A second proof of the Payne-pólya-Weinberger conjecture Commun. Math. Phys. 147 181–90
- [BFM07] Blanchard Ph, Figari R and Mantile A 2007 Point interaction Hamiltonians in bounded domains J. Math. Phys. 48 082108
- [Br83] Brezis H 1983 Analyse Fonctionelle (Paris: Masson)
- [Ev98] Evans L C 1998 Partial Differential Equations (Providence, RI: American Mathematical Society)
- [EGST96] Exner P, Gawlista R, Šeba P and Tater M 1996 Point interactions in a strip Ann. Phys. 252 133-79
- [EN02] Exner P and Němcová K 2002 Quantum mechanics of layers with a finite number of point perturbations J. Math. Phys. 43 1152–84
- [ES96] Exner P and Šeba P 1996 Point interactions in dimension two and three as models of small scatterers Phys. Lett. A 222 1–4
- [Fa23] Faber G 1923 Beweiss das unter allen homogenen Membranen von Gleicher Fläche und gleicher Spannung die kreisförmige den Tiefsten Grundton gibt Sitzungber. der math.-phys. Klasse der Bayerische Akad. der Wiss. zu München 169–72
- [FT93] Figari R and Teta A 1993 A boundary value problem of mixed type on perforated domains Asymptot. Anal. 6 271–84
- [HKK01] Harrell E M, Kröger P and Kurata K 2001 On the placement of an obstacle or a well so as to optimize the fundamental eigenvalue SIAM J. Math. Anal. 33 240–59
  - [He63] Hersch J 1963 The method of interior parallels applied to polygonal or multiply connected membranes Pac. J. Math. 13 1229–38
  - [Kr25] Krahn E 1925 Über eine von Rayleigh formulierte minimal Eigenschaft des Kreises Ann. Math. 94 97–100
- [PPW55] Payne L E, Pólya G and Weinberger H F 1955 Sur le quotient de deux fréquences propres consecutives Comp. Rend. 241 917–9
- [RS75] Reed M and Simon B 1975 Methods of Modern Mathematical Physics, II. Fourier Analysis, Self-Adjointness (New York: Academic)
- [RS78] Reed M and Simon B 1978 Methods of Modern Mathematical Physics, IV. Analysis of Operators (New York: Academic)
- [Sh03] Shimada S-i 2003 Resolvent convergence of sphere interactions to point interactions *J. Math. Phys.* 44 990–1005