ABSTRACT

On Critical Dipoles in Dimensions $n \geqslant 3$

S. Blake Allan

Director: Fritz Gesztesy, Ph. D.

We consider generalizations of Hardy's inequality corresponding to the case of (point) dipole potentials $V_\gamma(x) = \gamma(u,x)|x|^{-3}$, $x \in \mathbb{R}^n \backslash \{0\}$, $\gamma \in [0,\infty)$, $n \in \mathbb{N}$, $n \geqslant 3$. More precisely, for $n \geqslant 3$, we prove the existence of a critical dipole coupling constant $\gamma_{c,n} > 0$, such that

$$\text{for all } \gamma \in [0, \gamma_{c,n}],$$
$$\int_{\mathbb{R}^n} d^n x \, |(\nabla f)(x)|^2 \geqslant \gamma \int_{\mathbb{R}^n} d^n x \, (u,x)|x|^{-3}|f(x)|^2, \quad f \in C_0^\infty(\mathbb{R}^n \backslash \{0\}).$$

Here $\gamma_{c,n}$ is optimal, that is, the largest possible such constant, and we discuss a numerical scheme for its computation.

This quadratic form inequality will be a consequence of the fact,

$$\overline{\big[-\Delta + \gamma(u,x)|x|^{-3}\big]\big|_{C_0^\infty(\mathbb{R}^n \backslash \{0\})}} \geqslant 0 \text{ if and only if } 0 \leqslant \gamma \leqslant \gamma_{c,n},$$

where $\overline{T}$ represents the operator closure in $L^2(\mathbb{R}^n; d^n x)$.

APPROVED BY DIRECTOR OF HONORS THESIS:

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Dr. Fritz Gesztesy, Department of Mathematics

APPROVED BY THE HONORS PROGRAM:

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Dr. Elizabeth Corey, Director

DATE: ____________________

ON CRITICAL DIPOLES IN DIMENSIONS $N \geqslant 3$

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S. Blake Allan

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CHAPTER ONE

Introduction

The celebrated (multi-dimensional) Hardy inequality,

$$\begin{aligned} &\int_{\mathbb{R}^n} d^n x \, |(\nabla f)(x)|^2 \geqslant [(n-2)/2]^2 \int_{\mathbb{R}^n} d^n x \, |x|^{-2} |f(x)|^2, \\ &\qquad\qquad\qquad\qquad f \in C_0^\infty(\mathbb{R}^n \backslash \{0\}), \ n \in \mathbb{N}, \ n \geqslant 3, \end{aligned} \tag{1.1}$$

the first in an infinite sequence of higher-order Hardy-type inequalities, received enormous attention in the literature due to its ubiquity in self-adjointness and spectral theory problems associated with second-order differential operators with strongly singular coefficients, see, for instance, [AGG06], [Dav89, Sect. 1.5], [Dav95, Ch. 5], [Ges84], [GP80], [GM08], [GM11], [GM13, Part 1], [Kal72]–[KW72], [KMP07, Ch. 8], [OK90, Ch. 2], and [Sim83]. We also note that inequality (1.1) is closely related to Heisenberg's uncertainty relation as discussed in [Far78].

The basics behind the (point) dipole Hamiltonian $-\Delta + V_\gamma(x)$, with potential

$$V_\gamma(x) = \gamma \frac{(u,x)}{|x|^3}, \quad x \in \mathbb{R}^n \backslash \{0\}, \ \gamma \in [0,\infty), \ u \in \mathbb{R}^n, \ |u| = 1, \ n \in \mathbb{N}, \ n \geqslant 3 \tag{1.2}$$

(with (a,b) denoting the Euclidean scalar product of $a, b \in \mathbb{R}^n$), in the physically relevant case $n = 3$, has been discussed in great detail in the 1980 paper by Hunziker and Günther [HG80]. In particular, these authors point out some of the existing fallacies to be found in the physics literature in connection with dipole potentials and their ability to bind electrons. We will not repeat these clarifications of results in the literature at this point and note that the primary goal in this manuscript has been the attempt to extend the three-dimensional results on dipole potentials in [HG80] to the general case $n \geqslant 4$. The $L^2(\mathbb{R}^n; d^n x)$-realization of the differential expression $-\Delta + V_\gamma(x)$, $x \in \mathbb{R}^n \backslash \{0\}$, $n \geqslant 3$, is provided in Chapter 2.

Our principal new result derived in Chapter 3 then reads as follows: For each $n \geqslant 3$, we prove the existence of a critical dipole coupling constant $\gamma_{c,n} > 0$, such that

$$\text{for all } \gamma \in [0, \gamma_{c,n}],$$
$$\int_{\mathbb{R}^n} d^n x\, |(\nabla f)(x)|^2 \geqslant \gamma \int_{\mathbb{R}^n} d^n x\, (u, x)|x|^{-3}|f(x)|^2, \quad f \in C_0^\infty(\mathbb{R}^n \backslash \{0\}).$$

Here $\gamma_{c,n} > 0$ is optimal, that is, the largest possible such constant.

A numerical algorithm for the computation of $\gamma_{c,n}$ is discussed in Chapter 4.

Finally, in Chapter 5 we collect basic results on n-dimensional spherical harmonics and the Laplace–Beltrami operator in $L^2\big(S^{n-1}\big)$, $n \geqslant 2$.

CHAPTER TWO

The Dipole Hamiltonian

In this chapter we provide a discussion of the angular momentum decomposition of the n-dimensional Laplacian $-\Delta_n$ and then introduce the dipole Hamiltonian $H_n(\gamma)$, the principle object of this paper, and discuss an analogous decomposition of the latter.

In spherical coordinates (5.1), the Laplace differential expression in n dimensions takes the form

$$-\Delta_n = -\frac{\partial^2}{\partial r^2} - \frac{n-1}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}\Delta_{B,n} \tag{2.1}$$

with $-\Delta_{B,n}$ the Laplace–Beltrami operator[1] associated with the $(n-1)$-dimensional unit sphere S^{n-1} in $\mathbb{R}^n$, see (5.16). When acting in $L^2(\mathbb{R}^n; d^n x)$, which in spherical coordinates can be written as $L^2(\mathbb{R}^n; d^n x) \simeq L^2([0,\infty); r^{n-1}dr) \otimes L^2(S^{n-1}; d^{n-1}\omega)$, (2.1) becomes

$$-\left(\frac{d^2}{dr^2} + \frac{n-1}{r}\frac{d}{dr}\right) \otimes I_S - \frac{1}{r^2} \otimes \Delta_{B,n}, \tag{2.2}$$

where I_S represents the identity in $L^2(S^{n-1}; d^{n-1}\omega)$. The Laplace–Beltrami operator $-\Delta_{B,n}$ in $L^2(S^{n-1}; d^{n-1}\omega)$, with domain $\mathrm{dom}(-\Delta_{B,n}) = H^2\big(S^{n-1}\big)$ (cf. e.g., [BLP]), is known to be essentially self-adjoint and nonnegative on $C_0^\infty(S^{n-1})$ (cf. [Dav89, Theorem 5.2.3]). Recalling the treatment in [RS75, p. 160–161], one decomposes the

[1] We will call $-\Delta_n$ the Laplacian to guarantee nonnegativity of the underlying $L^2(\mathbb{R}^n)$-realization (and analogously for the $L^2(S^{n-1})$-realization of the Laplace–Beltrami operator $-\Delta_{B,n}$).

space $L^2(S^{n-1}; d^{n-1}\omega)$ into an infinite orthogonal sum, yielding

$$\begin{aligned} L^2(\mathbb{R}^n) &\simeq L^2([0,\infty); r^{n-1}dr) \otimes L^2(S^{n-1}; d^{n-1}\omega) \\ &= \bigoplus_{\ell=0}^{\infty} L^2([0,\infty); r^{n-1}dr) \otimes \mathcal{Y}_\ell^n, \end{aligned} \tag{2.3}$$

where $\mathcal{Y}_\ell^n$ is the eigenspace of $-\Delta_{B,n}$ corresponding to the eigenvalue $\ell(\ell+n-2)$, $\ell \in \mathbb{N}_0$, as

$$\sigma(-\Delta_{B,n}) = \{\ell(\ell+n-2)\}_{\ell\in\mathbb{N}_0}. \tag{2.4}$$

In particular, this results in

$$-\Delta_n = \bigoplus_{\ell=0}^{\infty} \bigg[-\frac{d^2}{dr^2} - \frac{n-1}{r}\frac{d}{dr} + \frac{\ell(\ell+n-2)}{r^2}\bigg] \otimes I_{\mathcal{Y}_\ell^n}, \tag{2.5}$$

in the space of (2.3), with $I_{\mathcal{Y}_\ell^n}$ the identity operator in $\mathcal{Y}_\ell^n$.

To simplify matters, replacing the measure $r^{n-1}dr$ by dr and simultaneously removing the term $(n-1)r^{-1}d/dr$, one introduces the unitary operator

$$U_n = \begin{cases} L^2([0,\infty); r^{n-1}dr) \to L^2([0,\infty); dr), \\ f(r) \mapsto r^{(n-1)/2} f(r), \end{cases} \tag{2.6}$$

under which (2.5) becomes

$$-\Delta_n = \bigoplus_{\ell=0}^{\infty} U_n^{-1} \bigg[-\frac{d^2}{dr^2} + \frac{[(n-1)(n-3)/4] + \ell(\ell+n-2)}{r^2}\bigg] U_n \otimes I_{\mathcal{Y}_\ell^n} \tag{2.7}$$

acting in the space (2.3). The precise self-adjoint L^2-realization of $-\Delta_n$ in the space (2.3) then is of the form

$$H_n = \bigoplus_{\ell=0}^{\infty} U_n^{-1} h_{n,\ell}\, U_n \otimes I_{\mathcal{Y}_\ell^n}, \tag{2.8}$$

where $h_{n,\ell}$, $\ell \in \mathbb{N}_0$, represents the Friedrichs extension of

$$\left[-\frac{d^2}{dr^2} + \frac{[(n-1)(n-3)/4] + \ell(\ell+n-2)}{r^2}\right]\bigg|_{C_0^\infty((0,\infty))}, \quad \ell \in \mathbb{N}_0,\ r > 0, \tag{2.9}$$

in $L^2((0,\infty);dr)$. Explicitly (see, e.g., [Ash+10, Sect. 10]),

$$\begin{aligned}
& h_{n,0} = -\frac{d^2}{dr^2} + \frac{(n-1)(n-3)/4}{r^2}, \quad r > 0, \\
& \operatorname{dom}(h_{n,0}) = \big\{f \in L^2((0,\infty);dr) \,\big|\, f, f' \in AC_{loc}((0,\infty));\ f_0 = 0; \\
& \qquad\qquad (-f'' + [(n-1)(n-3)/4]r^{-2}f) \in L^2((0,\infty);dr)\big\} \text{ for } n = 2,3,
\end{aligned} \tag{2.10}$$

$$\begin{aligned}
& h_{n,\ell} = -\frac{d^2}{dr^2} + \frac{[(n-1)(n-3)/4] + \ell(\ell+n-2)}{r^2}, \quad r > 0, \\
& \operatorname{dom}(h_{n,\ell}) = \big\{f \in L^2((0,\infty);dr) \,\big|\, f, f' \in AC_{loc}((0,\infty)); \\
& \qquad\qquad (-f'' + [((n-1)(n-3)/4) + \ell(\ell+n-2)]r^{-2}f) \in L^2((0,\infty);dr)\big\} \\
& \qquad\qquad\qquad\qquad \text{for } \ell \in \mathbb{N},\ n \geqslant 2 \text{ and } \ell = 0,\ n \geqslant 4,
\end{aligned} \tag{2.11}$$

where

$$f_0 = \begin{cases} \lim_{r\downarrow 0}[-r^{1/2}\ln(r)]^{-1}f(r), & n = 2, \\ f(0_+), & n = 3. \end{cases} \tag{2.12}$$

It is well-known (cf. [RS75, Sect. IX.7, Appendix to X.1]) that

$$H_n = -\Delta_n, \quad \operatorname{dom}(H_n) = H^2(\mathbb{R}^n), \tag{2.13}$$

$$H_n|_{C_0^\infty(\mathbb{R}^n)} \text{ is essentially self-adjoint,} \tag{2.14}$$

$$H_n|_{C_0^\infty(\mathbb{R}^n\setminus\{0\})} \text{ is essentially self-adjoint if and only if } n \geqslant 4. \tag{2.15}$$

Next, we turn to the dipole potential

$$V_\gamma(x) = \gamma\frac{(u,x)}{|x|^3}, \quad x \in \mathbb{R}^n,\ \gamma \geqslant 0,\ n \geqslant 3, \tag{2.16}$$

where $u \in \mathbb{R}^n$ is a unit vector in the direction of the dipole, the strength of the dipole equals γ (if $\gamma > 0$, which we assume without loss of generality), and $(\,\cdot\,,\,\cdot\,)$ represents the Euclidean scalar product in $\mathbb{R}^n$. Upon an appropriate rotation, one can always choose the coordinate system in such a manner that $(u, x) = |x| \cos(\theta_{n-1})$, implying

$$V_\gamma(x) = \gamma \frac{\cos(\theta_{n-1})}{|x|^2}, \quad n \geqslant 3. \tag{2.17}$$

In the following we primarily restrict ourselves to the case $n \geqslant 3$ and comment on the exceptional case $n = 2$ at the end of Chapter 3. The differential expression associated with Hamiltonian for this system then becomes

$$L_n(\gamma) = -\Delta_n + V_\gamma(x), \quad x \in \mathbb{R}^n \backslash \{0\},\ n \geqslant 3, \tag{2.18}$$

acting in $L^2(\mathbb{R}^n)$ which, in analogy to (2.2), can be represented as

$$L_n(\gamma) = -\left(\frac{d^2}{dr^2} + \frac{n-1}{r}\frac{d}{dr}\right) \otimes I_S + \frac{1}{r^2} \otimes \Lambda_n(\gamma), \quad n \geqslant 3, \tag{2.19}$$

acting in $L^2([0,\infty); r^{n-1} dr) \otimes L^2(S^{n-1}; d^{n-1}\omega)$, where

$$\Lambda_n(\gamma) = -\Delta_{B,n} + \gamma \cos(\theta_{n-1}), \quad \operatorname{dom}(\Lambda_n(\gamma)) = \operatorname{dom}(-\Delta_{B,n}), \quad n \geqslant 3, \tag{2.20}$$

is self-adjoint in $L^2(S^{n-1}; d^{n-1}\omega)$ (since $\gamma\cos(\theta_{n-1})$ is a bounded self-adjoint operator in $L^2(S^{n-1}; d^{n-1}\omega)$). Applying the angular momentum decomposition to $L_n(\gamma)$, but this time with respect to the eigenspaces of $\Lambda_n(\gamma)$, then results in

$$\begin{aligned} L^2(\mathbb{R}^n; d^n x) &= L^2([0,\infty); r^{n-1}\, dr) \otimes L^2(S^{n-1}; d^{n-1}\omega) \\ &= \bigoplus_{\ell=0}^{\infty} L^2([0,\infty); r^{n-1}\, dr) \otimes \mathcal{Y}_\ell^n(\gamma), \quad n \geqslant 3, \end{aligned} \tag{2.21}$$

where $\mathcal{Y}_\ell^n(\gamma)$ represents the eigenspace of $\Lambda_n(\gamma)$ corresponding to the eigenvalue

$\lambda_{n,\ell}(\gamma)$, as

$$\sigma(\Lambda_n(\gamma)) = \{\lambda_{n,\ell}(\gamma)\}_{\ell\in\mathbb{N}_0}. \tag{2.22}$$

We will order the eigenvalues of $\Lambda_n(\gamma)$ according to magnitude, that is,

$$\lambda_{n,\ell}(\gamma) \leqslant \lambda_{n,\ell+1}(\gamma), \quad \ell \in \mathbb{N}_0,\ n \geqslant 3, \tag{2.23}$$

repeating them according to their multiplicity. The analog of (2.7) in the space (2.21) then becomes

$$L_n(\gamma) = \bigoplus_{\ell=0}^{\infty} U_n^{-1}\left[-\frac{d^2}{dr^2} + \frac{[(n-1)(n-3)/4] + \lambda_{n,\ell}(\gamma)}{r^2}\right] U_n \otimes I_{\mathcal{Y}_\ell^n(\gamma)}, \quad n \geqslant 3, \tag{2.24}$$

with $I_{\mathcal{Y}_\ell^n(\gamma)}$ the identity operator in $\mathcal{Y}_\ell^n(\gamma)$.

Remark 2.1. *Since $e^{t\Delta_{B,n}}$, $t \geqslant 0$, has a continuous and nonnegative integral kernel (see, e,g., [Dav89, Theorem 5.2.1]), it is positivity improving in $L^2(S^{n-1}; d^{n-1}\omega)$. Hence, so is $e^{-t\Lambda_n(\gamma)}$, $t \geqslant 0$, by (a special case of) [RS78, Theorem XIII.45]. Thus, one concludes that*

$$\textit{the lowest eigenvalue } \lambda_{n,0}(\gamma) \textit{ of } \Lambda_n(\gamma) \textit{ is simple for all } \gamma \geqslant 0. \tag{2.25}$$

$\diamond$

In order to deal exclusively with operators which are bounded from below we now make the the following assumption.

Hypothesis 2.2. *Suppose that $n \in \mathbb{N}$, $n \geqslant 3$, and $\gamma > 0$ are such that*

$$\lambda_{n,0}(\gamma) \geqslant -(n-2)^2/4. \tag{2.26}$$

Inequality (2.26) is of course inspired by Hardy's inequality (1.1) (cf. [BEL15, Sect. 1.2], [Kat95, p. 345], [KMP07, Ch. 3], [KPS17, Ch. 1], [OK90, CH. 1]), which in turn implies

$$\left[-\frac{d^2}{dr^2}+\frac{c}{r^2}\right]\bigg|_{C_0^\infty((0,\infty))} \geqslant 0 \text{ if and only if } c \geqslant -1/4. \tag{2.27}$$

In fact, "$\geqslant 0$" in (2.27) can be replaced by "bounded from below". Assumption (2.26) is of course equivalent to

$$[(n-1)(n-3)/4] + \lambda_{n,\ell}(\gamma) \geqslant -1/4. \tag{2.28}$$

Remark 2.3. *Since the perturbation $\gamma\cos(\theta_{n-1})$, $\gamma \in [0,\infty)$, of $-\Delta_{B,n}$ in (2.20) is bounded from below and from above,*

$$-\gamma I_S \leqslant \gamma\cos(\theta_{n-1}) \leqslant \gamma I_S, \tag{2.29}$$

and $-\Delta_{B,n} \geqslant 0$, it is clear that

$$\lambda_{n,0}(\gamma) \geqslant -\gamma, \;\; \text{that is, } \; \Lambda_n(\gamma) \geqslant -\gamma I_S. \tag{2.30}$$

In particular, for $n \geqslant 3$ and $0 \leqslant \gamma$ sufficiently small, Hypothesis 2.2 will be satisfied. We're particularly interested in the existence of a critical $\gamma_{c,n} > 0$ such that

$$\lambda_{n,0}(\gamma_{c,n}) = -(n-2)^2/4, \tag{2.31}$$

and whether or not

$$\lambda_{n,0}(\gamma) < -(n-2)^2/4, \quad \gamma \in (\gamma_{c,n}, \gamma_2), \tag{2.32}$$

for a $\gamma_2 \in (\gamma_{c,n}, \infty)$, *with*

$$\lambda_{n,0}(\gamma) \geqslant -(n-2)^2/4, \quad \gamma \in (\gamma_2, \gamma_3), \tag{2.33}$$

for a $\gamma_3 \in (\gamma_2, \infty)$, *etc. This will be clarified in the next chapter (demonstrating that* $\gamma_2 = \infty$*).* $\diamond$

Given Hypothesis 2.2, the precise self-adjoint L^2-realization of $L_n(\gamma)$ in the space (2.21) is then of the form

$$H_n(\gamma) = \bigoplus_{\ell=0}^{\infty} U_n^{-1} h_{n,\ell}(\gamma) U_n \otimes I_{\mathcal{Y}_\ell^n(\gamma)}, \tag{2.34}$$

where $h_{n,\ell}(\gamma)$, $\ell \in \mathbb{N}_0$, represents the Friedrichs extension of

$$\left[-\frac{d^2}{dr^2} + \frac{[(n-1)(n-3)/4] + \lambda_{n,\ell}(\gamma)}{r^2}\right]\bigg|_{C_0^\infty((0,\infty))}, \quad \ell \in \mathbb{N}_0,\ r > 0, \tag{2.35}$$

in $L^2((0,\infty); dr)$. Explicitly, as discussed, for instance, in [GLN], the Friedrichs extension of $h_{n,\ell}(\gamma)$, $\ell \in \mathbb{N}_0$, can be determined from the fact that the Friedrichs extension $\widetilde{h}_{n,\alpha,F}$ in $L^2((0,\infty); dr)$ of

$$\widetilde{h}_{n,\alpha} = \left[-\frac{d^2}{dr^2} + \frac{\alpha^2 - (1/4)}{r^2}\right]\bigg|_{C_0^\infty((0,\infty))}, \quad \alpha \in [0,\infty),\ r > 0, \tag{2.36}$$

is given by

$$\widetilde{h}_{n,\alpha,F} = -\frac{d^2}{dr^2} + \frac{\alpha^2 - (1/4)}{r^2}, \quad \alpha \in [0,\infty),\ r > 0, \tag{2.37}$$

$$\begin{aligned} \operatorname{dom}\big(\widetilde{h}_{n,\alpha,F}\big) = \big\{ & f \in L^2((0,\infty); dr) \,\big|\, f, f' \in AC_{loc}((0,\infty));\ f_0 = 0; \\ & (-f'' + \big[\alpha^2 - (1/4)\big] r^{-2} f) \in L^2((0,\infty); dr)\big\}, \quad \alpha \in [0,1), \end{aligned} \tag{2.38}$$

$$\begin{aligned} \operatorname{dom}\big(\widetilde{h}_{n,\alpha,F}\big) = \big\{ & f \in L^2((0,\infty); dr) \,\big|\, f, f' \in AC_{loc}((0,\infty)); \\ & (-f'' + \big[\alpha^2 - (1/4)\big] r^{-2} f) \in L^2((0,\infty); dr)\big\}, \quad \alpha \in [1,\infty), \end{aligned} \tag{2.39}$$

where

$$f_0 = \begin{cases} \lim_{x\downarrow 0} f(x)/\big[x^{1/2}\ln(1/x)\big], & \alpha = 0, \\ \lim_{x\downarrow 0} f(x)/\big[(2\alpha)^{-1}x^{(1/2)-\alpha}\big], & \alpha \in (0,1). \end{cases} \tag{2.40}$$

Next we note the following fact.

Lemma 2.4. *Given the operator $\Lambda_n(\gamma)$ in $L^2(S^{n-1}; d^{n-1}\omega)$ as introduced in* (2.20)*, one infers that*

$$\lim_{\gamma\downarrow 0} \lambda_{n,\ell}(\gamma) = \ell(\ell+n-2), \quad \ell \in \mathbb{N}_0, \tag{2.41}$$

recalling that $\{\ell(\ell+n-2)\}_{\ell\in\mathbb{N}_0}$ are the corresponding eigenvalues of the unperturbed operator, the Laplace–Beltrami operator, $\Lambda_n(0) = -\Delta_{B,n}$.

Proof. This is a special case of Rellich's theorem in the form recorded, for instance, in [RS78, Theorems X.II.3 and X.II.13]. □

Lemma 2.5. *Assume Hypothesis* 2.2*. Then $H_n(\gamma)$ has purely absolutely continuous spectrum given by*

$$\sigma_{ac}(H_n(\gamma)) = [0,\infty). \tag{2.42}$$

Proof. First, one notes that $H_n(\gamma)$ is bounded from below if and only if each $h_{n,\ell}(\gamma)$, $\ell \in \mathbb{N}_0$, is bounded from below. The ordinary differential operators $h_{n,\ell}(\gamma)$, $\ell \in \mathbb{N}_0$, are well-known to have purely absolutely continuous spectrum equal to $[0,\infty)$, as proven, for instance in [EK07] and [GZ06]. Thus the result follows from the special case of direct sums (instead of direct integrals) in [RS78, Theorem XIII.85 (f)]. □

CHAPTER THREE

Criticality

We now turn to one of the principal questions – a discussion of which $\gamma > 0$ cause $H_n(\gamma)$ to be bounded from below.

Theorem 3.1. *Assume Hypothesis* 2.2. *Then for all $n \geqslant 3$, there exists a unique critical dipole moment $\gamma_{c,n} > 0$ as introduced in Remark* 2.3 (*cf.* (2.31)). *Moreover, $\lambda_{n,0}(\gamma)$ is strictly monotonically decreasing with respect to $\gamma \in [0, \infty)$ and*

$$\frac{d\lambda_{n,0}(\gamma)}{d\gamma} \leqslant \frac{\lambda_{n,0}(\gamma)}{\gamma} < 0 \ \ \textit{as well as} \ \ \lambda_{n,0}(\gamma) \geqslant -\gamma \tag{3.1}$$

hold. In particular, $H_n(\gamma)$ is bounded from below, and then $H_n(\gamma) \geqslant 0$, if and only if $0 < \gamma \leqslant \gamma_{c,n}$. Consequently,

$$\begin{aligned} &\textit{for all } \gamma \in [0, \gamma_{c,n}], \\ &\int_{\mathbb{R}^n} d^n x \, |(\nabla f)(x)|^2 \geqslant \gamma \int_{\mathbb{R}^n} d^n x \, (u, x)|x|^{-3}|f(x)|^2, \quad f \in C_0^\infty(\mathbb{R}^n \backslash \{0\}). \end{aligned} \tag{3.2}$$

The constant $\gamma_{c,n} > 0$ in (3.2) *is optimal* (*i.e., the largest possible*).

Proof. Existence of some critical dipole moment $\gamma_{c,n} > 0$ is clear from the discussion in Remark 2.3.

To prove the remaining claims in Theorem 3.1, we seek spherical harmonics dependent only on the final angle θ_{n-1}, as this is the only angular variable dependence of $V_\gamma(x)$. From (5.10) and (5.13), one infers these are precisely the ones indexed by the particular multi-indices $(\ell, 0, \dots, 0) \in \mathbb{N}_0^n$, that is (cf. (5.10)),

$$Y_{(\ell,0,\dots,0)}(\theta) = \left[\frac{[(n-2)/2](n-2)_\ell}{\ell!(\ell + [(n-2)/2])}\right]^{1/2} C_\ell^{(n-2)/2}(\cos(\theta_{n-1})). \tag{3.3}$$

With $\mathcal{Y}^n = \bigcup_{\ell \in \mathbb{N}_0} \mathcal{Y}_\ell^n$, one can define the subspace

$$\mathcal{L}^n = \{Y_{(\ell,0,\dots,0)} \in \mathcal{Y}^n \,|\, \ell \in \mathbb{N}_0\}. \tag{3.4}$$

Restricting the Laplace–Beltrami operator (5.16) to $\mathcal{L}^n$, one finds for (2.20),

$$\begin{aligned} \Lambda_{n,\mathcal{L}^n}(\gamma) &= -\frac{d^2}{d\theta_{n-1}^2} - (n-2)\cot(\theta_{n-1})\frac{d}{d\theta_{n-1}} + \gamma\cos(\theta_{n-1}) \\ &= -[\sin(\theta_{n-1})]^{2-n}\frac{d}{d\theta_{n-1}}\left[[\sin(\theta_{n-1})]^{n-2}\frac{d}{d\theta_{n-1}}\right] + \gamma\cos(\theta_{n-1}). \end{aligned} \tag{3.5}$$

Accordingly, restricting the measure $d^{n-1}\omega$ in (5.3) produces

$$d\omega_{\mathcal{L}^n} = \sin^{n-2}(\theta_{n-1})\, d\theta_{n-1}. \tag{3.6}$$

$\Lambda_{n,\mathcal{L}^n}(\gamma)$ then acts in the space $L^2([0,2\pi]; d\omega_{\mathcal{L}^n})$. Reverting from $d\omega_{\mathcal{L}^n}$ to Lebesgue measure $d\theta_{n-1}$ on $[0,\pi]$, one obtains the unitarily equivalent operator $\widetilde{\Lambda}_{n,\mathcal{L}^n}(\gamma)$ in $L^2([0,2\pi]; d\theta_{n-1})$ given by

$$\widetilde{\Lambda}_{n,\mathcal{L}^n}(\gamma) = -\frac{d}{d\theta_{n-1}}\left[[\sin(\theta_{n-1})]^{n-2}\frac{d}{d\theta_{n-1}}\right] + \gamma[\sin(\theta_{n-1})]^{n-2}\cos(\theta_{n-1}). \tag{3.7}$$

Introducing the change of variable $z = \cos(\theta_{n-1})$, one obtains

$$d\omega_{\mathcal{L}^n} = -\big(1 - z^2\big)^{(n-3)/2} dz, \quad z \in [-1, 1], \tag{3.8}$$

and

$$\Lambda_n(\gamma) = -\big(1-z^2\big)\frac{d^2}{dz^2} - (n-1)z\frac{d}{dz} + \gamma z \tag{3.9}$$

in $L^2\Big([-1,1]; -\big(1-z^2\big)^{(n-3)/2}dz\Big)$. Once more reverting to Lebesgue measure dz on $[-1,1]$ finally produces the unitarily equivalent operator $\widehat{\Lambda}_{n,\mathcal{L}^n}(\gamma)$ in $L^2([-1,1];dz)$ of the form

$$\widehat{\Lambda}_{n,\mathcal{L}^n}(\gamma) = -\big(1-z^2\big)^{(n-3)/2}\left(\big(1-z^2\big)\frac{d^2}{dz^2} - (n-1)z\frac{d}{dz}\right) + \gamma z. \tag{3.10}$$

To facilitate subsequent integration by parts, we rearrange (3.10) into the form

$$\widehat{\Lambda}_{n,\mathcal{L}^n}(\gamma) = -\frac{d}{dz}\left[\big(1-z^2\big)^{(n-1)/2}\frac{d}{dz}\right] + \gamma z, \tag{3.11}$$

still acting in $L^2([-1,1];dz)$. In analogy to [HG80], one now employs the min/max principle to bound $\lambda_{n,0}(\gamma)$ as follows. Choosing ψ real-valued and normalized, that is, $\|\psi\|_{L^2([-1,1];dz)} = 1$, one obtains

$$\begin{aligned}
\lambda_{n,0}(\gamma) &\leqslant \big(\psi, \widehat{\Lambda}_{n,\mathcal{L}^n}(\gamma)\psi\big)_{L^2([-1,1];dz)} \\
&= \int_{-1}^{1} dz\,\Big[\big(1-z^2\big)^{(n-1)/2}\psi'(z)^2 + \gamma z\psi(z)^2\Big] \\
&= \int_{-1}^{1} dz\,\bigg[\big(1-z^2\big)^{(n-1)/2}\psi'(z)^2 - (\gamma/2)\bigg[\frac{d}{dz}\big(1-z^2\big)\bigg]\psi(z)^2\bigg] \\
&= \int_{-1}^{1} dz\,\Big[\big(1-z^2\big)^{(n-1)/2}\psi'(z)^2 + \gamma\big(1-z^2\big)\psi(z)\psi'(z)\Big].
\end{aligned} \tag{3.12}$$

Employing the normalized trial function $\psi_\gamma(z) = [\gamma/(2\sinh(\gamma))]^{1/2} e^{-\gamma z/2}$, one gets

$$
\begin{aligned}
\lambda_{n,0}(\gamma) &\leqslant \big(\psi_\gamma, \widehat{\Lambda}_{n,\mathcal{L}^n}(\gamma)\psi_\gamma\big)_{L^2([-1,1];dz)} \\
&= \big[\gamma^3/(4\sinh(\gamma))\big] \int_{-1}^{1} dz \left[(1/2)\big(1-z^2\big)^{(n-1)/2} e^{-\gamma z} - \big(1-z^2\big)e^{-\gamma z}\right] \\
&= -\big[\gamma^3/(4\sinh(\gamma))\big] \int_{-1}^{1} dz \left[\Big((-(1/2)\big(1-z^2\big)^{(n-1)/2} + \big(1-z^2\big)\Big) e^{-\gamma z}\right] \\
&\leqslant -\big[\gamma^3/(8\sinh(\gamma))\big] \int_{-1}^{1} dz \left[\big(1-z^2\big)^{(n-1)/2} e^{-\gamma z}\right] < 0, \quad \gamma > 0.
\end{aligned} \tag{3.13}
$$

Thus, for all $\gamma > 0$, $\lambda_{n,0}(\gamma) < 0$.

Next, recalling that the lowest eigenvalue $\lambda_{n,0}(\gamma)$ of $\Lambda_n(\gamma)$ is simple for all $\gamma \geqslant 0$ (we note that $\Lambda_n(\gamma)$, $\widetilde{\Lambda}_n(\gamma)$, and $\widehat{\Lambda}_n(\gamma)$ all have the same lowest eigenvalue $\lambda_{n,0}(\gamma)$), we denote by $\psi_0(\gamma) \in L^2(S^{n-1}; d^{n-1}\omega)$ the corresponding normalized eigenfunction, that is,

$$
\Lambda_n(\gamma)\psi_0(\gamma) = \lambda_{n,0}(\gamma)\psi_0(\gamma), \quad \gamma \geqslant 0. \tag{3.14}
$$

Thus, one gets

$$
\begin{aligned}
\lambda_{n,0}(\gamma) &= (\psi_0(\gamma), \Lambda_n(\gamma)\psi_0(\gamma))_{L^2(S^{n-1}; d^{n-1}\omega)} \\
&= (\psi_0(\gamma), [-\Delta_{B,n} + \gamma\cos(\theta_{n-1})]\psi_0(\gamma))_{L^2(S^{n-1}; d^{n-1}\omega)}.
\end{aligned} \tag{3.15}
$$

Moreover, one observes that $\{\Lambda_n(\gamma)\}_{\gamma \in [0,\infty)}$ is a self-adjoint analytic (in fact, entire) family of type (A) in the sense of Kato (cf. [Kat95, Sect. VII.2, p. 375–379], [RS78, p. 16]), implying analyticity of $\lambda_{n,0}(\gamma)$ with respect to γ in a complex neighborhood of $[0,\infty)$. In particular, $\lambda_{n,0}(\gamma)$ is differentiable with respect to γ, and the Feynman–Hellmann Theorem [Thi81, p. 151] (see also [Sim15, Theorem 1.4.7]) yields that

$$
\frac{d\lambda_{n,0}(\gamma)}{d\gamma} = (\psi_0, \cos(\theta_{n-1})\psi_0)_{L^2(S^{n-1}; d^{n-1}\omega)}. \tag{3.16}
$$

Returning to the discussion of (2.30) in Remark 2.3,

$$\begin{aligned}
\lambda_{n,0}(\gamma) &= (\psi_0, \Lambda_n(\gamma)\psi_0)_{L^2(S^{n-1};d^{n-1}\omega)} \\
&= (\psi_0, [-\Delta_{B,n} + \gamma\cos(\theta_{n-1})]\psi_0)_{L^2(S^{n-1};d^{n-1}\omega)} \\
&\geqslant (\psi_0, \gamma\cos(\theta_{n-1})\psi_0)_{L^2(S^{n-1};d^{n-1}\omega)} \\
&\geqslant -\gamma, \qquad (3.17)
\end{aligned}$$

implying,

$$\frac{d\lambda_{n,0}(\gamma)}{d\gamma} = (\psi_0, \cos(\theta_{n-1})\psi_0)_{L^2(S^{n-1};d^{n-1}\omega)} \leqslant \frac{\lambda_{n,0}(\gamma)}{\gamma} < 0, \qquad (3.18)$$

by the strict negativity of $\lambda_{n,0}(\gamma)$ for $\gamma > 0$ derived in (3.13).

Finally, that $H_n(\gamma)$ is bounded from below, and then $H_n(\gamma) \geqslant 0$, if and only if $0 < \gamma \leqslant \gamma_{c,n}$ follows from (2.27), and (2.34), (2.35). The quadratic form inequality (3.2) is a special case of $H_n(\gamma) \geqslant 0$. □

Remark 3.2. (*i*) *One notices that the bound* (3.13) *on* $\lambda_{n,0}(\gamma)$ *is of order* γ^2 *as* $\gamma \downarrow 0$*. (Moreover, one can compute all integrals in* (3.13) *in terms of the modified Bessel function* $I_{n/2}(\gamma)$*, but we omit further details.) In the special case* $n = 3$*, Hunziker and Günther [HG80] also derive a lower bound that is of order* γ^2 *as* $\gamma \downarrow 0$

employing

$$
\begin{aligned}
&\big(\psi, \widehat{\Lambda}_{n,\mathcal{L}^n}(\gamma)\psi\big)_{L^2([-1,1];dz)} \\
&\quad = \int_{-1}^{1} dz \, \big[\big(1-z^2\big)\psi'(z)^2 + \gamma z \psi(z)^2\big] \\
&\quad = \int_{-1}^{1} dz \, \big[\big(1-z^2\big)\psi'(z)^2 + \gamma\big(1-z^2\big)\psi(z)\psi'(z)\big] \\
&\quad = \int_{-1}^{1} dz \, \big[\big(1-z^2\big)[\psi'(z) - (\gamma/2)\psi(z)]^2 - \big[\gamma^2/4\big]\psi(z)^2\big] \\
&\quad \geqslant -\big[\gamma^2/4\big] \int_{-1}^{1} dz \, \psi(z)^2 \\
&\quad = -\gamma^2/4,
\end{aligned} \tag{3.19}
$$

and hence,

$$
\lambda_{n,0}(\gamma) \geqslant -\gamma^2/4. \tag{3.20}
$$

We have not been able to prove an analog of (3.20) *for* $n \geqslant 4$.

(*ii*) *For* $n = 3$, *the existence and value of* $\gamma_{c,n}$ *are widely documented, beginning with [FT47] (and continuing in [BR67], [CG07], [HG80], [Lév67], [Tur77], and [TF66]), but we were particularly interested in analogous results for* $n \geqslant 4$.

(*iii*) *Theorem* 3.1 *demonstrates that* $\gamma_2 = \infty$ *in Remark* 2.3.

(*iv*) *We conjecture (but did not prove) that in analogy to the standard Hardy inequality, also inequality* (3.2) *is strict, that is, equality holds in* (3.2) *if and only if* $f = 0$. $\diamond$

Finally we briefly discuss the remaining case $n = 2$. In this case, the Laplace–

Beltrami operator $-\Delta_{B,2}$ in $L^2\big(S^1; d\omega\big)$ can be characterized by

$$
\begin{aligned}
&(-\Delta_{B,2} f)(\theta_1) = -f''(\theta_1), \quad \theta_1 \in [0, 2\pi], \\
&f \in \operatorname{dom}(-\Delta_{B,2}) = \big\{ g \in L^2([0, 2\pi]; d\theta_1) \,\big|\, g, g' \in AC([0, 2\pi]); \\
&\qquad\qquad\qquad g(0) = g(2\pi),\, g'(0) = g'(2\pi);\, g'' \in L^2([0, 2\pi]; d\theta_1) \big\},
\end{aligned} \tag{3.21}
$$

with

$$
\sigma(-\Delta_{B,2}) = \big\{\ell^2\big\}_{\ell \in \mathbb{N}_0}, \tag{3.22}
$$

$$
-\Delta_{B,2} e^{\pm i\ell\theta_1} = \ell^2 e^{\pm i\ell\theta_1}, \quad \theta_1 \in [0, 2\pi],\ \ell \in \mathbb{N}_0. \tag{3.23}
$$

The resulting Mathieu operator $\Lambda_2(\gamma)$ in $L^2([0, 2\pi]; d\theta_1)$ (cf. (2.20)), of the form

$$
\Lambda_2(\gamma) = -\Delta_{B,2} + \gamma \cos(\theta_1), \quad \operatorname{dom}(\Lambda_2(\gamma)) = \operatorname{dom}(-\Delta_{B,2}), \tag{3.24}
$$

has extensively been studied in the literature, see, for instance [MS54, Ch. 2]. More generally, the least periodic eigenvalue of Hill operators (i.e., situations where $\cos(\theta_1)$ is replaced by a 2π-periodic, locally integrable potential $q(\theta_1)$) has received enormous attention, see for instance, [Blu63], [GGS92], [Kat52], [Moo57], [Put51], [Sta79], [Ung61], and [Win51]. Applied to the Mathieu operator $\Lambda_2(\gamma)$ at hand, the results obtained (cf. the discussion in [GGS92]) imply,

$$
-\gamma^2\big/\big[8\pi^2\big] < \lambda_{2,0}(\gamma) < 0, \quad \gamma \in (0, \infty), \tag{3.25}
$$

$$
\text{there exists } c_0 \in (0, \infty) \text{ such that } \lambda_{2,0}(\gamma) \leqslant -c_0 \gamma^2, \quad \gamma \in [0, 1]. \tag{3.26}
$$

In particular, this proves the absence of a critical coupling constant $0 < \gamma_{c,2}$ for $n = 2$ (equivalently, the critical constant in two dimensions equals zero, $\gamma_{c,2} = 0$), explaining why we had to limit ourselves to $n \geqslant 3$ in the bulk of this chapter.

CHAPTER FOUR

A Numerical Approach

Having demonstrated the existence and uniqueness of critical dipole moments $\gamma_{c,n}$ for all dimensions $n \geqslant 3$, and having shown some of the properties of $\lambda_{n,0}(\gamma)$, this chapter is devoted to a description of a numerical method for computing $\gamma_{c,n}$, in analogy to the Legendre expansion in [CG07].

To set up the numerical algorithm we argue as follows: Given (3.14), that is, $\Lambda_n(\gamma)\psi_0(\gamma) = \lambda_{n,0}(\gamma)\psi_0(\gamma)$, $\gamma \geqslant 0$, we are interested in solving this eigenvalue problem in the particular scenario where γ ranges from 0 to $\gamma_{c,n}$, observing that $\lambda_{n,0}(\gamma_{c,n}) = -(n-2)^2/4$ (cf. (2.31)). Restricting the Laplace–Beltrami operator (5.16) to $\mathcal{L}^n$ as in (3.3)–(3.5), the first line of (3.5) thus amounts to solving the eigenvalue problem

$$\begin{aligned}
&-\frac{d^2\Psi(\theta_{n-1})}{d\theta_{n-1}^2} - (n-2)\cot(\theta_{n-1})\frac{d\Psi(\theta_{n-1})}{d\theta_{n-1}} + \gamma_{c,n}\cos(\theta_{n-1})\Psi(\theta_{n-1}) \\
&\quad = \lambda_{n,0}(\gamma_{c,n})\Psi(\theta_{n-1}), \quad \lambda_{n,0}(\gamma_{c,n}) = -(n-2)^2/4.
\end{aligned} \tag{4.1}$$

Expanding $\Psi(\,\cdot\,)$ in normalized Gegenbauer polynomials, one obtains

$$\Psi(\theta_{n-1}) = \sum_{\ell=0}^{\infty} d_\ell \left[\frac{\ell!(2\ell+n-2)}{2^{4-n}\pi\Gamma(\ell+n-2)}\right]^{1/2} \Gamma((n-2)/2)C_\ell^{(n-2)/2}(\cos(\theta_{n-1})) \tag{4.2}$$

where d_ℓ are appropriate expansion coefficients. Since the Gegenbauer polynomials are eigenfunctions of $-\Delta_{B,n}$ corresponding to the eigenvalue $\ell(\ell+n-2)$, (4.1) becomes

$$\sum_{\ell=0}^{\infty}\Big((\ell(\ell+n-2)+\gamma_{c,n}\cos(\theta_{n-1})-\lambda_{n,0}(\gamma_{c,n})\Big)d_\ell\left[\frac{\ell!(2\ell+n-2)}{2^{4-n}\pi\Gamma(\ell+n-2)}\right]^{1/2}$$
$$\times\,\Gamma((n-2)/2)C_\ell^{(n-2)/2}(\cos(\theta_{n-1})) \tag{4.3}$$

Next, we will exploit the following recurrence relation of Gegenbauer polynomials,

$$\cos(\theta_{n-1})C_\ell^{(n-2)/2}(\cos(\theta_{n-1}))$$
$$=\frac{\ell+1}{2\ell+n-2}\left(C_{\ell+1}^{(n-2)/2}(\cos(\theta_{n-1}))+\frac{\ell+n-3}{\ell+1}C_{\ell-1}^{(n-2)/2}(\cos(\theta_{n-1}))\right),$$
$$\ell\in\mathbb{N}_0, \tag{4.4}$$

to expand the term $\gamma_{c,n}\cos(\theta_{n-1})$. For the $(\ell-1)$-term, one infers

$$\gamma_{c,n}\cos(\theta_{n-1})d_{\ell-1}\left[\frac{(\ell-1)!(2\ell+n-4))^2}{2^{4-n}\pi\Gamma(\ell+n-3)}\right]^{1/2}\Gamma((n-2)C_{\ell-1}^{(n-2)/2}(\cos(\theta_{n-1}))$$
$$=\gamma_{c,n}d_{\ell-1}\left[\frac{(\ell-1)!(2\ell+n-4)}{2^{4-n}\pi\Gamma(\ell+n-3)}\right]^{1/2}\frac{\ell\Gamma((n-2)/2)}{2\ell+n-4}C_\ell^{(n-2)/2}(\cos(\theta_{n-1})),$$
$$\ell\in\mathbb{N}_0, \tag{4.5}$$

and for the $(\ell+1)$-term, one obtains

$$\gamma_{c,n}\cos(\theta_{n-1})d_{\ell+1}\left[\frac{(\ell+1)!(2\ell+n)}{2^{4-n}\pi\Gamma(\ell+n-1)}\right]^{1/2}\Gamma((n-2)/2)C_{\ell+1}^{(n-2)/2}(\cos(\theta_{n-1}))$$
$$=\gamma_{c,n}d_{\ell+1}\left[\frac{\ell+1)!(2\ell+n)}{2^{4-n}\pi\Gamma(\ell+n-1)}\right]^{1/2}\Gamma((n-2)/2)\frac{\ell+n-2}{2\ell+n}C_\ell^{(n-2)/2}(\cos(\theta_{n-1})),$$
$$\ell\in\mathbb{N}_0. \tag{4.6}$$

The ℓ-term maintains its form

$$\Big(\ell(\ell+n-2)-\lambda_{n,0}(\gamma_{c,n})\Big)d_\ell\left[\frac{\ell!(2\ell+n-2)}{2^{4-n}\pi\Gamma(\ell+n-2)}\right]^{1/2}\Gamma((n-2)/2)$$
$$\times\, C_\ell^{(n-2)/2}(\cos(\theta_{n-1})),\quad \ell\in\mathbb{N}_0, \tag{4.7}$$

so one can divide all terms by the normalizing factor from (4.2) (since the orthogonality of the Gegenbauer polynomials mandates every term in the sum be zero), obtaining

$$\sum_{\ell=0}^{\infty}\Bigg[\Big(\ell(\ell+n-2)-\lambda_{n,0}(\gamma_{c,n})\Big)d_\ell$$
$$+\gamma_{c,n}\left(\left[\frac{(2\ell+n-4)(\ell+n-3)}{\ell(2\ell+n-2)}\right]^{1/2}\frac{\ell}{2\ell+n-4}d_{\ell-1}\right.$$
$$\left.+\left[\frac{(\ell+1)(2\ell+n)}{2\ell+n-2)(\ell+n-2)}\right]^{1/2}\frac{\ell+n-2}{2\ell+n}d_{\ell+1}\right)\Bigg]C_\ell^{(n-2)/2}(\cos(\theta_{n-1}))=0. \tag{4.8}$$

Inserting the critical value of $\lambda_{n,0}(\gamma_{c,n})=-(n-2)^2/4$, one can set each coefficient equal to zero:

$$\begin{aligned}&\Big(\ell(\ell+n-2)+\big[(n-2)^2/4\big]\Big)d_\ell+\gamma_{c,n}\left(\left[\frac{\ell(\ell+n-3)}{(2\ell+n-4)(2\ell+n-2)}\right]^{1/2}d_{\ell-1}\right.\\&\quad\left.+\left[\frac{(\ell+1)(\ell+n-2)}{(2\ell+n-2)(2\ell+n)}\right]^{1/2}d_{\ell+1}\right)=0,\quad \ell\in\mathbb{N}_0.\end{aligned} \tag{4.9}$$

One can rewrite (4.9) as

$$\left[\frac{(\ell+1)(\ell+n-2)}{(2\ell+n-2)(2\ell+n)}\right]^{1/2}d_{\ell+1}+\left[\frac{\ell(\ell+n-3)}{(2\ell+n-4)(2\ell+n-2)}\right]^{1/2}d_{\ell-1}$$
$$=-\frac{1}{\gamma_{c,n}}\Big(\ell(\ell+n-2)+\big[(n-2)^2/4\big]\Big)\,d_\ell,\quad \ell\in\mathbb{N}_0. \tag{4.10}$$

This can be expressed as the generalized Jacobi operator eigenvalue problem in

$\ell^2(\mathbb{N}_0; w)$,

$$Jd = -\frac{1}{\gamma_{c,n}} wd, \tag{4.11}$$

where

$$Jd = \begin{cases} a_{\ell+1} d_{\ell+1} + a_\ell d_{\ell-1}, & \ell \in \mathbb{N}, \\ a_1 d_1, & \ell = 0, \end{cases} \qquad wd = \big(w_\ell d_\ell\big)_{\ell \in \mathbb{N}_0}, \tag{4.12}$$

and

$$a_\ell = \left[\frac{\ell(\ell+n-3)}{(2\ell+n-4)(2\ell+n-2)}\right]^{1/2}, \quad w_\ell = \ell(\ell+n-2) + \big[(n-2)^2/4\big], \tag{4.13}$$
$$\ell \in \mathbb{N}_0.$$

Since we are interested in varying γ from 0 to $\gamma_{c,n}$, this implies we are searching for the *smallest negative eigenvalue* of the operator J in $\ell^2(\mathbb{N}_0; w)$.

Explicitly, (4.12) yields the self-adjoint Jacobi operator J in $\ell^2(\mathbb{N}_0; w)$

$$\begin{aligned} Jd &= \begin{pmatrix} 0 & a_1 & 0 & \dots & & & \\ a_1 & 0 & a_2 & 0 & \dots & & \\ 0 & a_2 & 0 & a_3 & 0 & \dots & \\ \vdots & 0 & a_3 & 0 & a_4 & 0 & \dots \\ & \vdots & 0 & \ddots & \ddots & \ddots & \end{pmatrix} \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ \vdots \\ \\ \end{pmatrix} \\ &= -\frac{1}{\gamma_{c,n}} \begin{pmatrix} w_0 & 0 & \dots & & & & \\ 0 & w_1 & 0 & \dots & & & \\ \vdots & 0 & w_2 & 0 & \dots & & \\ & \vdots & 0 & w_3 & 0 & \dots & \\ & & \vdots & \ddots & \ddots & \ddots & \end{pmatrix} \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ \vdots \\ \\ \end{pmatrix} = -\frac{1}{\gamma_{c,n}} wd. \end{aligned} \tag{4.14}$$

One would like to calculate $\gamma_{c,n}$ approximately using finite truncations of this matrix - a notion which will be made more precise below. In order for these approximants to converge, a transformation to a compact Jacobi operator becomes necessary. For this purpose one introduces the operator

$$V = \begin{cases} \ell^2(\mathbb{N}_0; w) \to \ell^2(\mathbb{N}_0), \\ b \mapsto w^{1/2} b. \end{cases} \tag{4.15}$$

That V is unitary may be seen from

$$||Vb||_{\ell^2(\mathbb{N}_0)} = ||w^{1/2}b||_{\ell^2(\mathbb{N}_0)} = ||b||_{\ell^2(\mathbb{N}_0;w)}, \quad b \in \ell^2(\mathbb{N}_0; w), \tag{4.16}$$

and the fact that V is surjective and defined on all of $\ell^2(\mathbb{N}_0; w)$. Next, one transforms (4.14) into

$$V^{-1}JV^{-1}Vd = -\frac{1}{\gamma_{c,n}} Vd, \quad d \in \ell^2(\mathbb{N}_0; w), \tag{4.17}$$

which can equivalently be expressed as

$$w^{-1/2}Jw^{-1/2}d' = -\frac{1}{\gamma_{c,n}} d', \quad d' = Vd \in \ell^2(\mathbb{N}_0). \tag{4.18}$$

With the definition $K := w^{-1/2} J w^{-1/2}$, one can write (4.18) in the form

$$
\begin{aligned}
Kd' &= \begin{pmatrix} 0 & a_1' & 0 & \dots & & & \\ a_1' & 0 & a_2' & 0 & \dots & & \\ 0 & a_2' & 0 & a_3' & 0 & \dots & \\ \vdots & 0 & a_3' & 0 & a_4' & 0 & \dots \\ & \vdots & 0 & \ddots & \ddots & \ddots & \end{pmatrix} \begin{pmatrix} d_0' \\ d_1' \\ d_2' \\ \vdots \\ \end{pmatrix} \\
&= -\frac{1}{\gamma_{c,n}} \begin{pmatrix} d_0' \\ d_1' \\ d_2' \\ \vdots \\ \end{pmatrix} = -\frac{1}{\gamma_{c,n}} d',
\end{aligned} \tag{4.19}
$$

in analogy with (4.14), with

$$
\begin{aligned}
a_\ell' &= w_\ell^{-1/2} a_\ell \, w_{\ell-1}^{-1/2} \\
&= \Big[\ell(\ell+n-2) + [(n-2)^2/4]\Big]^{-1/2} \Big[(\ell-1)(\ell+n-3) + [(n-2)^2/4]\Big]^{-1/2} \\
&\quad \times \left[\frac{\ell(\ell+n-3)}{(2\ell+n-4)(2\ell+n-2)}\right]^{1/2} \underset{\ell\to\infty}{=} O\big(\ell^{-2}\big).
\end{aligned} \tag{4.20}
$$

Once again, we are searching for the *smallest negative eigenvalue* of the operator K in $\ell^2(\mathbb{N}_0)$.

A few elementary facts about K follow from elementary analysis of its entries.

Proposition 4.1. *One has* $K \in \mathcal{B}_\infty(\ell^2(\mathbb{N}_0))$, *and*[1]

$$
||K||_{\mathcal{B}(\ell^2(\mathbb{N}_0))} \leqslant \begin{cases} \frac{8}{3\sqrt{3}}, & n = 3, \\ 2\max\{a_{\ell_{r,n}}', a_{\ell_{r,n}-1}'\}, & n \geqslant 4, \end{cases} \tag{4.21}
$$

[1] We temporarily indicate the n-dependence of a' by emplying the additional subscript n.

where

$$r(n) = \frac{1}{4}\left(6 - 2n + \left\{2\left[26 - 18n + 3n^2\right]\right\}^{1/2}\right), \quad \ell_{r,n} = \lceil r(n) \rceil, \tag{4.22}$$

with $\lceil x \rceil = \inf\{m \in \mathbb{N}_0 \,|\, m \geqslant x\}$, *the ceiling function.*

Proof. The compactness assertion follows from the limiting behavior $a'_\ell \underset{\ell\to\infty}{\to} 0$, see, for instance, [Van96, p. 201]. To obtain the norm bound, one applies [Tes99, Theorem 1.5] after calculating $||a'||_{\ell^\infty(\mathbb{N}_0)}$. As $a'_{\ell,n}$ is bounded and tends to 0 as $\ell \to \infty$ for all $n \geqslant 3$, it attains its supremum. To find the index where this occurs, one considers ℓ as a continuous variable, and solves $\frac{da'_{\ell,n}}{d\ell} = 0$. The value $r(n)$ emerges as the root of this expression, but as $0 < r(n) \in \mathbb{R} \setminus \mathbb{N}$ for $n \geqslant 4$, the ceiling function in (4.21) and maximum in (4.22) are required. Since $r(3) \in \mathbb{C} \setminus \mathbb{R}$, the norm $||a'_{\ell,3}||_{\ell^\infty(\mathbb{N}_0)}$ must be computed separately as $||a'_{\ell,3}||_{\ell^\infty(\mathbb{N}_0)} = |a'_{1,3}| = \frac{8}{3\sqrt{3}}$. □

To introduce the notion of finite truncations, one considers the operators

$$P_m = \begin{pmatrix} I_m & 0 \\ 0 & 0 \end{pmatrix} = I_m \oplus 0, \quad K_m = P_m K P_m, \quad m \in \mathbb{N}, \tag{4.23}$$

on $\ell^2(\mathbb{N}_0)$, where I_m denotes the identity operator in $\mathbb{C}^m$, $m \in \mathbb{N}$.

We also introduce the finite $N \times N$ tri-diagonal Jacobi matrices $J_N(a'_0, \ldots, a'_{N-1})$ in $\mathbb{C}^N$, $N \in \mathbb{N}$, $N \geqslant 2$, denoted by

$$J_N(a'_1, \ldots, a'_{N-1}) = \begin{pmatrix} 0 & a'_1 & & & & \\ a'_1 & 0 & a'_2 & & \mathbf{0} & \\ & a'_2 & 0 & a'_3 & & \\ & & a'_3 & 0 & \ddots & \\ & \mathbf{0} & & \ddots & \ddots & a'_{N-1} \\ & & & & a'_{N-1} & 0 \end{pmatrix}, \quad N \in \mathbb{N}, N \geqslant 2, \tag{4.24}$$

in particular,

$$
\begin{aligned}
&\det_{\mathbb{C}^N}(zI_N - J_N(a_1',\dots,a_{N-1}')) = z\det_{\mathbb{C}^{N-1}}(zI_{N-1} - J_{N-1}(a_2',\dots,a_{N-1}')) \\
&\qquad - [a_1']^2\det_{\mathbb{C}^{N-2}}(zI_{N-2} - J_{N-2}(a_3',\dots,a_{N-1}')), \quad z \in \mathbb{C}, \\
&\quad = \begin{cases} zP_{(N-1)/2}\big(z^2\big), \quad P_{(N-1)/2}(0) \neq 0, & N \text{ odd}, \\ Q_{N/2}\big(z^2\big), \quad Q_{N/2}(0) \neq 0, & N \text{ even}, \end{cases}
\end{aligned} \tag{4.25}
$$

where $P_{(N-1)/2}(\,\cdot\,)$ and $Q_{N/2}(\,\cdot\,)$ are monic polynomials of degree $(N-1)/2$ and $N/2$, respectively.

Thus, the spectrum of each $J_N(a_0',\dots,a_{N-1}')$ consists of N real eigenvalues, symmetric with respect to the origin, the eigenvalues being simple as long as $a_j' > 0$, $1 \leqslant j \leqslant N-1$. Explicitly,

$$
\begin{aligned}
&\det_{\mathbb{C}^2}((zI_2 - J_2(a_1')) = z^2 - [a_1']^2, \\
&\det_{\mathbb{C}^3}((zI_3 - J_3(a_1',a_2')) = z\big\{z^2 - [a_1']^2 - [a_2']^2\big\}, \\
&\det_{\mathbb{C}^4}((zI_4 - J_4(a_1',a_2',a_3')) = z^4 - \big\{[a_1']^2 + [a_2']^2 + [a_3']^2\big\}z^2 + [a_1']^2[a_3']^2, \\
&\det_{\mathbb{C}^5}((zI_5 - J_5(a_1',a_2',a_3',a_4')) = z\big\{z^4 - \big\{[a_1']^2 + [a_2']^2 + [a_3']^2 + [a_4']^2\big\}z^2 \\
&\qquad\qquad + [a_1']^2[a_3']^2 + [a_1']^2[a_4']^2 + [a_2']^2[a_4']^2\big\},
\end{aligned} \tag{4.26}
$$

etc.

In addition, we introduce the unitary, self-adjoint, diagonal operator U in $\ell^2(\mathbb{N}_0)$ as

$$
U = \big((-1)^p\delta_{p,q}\big)_{(p,q)\in\mathbb{N}_0^2}, \quad U^{-1} = U = U^*. \tag{4.27}
$$

Theorem 4.2. *With K, K_m, $m \in \mathbb{N}$, and U as in* (4.19), (4.23)–(4.27), *one concludes* *that K and $-K$ as well as K_m and $-K_m$ are unitarily equivalent,*

$$-K = UKU^{-1}, \quad -K_m = UK_mU^{-1}, \ m \in \mathbb{N}, \tag{4.28}$$

and hence the spectra of K and K_m, $m \in \mathbb{N}$, are symmetric with respect to zero. Moreover, all nonzero eigenvalues of K are simple,

$$\lim_{m\to\infty} \|K_m - K\|_{\mathcal{B}(\ell^2(\mathbb{N}_0))} = 0, \tag{4.29}$$

and[2]

$$\sigma(K) = \lim_{m\to\infty} \sigma(K_m) \ \text{ and } \ \sigma_e(K) = \sigma_e(K_m) = \{0\}, \ m \in \mathbb{N}. \tag{4.30}$$

Equivalently, $\lambda \in \sigma(K)$ if and only if there is a sequence $(\lambda_m)_{m\in\mathbb{N}}$ with $\lambda_m \in \sigma(K_m)$ such that $\lambda_m \underset{m\to\infty}{\longrightarrow} \lambda$.

Proof. The symmetry fact (4.28) follows from an elementary computation. That all eigenvalues of K are simple follows from the fact that K is a half-lattice operator with $a'_\ell > 0$, $\ell \in \mathbb{N}$, and hence the half-lattice does not decouple into a disjoint union of subsets (resp., K does not reduce to a direct sum of operators).

One notices that $\text{s-lim}_{m\to\infty} P_m = I$, where I denotes the identity operator in $\ell^2(\mathbb{N}_0)$, and strong operator convergence is abbreviated by s-lim. Together with the compactness of K given in Proposition 4.1, one obtains

$$\lim_{m\to\infty} \|P_mK - K\|_{\mathcal{B}(\ell^2(\mathbb{N}_0))} = 0, \tag{4.31}$$

applying [Amr81, Proposition 3.11]. The norm convergence in (4.31), together with the uniform bound $\|P_m\|_{\mathcal{B}(\ell^2(\mathbb{N}_0))} = 1$, $m \in \mathbb{N}$, yields (4.29). The latter implies

[2] Here $\sigma_e(\,\cdot\,)$ denotes the essential spectrum.

(4.30) as a consequence of [RS72, Theorem VIII.23 (a) and Theorem VIII.24 (a)] (see also [Wei00, Satz 9.24 *a*)]), taking into account that norm resolvent convergence of a sequence of self-adjoint operators is equivalent to norm convergence of a uniformly bounded sequence of self-adjoint operators in a complex Hilbert space (see [RS72, Theorem VII.18], [Wei00, Satz 9.22 a) (*ii*)]). □

A more precise version of the eigenvalue convergence result can most efficiently be obtained from Courant's max-min theorem. The proof of the following result is due to [EM].

Theorem 4.3. *Let $\mathcal{H}$ be a complex, separable Hilbert space, $0 \leqslant C_\infty \in \mathcal{B}(\mathcal{H})$, and $0 \leqslant C_n \in \mathcal{B}_\infty(\mathcal{H})$, $n \in \mathbb{N}$, with $||C_n - C_\infty||_{\mathcal{B}(\mathcal{H})} \underset{n\to\infty}{\to} 0$. Then, $C_\infty \in \mathcal{B}_\infty(\mathcal{H})$. Let $\lambda_{\infty,k}$, $\lambda_{n,k}$ be the eigenvalues of C_∞, C_n, ordered according to*

$$\begin{aligned} \lambda_{\infty,1} \geqslant \lambda_{\infty,2} \geqslant \dots, \\ \lambda_{n,1} \geqslant \lambda_{n,2} \geqslant \dots, \end{aligned} \tag{4.32}$$

counting multiplicity. Then, for each $k \in \mathbb{N}$

$$\lim_{n\to\infty} \lambda_{n,k} = \lambda_{\infty,k}. \tag{4.33}$$

Proof. Using Courant's max-min theorem,

$$\lambda_{n,k} = \max_{\substack{W_k \subset \mathcal{H} \\ \dim(W_k)=k}} \min_{\substack{f \in W_k \\ ||f||_{\mathcal{H}}=1}} (f, C_n f)_{\mathcal{H}}, \tag{4.34}$$

and similarly with $\lambda_{n,k}, C_n$ replaced by $\lambda_{\infty,k}, C_\infty$. Pick $\varepsilon > 0$, then there exists some $N = N(\varepsilon) \in \mathbb{N}$ such that

$$(f, C_\infty f)_{cH} - \varepsilon ||f||^2_{\mathcal{H}} \leqslant (f, C_n f)_{\mathcal{H}} \leqslant (f, C_\infty f)_{\mathcal{H}} + \varepsilon ||f||^2_{\mathcal{H}}, \quad n \geqslant N, n \in \mathbb{N}, f \in \mathcal{H}, \tag{4.35}$$

and hence by the min-max theorem,

$$\lambda_{\infty,k} - \varepsilon \leqslant \lambda_{n,k} \leqslant \lambda_{\infty,k} + \varepsilon, \tag{4.36}$$

proving (4.33). □

Remark 4.4. *Theorem* 4.3 *requires* $C \geqslant 0$*, a hypothesis not satisfied by* K *in Theorem* 4.2*. However, Theorem* 4.3 *applies separately to* $C_{\pm} = [|C| \pm C]/2$*, equivalently, one restricts the subspaces* W_k *in* (4.34) *in such a manner that*

$$(f, C_\infty f)_{\mathcal{H}} \geqslant 0, \ \ resp., \ (f, C_\infty f)_{\mathcal{H}} \leqslant 0, \quad f \in W_k. \tag{4.37}$$

See [Heu86, Sect. 32] for details.

Returning to the dipole context, one may now compute approximants of $\gamma_{c,n}$ by approximating the largest negative eigenvalues of K in terms of the largest negative eigenvalue of K_m with increasing $m \in \mathbb{N}$. Using K_7, (which produced 16 stable digits in the case $n = 3$), one obtains the following critical values for $3 \leqslant n \leqslant 10$:

n	$\gamma_{c,n}$
3	1.279
4	3.790
5	7.584
6	12.672
7	19.058
8	26.742
9	35.725
10	46.006

The result for $n = 3$ is in excellent agreement with the ones found in the literature (see, e.g., [AG78], [BR67], [CG07], [Cra67], [FT47], [Lév67], [Tur77], and [TF66]).

The approximate values of $\gamma_{c,n}$ for $n \geqslant 4$ are in good agreement with those obtained in [FMT08, p. 99], which were obtained by entirely different methods.

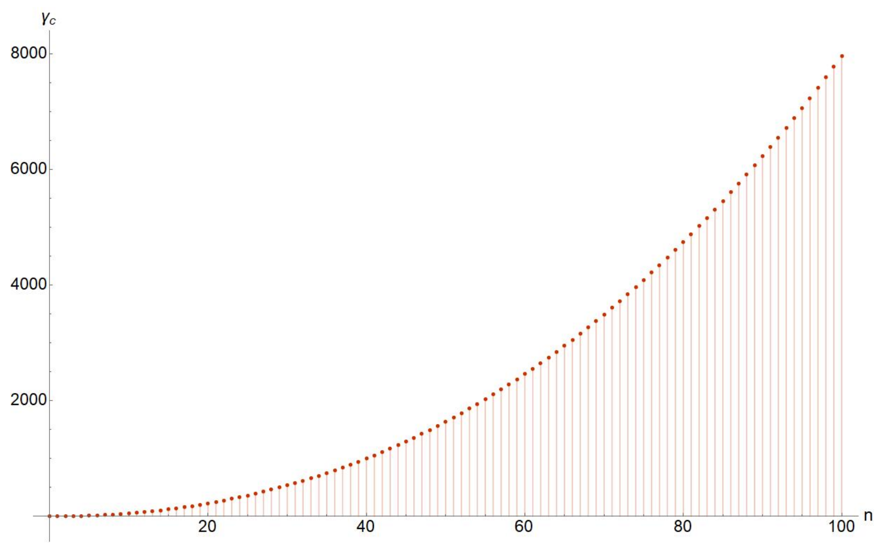

Figure 4.1: Dimension vs. Critical Dipole Moment

Combining the results of this manuscript with those in [Ges+16] one can extend the scope of this investigation to include multi-polar dipole interactions, that is, sums of point dipoles supported on an infinite discrete set (a set of distinct points spaced apart by a minimal distance $\varepsilon > 0$). In this context one can extend existing results of [FMT08], [FMT09] regarding quadratic form estimates, a topic we will return to at a later stage.

CHAPTER FIVE

Spherical Harmonics and the Laplace–Beltrami Operator

In this appendix we summarize some of the results on spherical harmonics and the Laplace–Beltrami operator on the unit sphere S^{n-1} in dimensions $n \in \mathbb{N}$, $n \geqslant 2$, following [AH12, Chs. 2,3], [DX13, Ch. 1], and [Her99, Ch. 2].

Denoting the unit sphere in $\mathbb{R}^n$ by S^{n-1}, $n \in \mathbb{N}$, $n \geqslant 2$, cartesian and polar coordinates (cf. e.g., [Blu60]) are given by

$$\begin{aligned}
&x = (x_1, \dots, x_n) = (r, \theta_1, \theta_2, \dots, \theta_{n-1}) \in \mathbb{R}^n, \\
&x = r\theta,\ \theta = (\theta_1, \theta_2, \dots, \theta_{n-1}) = x/|x| \in S^{n-1}, \\
&x_k \in \mathbb{R},\ 1 \leqslant k \leqslant n,\ r = |x| \in [0, \infty),\ \theta_1 \in [0, 2\pi],\ \theta_j \in [0, \pi],\ 2 \leqslant j \leqslant n-1,
\end{aligned} \tag{5.1}$$

where (cf., e.g., [Blu60], [DX13, Sect. 1.5])

$$\begin{cases}
x_1 = r\sin(\theta_1) \prod_{j=2}^{n-1} \sin(\theta_j), \\
x_2 = r\cos(\theta_1) \prod_{j=2}^{n-1} \sin(\theta_j), \\
\vdots \\
x_{n-1} = r\cos(\theta_{n-2})\sin(\theta_{n-1}), \\
x_n = r\cos(\theta_{n-1}).
\end{cases} \tag{5.2}$$

The surface measure $d^{n-1}\omega$ on S^{n-1} and the volume element in $\mathbb{R}^n$ then read

$$d^{n-1}\omega(\theta) = d\theta_1 \prod_{j=2}^{n-1} [\sin(\theta_j)]^{j-1} d\theta_j, \quad d^n x = r^{n-1} dr\, d^{n-1}\omega, \tag{5.3}$$

in particular, the area ω_n of the unit sphere S^{n-1} in $\mathbb{R}^n$ is given by (cf. [Mül66, p. 2])

$$\omega_n = \int_{S^{n-1}} d^{n-1}\omega(\theta) = 2\pi^{n/2}/\Gamma(n/2). \tag{5.4}$$

Turning to spherical harmonics next, we recall that a homogeneous polynomial $P(x_1, \dots, x_n)$ of degree $\ell \in \mathbb{N}_0$ (in n variables) satisfies $P(tx_1, \dots, tx_n) = t^n P(x_1, \dots, x_n)$ and is a linear combination of terms of degree ℓ. The space of such polynomials with real coefficients is denoted $\mathscr{P}_\ell^n$. We define the harmonic homogeneous polynomials of degree ℓ in n variables by

$$\mathscr{H}_\ell^n = \{P \in \mathscr{P}_\ell^n \,|\, \Delta_n P = 0\}, \tag{5.5}$$

where Δ_n represents the Laplace differential expression on $\mathbb{R}^n$. Restricting the elements of $\mathscr{H}_\ell^n$ to the sphere S^{n-1}, one obtains $\mathcal{Y}_\ell^n$, the space of spherical harmonics of degree ℓ in n dimensions. Spaces of different degrees are orthogonal with respect to the real inner product on the sphere,

$$\begin{split} (Y, Z)_{L^2(S^{n-1};d^{n-1}\omega)} = \int_{S^{n-1}} d^{n-1}\omega(\theta)\, Y(\theta)Z(\theta) = 0, \\ Y \in \mathcal{Y}_\ell^n,\ Z \in \mathcal{Y}_{\ell'}^n,\ \ell, \ell' \in \mathbb{N}_0,\ \ell \neq \ell'. \end{split} \tag{5.6}$$

The dimension of $\mathcal{Y}_\ell^n$ equals that of $\mathscr{H}_\ell^n$ and is given by ([DX13, Corollary 1.1.4])

$$\dim(\mathscr{H}_\ell^n) = \binom{\ell+n-1}{\ell} - \binom{\ell+n-3}{\ell-2} = \frac{2\ell+n-2}{\ell+n-2}\binom{\ell+n-2}{n-2}, \tag{5.7}$$

where we use the convention that the second binomial coefficient equals 0 when $\ell = 0, 1$, and replace the final fraction by 1 in the case where $n = 2$ and $\ell = 0$. This is equivalently formulated in [Mül66, Lemma 3, p. 4] as the generating series

$$\frac{1+x}{(1-x)^{n-1}} = \sum_{\ell=0}^{\infty} \dim(\mathcal{Y}_\ell^n)\, x^\ell. \tag{5.8}$$

Most importantly, the spherical harmonics are the eigenfunctions of the Laplace–Beltrami operator $\Delta_{B,n}$ in $L^2\big(S^{n-1}; d^{n-1}\omega\big)$, satisfying the eigenvalue equation

$$(-\Delta_{B,n} Y)(\theta) = \ell(\ell+n-2) Y(\theta), \quad Y \in \mathcal{Y}_\ell^n,\ \ell \in \mathbb{N}_0. \tag{5.9}$$

Following [DX13, Sect. 1.5] an explicit characterization for the spherical harmonics reads as follows: Introducing the multi-index $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$, with $|\alpha| = \sum_{j=1}^{n} \alpha_j$, and $\theta = (\theta_1, \dots, \theta_{n-1}) \in S^{n-1}$, the spherical harmonics are of the form

$$Y_\alpha(\theta) = [N_\alpha]^{-1} g_\alpha(\theta_1) \prod_{j=1}^{n-2} [\sin(\theta_{n-j})]^{|\alpha^{j+1}|} C_{\alpha_j}^{\nu_j}(\cos(\theta_{n-j})), \tag{5.10}$$

where

$$|\alpha^j| = \sum_{k=j}^{n-1} \alpha_k, \quad \nu_j = |\alpha^{j+1}| + [(n-j-1)/2], \tag{5.11}$$

$$g_\alpha(\theta_1) = \begin{cases} \cos(\alpha_{n-1}\theta_1), & \alpha_n = 0, \\ \sin(\alpha_{n-1}\theta_1), & \alpha_n = 1, \end{cases} \tag{5.12}$$

$$[N_\alpha]^2 = b_\alpha \prod_{j=1}^{n-2} \frac{[\alpha_j!]([(n-j+1)/2])_{|\alpha^{j+1}|}(\alpha_j+\nu_j)}{(2\nu_j)_{\alpha_j}([(n-j)/2])_{|\alpha^{j+1}|}\nu_j}, \quad b_\alpha = \begin{cases} 2, & \alpha_{n-1}+\alpha_n > 0, \\ 1, & \text{otherwise.} \end{cases} \tag{5.13}$$

Here the Pochhammer symbol $(x)_a$ is defined by

$$(x)_0 = 1, \quad (x)_n = \Gamma(x+n)/\Gamma(n) = x(x+1)\cdots(x+n-1), \quad n \in \mathbb{N}, \tag{5.14}$$

and $C_n^{\lambda}(\,\cdot\,)$ represent the Gegenbauer (or ultrasperical) polynomials, see, for instance, [AS64, Ch. 22], [DX13, Appendix B].

The set $\{Y_\alpha \,|\, |\alpha| = \ell, \alpha_n = 0, 1\}$ represents an orthonormal basis of $\mathcal{Y}_\ell^n$.

Finally, we recall the expression of the Laplace–Beltrami differential expression on S^{n-1} in spherical coordinates. From [AH12, p. 94], [DX13, Lemma 1.4.2], one obtains the recursion

$$\begin{aligned} -\Delta_{B,2} &= -\frac{\partial^2}{\partial\theta_1^2}, \qquad (5.15)\\ -\Delta_{B,n} &= -\frac{\partial^2}{\partial\theta_{n-1}^2} - (n-2)\cot(\theta_{n-1})\frac{\partial}{\partial\theta_{n-1}} - [\sin(\theta_{n-1})]^{-2}\Delta_{B,n-1}, \quad n \geqslant 3. \end{aligned}$$

Explicitly (cf. [DX13, p. 19]),

$$\begin{aligned} -\Delta_{B,n} &= -[\sin(\theta_{n-1})]^{2-n}\frac{\partial}{\partial\theta_{n-1}}\left[[\sin(\theta_{n-1})]^{n-2}\frac{\partial}{\partial\theta_{n-1}}\right] \\ &\quad - \sum_{j=1}^{n-2}\left(\prod_{k=j+1}^{n-1}[\sin(\theta_k)]^{-2}\right)[\sin(\theta_j)]^{1-j}\frac{\partial}{\partial\theta_j}\left[[\sin(\theta_j)]^{j-1}\frac{\partial}{\partial\theta_j}\right] \qquad (5.16)\\ &= -\sum_{j=1}^{n-1}\left(\prod_{k=1}^{j-1}[\sin(\theta_{n-k})]^{-2}\right)[\sin(\theta_{n-j})]^{1-j-n} \\ &\qquad \times \frac{\partial}{\partial\theta_{n-j}}\left[[\sin(\theta_{n-j})]^{n-j-1}\frac{\partial}{\partial\theta_{n-j}}\right]. \qquad (5.17) \end{aligned}$$

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