SEMICLASSICAL SZEGÖ LIMIT OF EIGENVALUE CLUSTERS FOR THE HYDROGEN ATOM ZEEMAN HAMILTONIAN

MISAEL AVENDAÑO-CAMACHO, PETER D. HISLOP,
AND CARLOS VILLEGAS-BLAS

Abstract. We prove a limiting eigenvalue distribution theorem (LEDT) for suitably scaled eigenvalue clusters around the discrete negative eigenvalues of the hydrogen atom Hamiltonian formed by the perturbation by a weak constant magnetic field. We study the hydrogen atom Zeeman Hamiltonian $H_V(h,B) = (1/2)(-\imath h\nabla - \mathbf{A}(h))^2 - |\mathbf{x}|^{-1}$, defined on $L^2(\mathbb{R}^3)$, in a constant magnetic field $\mathbf{B}(h) = \nabla \times \mathbf{A}(h) = (0,0,\epsilon(h)B)$ in the weak field limit $\epsilon(h) \to 0$ as $h \to 0$. We consider the Planck's parameter h taking values along the sequence $h = 1/(N+1)$, with $N = 0,1,2,\ldots$, and $N \to \infty$. We prove a semiclassical $N \to \infty$ LEDT of the Szegö-type for the scaled eigenvalue shifts and obtain both (**i**) an expression involving the regularized classical Kepler orbits with energy $E = -1/2$ and (**ii**) a weak limit measure that involves the component ℓ_3 of the angular momentum vector in the direction of the magnetic field. This LEDT extends results of Szegö-type for eigenvalue clusters for bounded perturbations of the hydrogen atom to the Zeeman effect. The new aspect of this work is that the perturbation involves the unbounded, first-order, partial differential operator $w(h,B) = \frac{(\epsilon(h)B)^2}{8}(x_1^2 + x_2^2) - \frac{\epsilon(h)B}{2} hL_3$, where the operator hL_3 is the third component of the usual angular momentum operator and is the quantization of ℓ_3. The unbounded Zeeman perturbation is controlled using localization properties of both the hydrogen atom coherent states $\Psi_{\boldsymbol{\alpha},N}$, and their derivatives $L_3(h)\Psi_{\boldsymbol{\alpha},N}$, in the large quantum number regime $N \to \infty$.

Contents

1. Introduction: Limiting eigenvalue distribution theorems.

The behavior of eigenvalue clusters resulting from the perturbation of highly degenerate eigenvalues of elliptic operators on compact manifolds has been studied by many researchers, notably by V. Guillemin [9, 10], and by A. Weinstein [21].

This is the second paper in which we study the behavior of resonance and eigenvalue clusters associated with a fixed eigenvalue of a family of hydrogen atom Hamiltonians, labeled by the Planck's parameter h, under perturbations by external electric and magnetic fields in the weak field limit. In [12], we studied the resonance cluster associated with the hydrogen atom Stark Hamiltonian in the small electric field regime and proved a Szegö-type result for the resonance shifts. In this paper, we treat the eigenvalue clusters formed by a magnetic field (the Zeeman effect).

The behavior of eigenvalue clusters for smooth real-valued perturbations V of the Laplacian on rank one symmetric spaces was studied by V. Guillemin [9, 10]. A. Weinstein [21] established a **limiting eigenvalue distribution theorem** (LEDT) for the Laplacian Δ_M on a compact Riemannian manifold M all of whose geodesics are closed perturbed by a smooth real-valued potential V. The spectrum of the Laplacian Δ_M consists of eigenvalues E_N with multiplicity d_N that grows polynomially with N. In this case, the semiclassical parameter is the index N of the unperturbed eigenvalue E_N. Since V is bounded, the spectrum of $\Delta_M + V$ consists of eigenvalues that form clusters around the unperturbed eigenvalues.

To explain the LEDT introduced by Weinstein [21], we denote by $E_{N,j}$, $j = 1, \ldots, d_N$, the eigenvalues in the cluster around E_N, and by $\nu_{N,j} = E_{N,j} - E_N$ the eigenvalue shifts. The LEDT states that for a continuous, real-valued function $\rho : \mathbb{R} \to \mathbb{R}$ we have

$$\lim_{N\to\infty} \frac{1}{d_N} \sum_{j=1}^{d_N} \rho\left(\nu_{N,j}\right) = \int_\Gamma \rho(\hat{V}(\gamma))\ d\mu_\Gamma(\gamma), \tag{1}$$

where Γ denotes the space of oriented geodesics of M. These are the classical orbits of the unperturbed problem describing a particle moving on the manifold M with no potential. The function $\hat{V} : \Gamma \to \mathbb{R}$ is the Radon transform of the potential V. Namely, $\hat{V}(\gamma)$ denotes the average of V along the geodesic γ parameterized with respect to arc-length. The measure $\mathrm{d}\mu_\Gamma$ is the normalized measure on the space Γ obtained from the restriction to the unit cotangent bundle $T_1^* M$ of the Liouville measure associated to the canonical simplectic form on the symplectic manifold T^*M. Weinstein actually proves a LEDT for perturbations given by pseudo-differential operators of order zero. Here we only state the result for multiplicative potentials for simplicity.

R. Brummelhuis and A. Uribe [4] extended these results to the study of the semiclassical Schrödinger operator $H_h(V) = -h^2\Delta + V$ on $L^2(\mathbb{R}^n)$. The potential $V \geq 0$ is smooth with $V_\infty \equiv \liminf_{|\mathbf{x}|\to\infty} V(x) > 0$. They studied the semiclassical behavior of the eigenvalue cluster near an energy $0 < E^2 < V_\infty$. They proved an asymptotic expansion of $Tr\rho[(H_h(V)^{1/2} - E)h^{-1}]$ as $h \to 0$ and related the coefficients to the classical flow for $|\mathbf{p}|^2 + V$ on the energy surface E. For other results on the clustering of eigenvalues for h-pseudodifferential operators with periodic flows see, for example, [11, 6].

A. Uribe and C. Villegas-Blas [19] extended these results by considering perturbations of the family of hydrogen atom Hamiltonians $H_V(h) = -(1/2)h^2\Delta - |\mathbf{x}|^{-1}$ defined on $L^2(\mathbb{R}^n)$, $n \geq 2$, by operators of the form $\epsilon(h)Q_h$ where Q_h is a zero-order pseudo-differential operator uniformly bounded in h and $\epsilon(h) = h^{1+\delta}$, for $\delta > 0$. Here and in the sequel V denotes the Coulomb potential $V = -|\mathbf{x}|^{-1}$. The spectrum of $H_V(h)$ consists of discrete eigenvalues $E_k(h) = -\frac{1}{2h^2\left(k+\left(\frac{n-1}{2}\right)\right)^2}$, $k \in \mathbb{N}^*$, with multiplicity $d_k = O(k^{n-1})$ together with the continuous spectrum $[0, \infty)$. Here, we denote by $\mathbb{N}^* = \mathbb{N} \cup \{0\}$ the set of non-negative integers and by $\mathbb{N}$ the set of natural numbers $\{1, 2, \ldots\}$. They considered the Planck's parameter taking values along the following sequence converging to zero: $h = 1/(N + \frac{n-1}{2})$ with $N \in \mathbb{N}^*$. Thus for N given and taking $k = N$, we have that the number $E = E_{k=N}(h = 1/(N + \frac{n-1}{2})) = -1/2$ is an eigenvalue of $H_V(h = 1/(N + \frac{n-1}{2}))$ with multiplicity $d_N = O(N^{n-1})$.

In this setting, Uribe and Villegas-Blas [19] established a LEDT similar to formula (1) but with (**i**) the clusters of eigenvalues around the number $E = -1/2$, **(ii)** the eigenvalue shifts scaled by $\epsilon(h)$,**(iii)** the right-hand side involving averages of the principal symbol of Q_h along the classical orbits of the regularized Kepler problem on the energy surface

$$\Sigma(-1/2) = \left\{(\mathbf{x}, \mathbf{p}) \in \mathbb{T}^*(\mathbb{R}^3 - \{0\}) \mid \frac{|\mathbf{p}|^2}{2} - \frac{1}{|\mathbf{x}|} = -1/2\right\}, \tag{2}$$

and **(iv)** the integration being with respect to the normalized Liouville measure on the energy surface $\Sigma(-1/2)$.

The semiclassical limit is achieved by taking $N \to \infty$ or equivalently $h \to 0$. A novelty comes in the work of Uribe and Villegas-Blas [19] from the fact that for a fixed negative energy, there are two types of (phase space) classical orbits for the classical Hamiltonian flow with Hamiltonian $G(\mathbf{x}, \mathbf{p}) = \frac{|\mathbf{p}|^2}{2} - \frac{1}{|\mathbf{x}|}$ (the Kepler problem). Namely, (i) bounded periodic orbits corresponding to nonzero angular momentum, and (ii) unbounded collision orbits with zero angular momentum. Uribe and Villegas-Blas used Moser's regularization of collision orbits (see Appendix 1, section 8) so that all the collision orbits on $\Sigma(-1/2)$ can be considered periodic orbits after a time re-parametrization. In this regularization, all orbits on $\Sigma(-1/2)$ correspond to geodesics on the sphere $\mathbb{S}^n$ through the Moser map $\mathcal{M} : T^*(\mathbb{R}^3) \to T^*(\mathbb{S}^3_o)$ with $\mathbb{S}^3_o$ denoting the 3-sphere with the north pole removed (see Appendix 1, section 8 for a review of $\mathcal{M}$). Those passing through the north pole are the collision orbits. The geodesics on $\mathbb{S}^n$ are parameterized by the quotient of the subset $\mathcal{A} = \{\boldsymbol{\alpha} \in \mathbb{C}^{n+1} \mid |\Re\boldsymbol{\alpha}| = |\Im\boldsymbol{\alpha}| = 1,\ \Re\boldsymbol{\alpha} \cdot \Im\boldsymbol{\alpha} = 0\}$ of the null quadric in $\mathbb{C}^{n+1}$ with respect to the circle action (see Appendix 2, section 9). The set $\mathcal{A}$ corresponds to the unit cotangent bundle $T_1^*\mathbb{S}^n$ of $\mathbb{S}^n$ under the map $\sigma : \mathcal{A} \to T_1^*\mathbb{S}^n$ with $\sigma(\boldsymbol{\alpha}) = (\Re\boldsymbol{\alpha}, -\Im\boldsymbol{\alpha})$.

In this paper, we extend these results to eigenvalue clusters of the hydrogen atom Zeeman Hamiltonian defined on $L^2(\mathbb{R}^3)$. We prove a LEDT on the semi-classical behavior of the distribution of the eigenvalue shifts. To explain this in more detail, let us consider the same setting as Uribe and Villegas-Blas. We regard $E = -1/2$ as an eigenvalue of the family of hydrogen atom Hamiltonians $H_V(h = 1/(N+1))$ with multiplicity $d_N = (N+1)^2$. We consider the atom in an external, constant magnetic field $\mathbf{B}(h) = (0, 0, \epsilon(h)B)$, with the constant $B \geq 0$ and $\epsilon(h) = h^{K+\delta}$, $\delta > 0$, for some suitably chosen $K > 0$, see Theorem 1.1. We consider $\mathbf{B}(h) \to 0$ as $h \to 0$. We refer to this as the weak field limit.

The resulting Hamiltonian

$$\begin{aligned} H_V(h, B) &= (1/2)(-\imath h\nabla - \mathbf{A}(h))^2 - |\mathbf{x}|^{-1} \\ &= H_V(h) + \frac{(\epsilon(h)B)^2}{8}(x_1^2 + x_2^2) - \frac{\epsilon(h)B}{2} hL_3 \end{aligned} \tag{3}$$

is called the *hydrogen atom Zeeman Hamiltonian.* Here, $\mathbf{x} = (x_1, x_2, x_3)$ denotes Cartesian coordinates for $\mathbb{R}^3$, $\nabla = (\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3})$ and the operator $hL_3 = -\imath h\left(x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1}\right)$ is the component of the angular momentum operator $h\mathbf{L} = \mathbf{x} \times (-\imath h)\nabla$ along the direction of the magnetic field $\mathbf{B}(h)$. We are working in the symmetric gauge for the vector potential $\mathbf{A}(h) = \frac{\epsilon(h)B}{2}(-x_2, x_1, 0)$.

Although the perturbation $\frac{(\epsilon(h)B)^2}{8}(x_1^2 + x_2^2) - \frac{\epsilon(h)B}{2}hL_3$ is not bounded, we still have an eigenvalue stability theorem that follows from the work of J. Avron, I. Herbst, and B. Simon [1]. Following [1], we show that under the perturbation by the effective magnetic field $\epsilon(h)B$, the eigenvalue $E = -1/2$ gives rise to a cluster of nearby eigenvalues $E_{N,j}(h, B) = E_{N,j}(1/(N+1), B), j = 1, \ldots, d_N$, with total geometric multiplicity equal to d_N (see Theorem 3.1 on eigenvalue stability). We obtain explicit relative bounds on the perturbation that allow an estimate on the size of the cluster. Our main result is the following LEDT for this eigenvalue cluster in the large N limit corresponding to a weak magnetic field:

Theorem 1.1. *Let $B > 0$ be fixed, and let ρ be a continuous function on $\mathbb{R}$. Let $\epsilon(h) = h^{33/2+\delta}$, for some $\delta > 0$, and take $h = 1/(N+1)$, with $N \in \mathbb{N}^*$. For the eigenvalue cluster $\{E_{N,j}(1/(N+1), B)\}$, with $j = 1, 2, \ldots, d_N$, near $E_N(1/(N+1)) = -1/2$, we have*

$$\begin{aligned} \lim_{N\to\infty} \frac{1}{d_N} \sum_{j=1}^{d_N} \rho\left(\frac{E_{N,j}(1/(N+1), B) - E_N(1/(N+1))}{\epsilon(1/(N+1))}\right) \\ = \int_{\Sigma(-1/2)} \rho\left(-\frac{B}{2}\ell_3(\mathbf{x}, \mathbf{p})\right)\, d\mu_L(\mathbf{x}, \mathbf{p}), \end{aligned} \tag{4}$$

where $\ell_3(\mathbf{x},\mathbf{p}) = x_1p_2 - x_2p_1$ *is the component of the classical angular momentum vector* $\boldsymbol{\ell} = \mathbf{x}\times\mathbf{p}$ *along the direction of the magnetic field* $\mathbf{B}(h)$ *on the energy surface* $\Sigma(-1/2)$ *with collision orbits treated as in* [19]*. The measure* $d\mu_L$ *is the normalized restriction of the Liouville measure to the energy surface* $\Sigma(-1/2)$*. Here* $\mathbb{T}^*(R^3 - \{\mathbf{0}\})$ *is endowed with its canonical symplectic form.*

We recall the proof in Appendix 1, section 8, that ℓ_3 is conserved and bounded on the Kepler orbits on the energy surface $\Sigma(-1/2)$, so there is no problem working with arbitrary continuous functions.

Theorem 1.1 parallels and extends the result of Uribe and Villegas-Blas [19] on eigenvalue clusters formed by bounded perturbations Q_h of the hydrogen atom Hamiltonian. These ideas were applied by two of the authors [12] to the hydrogen atom Stark Hamiltonian. The main result of [12] is a limiting resonance distribution theorem for resonance clusters associated with a hydrogen atom eigenvalue under the Stark perturbation by an external electric field. Theorem 1.1 considers the case of eigenvalue clusters formed when a hydrogen atom is placed in a constant magnetic field. Both of these works have in common an unbounded perturbation. As in [12], control of the unbounded Zeeman perturbation is obtained through localization properties of coherent states of the hydrogen atom Hamiltonian. However, since the Zeeman perturbation is a first order differential operator, we have to extend these localization results to the derivatives of the coherent states. This requires an additional analysis (see section 5.1).

We remark that the size of the exponent K in Theorem 1.1 is far from optimal. Roughly speaking, if we suppose that the perturbation proportional to $(x_1^2+x_2^2)$ is bounded, the size of the eigenvalue cluster around the eigenvalue $-1/2$ is N^{-K}. For the eigenvalue clusters to be well separated, we need $N^{-K} \approx N^{-1}$, so $K > 1$. But, the perturbation is unbounded, and this forces us to take K much larger in order to control the error in the estimate of the difference of resolvents in Lemma 3.1 and Theorem 3.1.

Let $d\mu$ be defined as the normalized SO(4)-invariant measure on $\mathcal{A} \subset \mathbb{C}^{n+1}$ defined above. In Proposition 5.2, section 5, we show that the Liouville measure $d\mu_L$ on the energy surface $\Sigma(-1/2)$ is the push-forward measure of $d\tilde{\mu}$ by the map $\mathcal{M}^{-1} \circ \sigma$, where $d\tilde{\mu}$ is the restriction of $d\mu$ to a subset $\tilde{\mathcal{A}}$ of $\mathcal{A}$ with $\mu(\mathcal{A} - \tilde{\mathcal{A}}) = 0$, see equation (108) . Thus the right hand side of (4) can be written in terms of an integral over $\mathcal{A}$. This allows the following reformulation of Theorem 1.1.

Theorem 1.2. *Under the same hypothesis as in Theorem 1.1, we have*

$$\lim_{N\to\infty} \frac{1}{d_N} \sum_{j=1}^{d_N} \rho\left(\frac{E_{N,j}(1/(N+1),B) - E_N(1/(N+1))}{\epsilon(1/(N+1))}\right) = \int_{\mathcal{A}} \rho\left(-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right)\, d\mu(\boldsymbol{\alpha}), \tag{5}$$

where, for all $\boldsymbol{\alpha} \in \mathcal{A}$*, we have* $\ell_3(\boldsymbol{\alpha}) = (\Re\alpha)_1(\Im\alpha)_2 - (\Re\alpha)_2(\Im\alpha)_1$*. The function* $\ell_3(\boldsymbol{\alpha})$ *can be thought of as a continuous extension of the assignment* $\boldsymbol{\alpha} \to$

$(\mathbf{x},\mathbf{p}) \mapsto \ell_3(\mathbf{x},\mathbf{p})$ thorough the map $\mathcal{M}^{-1} \circ \sigma(\alpha)$ which is well defined as long as $\Re\boldsymbol{\alpha}$ is not the north pole of $\mathbb{S}^3$.

We can think of the right-hand side of (5) as a linear positive functional on $C_0^\infty(\mathbb{R})$. By a Riesz Representation Theorem, there exists a measure $d\kappa$ on the real line such that the right-hand side of (5) can be written as the integral of ρ with respect to $d\kappa$. The measure $d\kappa$ can be seen as the push-forward measure of $d\mu(\boldsymbol{\alpha})$ under the map $-\frac{B}{2}\ell_3 : \mathcal{A} \to \mathbb{R}$. By using an explicit expression for $d\mu$ in terms of coordinates for both the classical angular momentum vector $\boldsymbol{\ell}$ and the Runge-Lenz vector $\mathbf{a}$, and the relative angle between the position vector $\mathbf{x}$ and $\mathbf{a}/|\mathbf{a}|$ (see [20]), we can actually provide an explicit expression for $d\kappa$. This leads to another formulation of Theorem 1.1 :

Theorem 1.3. *Under the same hypothesis as in Theorem 1.1, we have:*

$$\lim_{N\to\infty} \frac{1}{d_N} \sum_{j=1}^{d_N} \rho\left(\frac{E_{N,j}(1/(N+1),B) - E_N(1/(N+1))}{\epsilon(1/(N+1))}\right) = \int_{[-1,1]} \rho\left(-\frac{B}{2}u\right)(1-|u|)\,du, \tag{6}$$

where du denotes the Lebesgue measure on the interval $[-1,1]$. The variable u can be thought of as the component ℓ_3 of the classical angular momentum vector $\boldsymbol{\ell}$.

The measure $d\kappa = \frac{2}{B}(1 - \frac{2}{B}|\mathbf{x}|)\,dx$ is supported on the interval $[-\frac{B}{2}, \frac{B}{2}]$ (for $B > 0$), where dx is the Lebesgue measure on $\mathbb{R}$. This measure gives us a precise picture of how, for N large, the scaled eigenvalue shifts

$$\frac{E_{N,j}(1/(N+1),B) - E_N(1/(N+1))}{\epsilon(1/(N+1))}, \quad j = 1,\ldots,d_N,$$

are distributed in the interval $[-\frac{B}{2}, \frac{B}{2}]$. The distribution around the origin in the interval $[-\frac{B}{2}, \frac{B}{2}]$ is determined according to the probability density function $P(x) = \frac{2}{B}(1 - \frac{2}{B}|\mathbf{x}|)$.

Theorems 1.1, 1.2 and 1.3 give a rather complete analytical and geometric description of the limiting eigenvalue distribution for the eigenvalue clusters formed by the Zeeman perturbation of the hydrogen atom Hamiltonian.

We remark that Theorem 1.3 can actually be shown in a different way than using Theorem 1.2 and the expression for $d\mu$ mentioned above. One can use a suitable eigenvalue approximation for the cluster around $E_N(1/(N+1))$ and then evaluate the left hand side of (6) by means of Riemann sums. This is shown in section 7. This procedure, however, completely masks the beautiful geometric foundations of the problem appearing in Theorems 1.1 and 1.2.

1.1. **Contents.** In section 2, we scale the hydrogen atom Zeeman Hamiltonian using the dilation group. This establishes a countable family of scaled hydrogen atom Zeeman Hamiltonians $S_V(\lambda) = S_V + W(\lambda)$. The operator S_V is a fixed, h-independent, hydrogen atom Hamiltonian $S_V = -\frac{1}{2}\Delta - \frac{1}{|\mathbf{x}|}$. The magnetic perturbation is $W(\lambda) = \frac{\lambda^2}{8}(x_1^2 + x_2^2) - \frac{\lambda}{2}L_3$, where the effective magnetic field strength is $\lambda(h,B) = h^3\epsilon(h)B$, and $L_3 = -\imath\left(x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1}\right)$. In this new framework, we want to establish conditions on the size of $\epsilon(h)$ in order to show the existence of clusters of eigenvalues around $E_N = -\frac{1}{2(N+1)^2}$, for N sufficiently large, with $h = 1/(N+1)$.

In section 3, we provide the description of known results on the spectrum of the operator $S_V(\lambda)$, with λ fixed, based on references [1] and [8]. Then we mention and prove a key result of Avron, Herbst, and Simon [1, 2] on the norm convergence $V(S_0(\lambda) - \mathbf{z})^{-1} \to V(S_0 - \mathbf{z})^{-1}$ as $\lambda \to 0$ for $\mathbf{z} \notin [0,\infty)$, with

$$S_0 = -\frac{1}{2}\Delta \quad \text{and} \quad S_0(\lambda) = S_0 + W(\lambda), \tag{7}$$

by presenting several important resolvent estimates necessary for our work. Moreover, we study such a rate of convergence with $\lambda(h,B) = h^3\epsilon(h)B$ and $h = 1/(N+1)$ when $N \to \infty$ and $\mathbf{z}$ is in a circle of radius $O(N^{-3})$ with center E_N. Then we are able to show an eigenvalue stability theorem, Theorem 3.1, by estimating the difference between corresponding spectral projectors associated to the perturbed and unperturbed Hamiltonians on a small disk around E_N.

In section 4, we use the stability theorem in order to show that the averages appearing on the left hand side of equation (4) (with a factor h^2 included in the denominator due to scaling) can be approximated by the normalized trace of $\frac{1}{d_N}\rho\left(\Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N\right)$ with Π_N the projector onto the eigenspace of the unperturbed operator S_V with eigenvalue E_N. Next, in section 5, we take the semiclassical limit $N \to \infty$ of this last trace by using the Stone-Weierstrass Theorem, the coherent states for the hydrogen atom introduced in [18], and the stationary phase method in order to estimate the expected value of $\left(-\frac{B}{2}hL_3\right)^m$, $m \in \mathbb{N}^*$, between coherent states. We use decay properties of coherent states shown in [18] but, in addition, we need to estimate decay of their derivatives.

Finally, an alternate proof of Theorem 1.3 is presented in section 7.

We include two appendices. The Kepler problem and the Moser map are briefly described in the first appendix in section 8. In the second appendix, section 9, details of the coherent states for the hydrogen atom are presented.

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2. The basic operators and scaling.

The hydrogen atom Hamiltonian $H_V(h)$ with the semiclassical parameter h acts on the dense domain $H^2(\mathbb{R}^3)$ in the Hilbert space $L^2(\mathbb{R}^3)$. The operator is self-adjoint on this domain and given by

$$H_V(h) = -\frac{h^2}{2}\Delta - \frac{1}{|\mathbf{x}|}. \tag{8}$$

We denote the Coulomb potential by $V(x) = -1/|\mathbf{x}|$. The discrete spectrum consists of an infinite family of eigenvalues $E_k(h)$

$$E_k(h) = \frac{-1}{2h^2(k+1)^2}, \; k = 0, 1, 2, \ldots \tag{9}$$

each eigenvalue having multiplicity $d_k := (k+1)^2$. The essential spectrum is $[0, \infty)$. With the choice of $h = 1/(N+1)$ and $k = N$, we see that $E_{k=N}(h = 1/(N+1)) = -1/2$ is in the spectra of the countable family of Hamiltonians $H_V(1/(N+1))$, $N \in \mathbb{N}$. The multiplicity of the eigenvalue $-1/2$ is $d_N = (N+1)^2$.

We next consider a hydrogen atom in a constant magnetic field. We assume, without loss of generality, that the magnetic field has the form $\mathbf{B}(h) = (0, 0, \epsilon(h)B)$. We keep $B \geq 0$ fixed and use it only to control whether the magnetic field is on or not. We control the strength of the magnetic field by taking $\epsilon(h) = h^K$, with a constant $K > 0$ chosen below. We choose the gauge such that the vector potential $\mathbf{A}(h)$ is given by $\mathbf{A}(h) = \frac{\epsilon(h)B}{2}(-x_2, x_1, 0)$. The **unscaled Zeeman hydrogen Hamiltonian** is

$$\begin{aligned} H_V(h, B) &= \frac{1}{2}(-\imath h\nabla - \mathbf{A}(h))^2 - \frac{1}{|\mathbf{x}|} \\ &= H_V(h) + w(h, B). \end{aligned} \tag{10}$$

where the **unscaled Zeeman perturbation** $w(h, B)$ is given by

$$w(h, B) = \frac{(\epsilon(h)B)^2}{8}(x_1^2 + x_2^2) - \frac{\epsilon(h)B}{2} h L_3, \tag{11}$$

with $L_3 = -\imath \left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} \right)$.

To implement scaling of these Hamiltonians, we use the dilation group D_α, $\alpha > 0$. The dilation group is a representation of the multiplicative group $\mathbb{R}^+$ and has a unitary implementation on $L^2(\mathbb{R}^3)$ given by

$$(D_\alpha f)(\mathbf{x}) = \alpha^{3/2} f(\alpha \mathbf{x}), \quad f \in L^2(\mathbb{R}^3). \tag{12}$$

Using the relation $D_\alpha L_3 D_{\alpha^{-1}} = L_3$, we scale the Hamiltonian in (10) by $\alpha = h^2$:

$$\begin{aligned} & D_{h^2} H_V(h, B) D_{h^{-2}} \\ &\quad = \frac{1}{h^2}\left[-\frac{1}{2}\Delta - \frac{1}{|\mathbf{x}|} + \frac{\left(h^3\epsilon(h)B\right)^2}{8}(x_1^2 + x_2^2) - \frac{h^3\epsilon(h)B}{2} L_3 \right] \\ &\quad =: \frac{1}{h^2} S_V(\lambda(h, B)). \end{aligned} \tag{13}$$

The **scaled Zeeman hydrogen Hamiltonian** $S_V(\lambda(h, B))$ is defined via the **effective magnetic field** $\lambda(h, B) = h^3\epsilon(h)B$ and the operator $S_V(\lambda)$ is given by:

$$\begin{aligned} S_V(\lambda) &= -\frac{1}{2}\Delta - \frac{1}{|\mathbf{x}|} + \frac{\lambda^2}{8}(x_1^2 + x_2^2) - \frac{\lambda}{2}L_3 \\ &= S_V + W(\lambda). \end{aligned} \tag{14}$$

where we write $S_V \equiv -\frac{1}{2}\Delta - \frac{1}{|\mathbf{x}|}$ for the scaled hydrogen atom Hamiltonian and the magnetic perturbation is

$$W(\lambda) = \frac{\lambda^2}{8}(x_1^2 + x_2^2) - \frac{\lambda}{2}L_3. \tag{15}$$

The **scaled Zeeman perturbation** is then given by $W(\lambda(h, B))$.

Note that we can make the effective magnetic field $\lambda(h, B)$ small by taking $h \to 0$. Equivalently, we may set $h = 1/(N + 1)$ and take $N \to \infty$. For $B = 0$, the eigenvalues of $S_V(0)$ are given by $E_k \equiv E_k(1) = -1/(2(k+1)^2)$, with $k \in \mathbb{N}^*$ and multiplicity $d_k = (k + 1)^2$.

Since the discrete spectra of the operators $H_V(h, B)$ and $S_V(\lambda(h, B))$ are the same up to the factor h^2, Theorem 1.1 will be proved by establishing a LEDT theorem for the family of operators $S_V(\lambda(h = 1/(N + 1), B))$, $N \in \mathbb{N}^*$, by studying the eigenvalue distribution in the cluster around $E_N(1) = -1/(2(N + 1)^2)$ and then taking the corresponding limit when $N \to \infty$. Since the perturbation $W(\lambda(h, B))$ is unbounded, the existence of these clusters of eigenvalues is by no means immediate. A suitable version of a stability theorem due to Avron, Herbst and Simon [1], together with an adequate choice of the exponent $K > 0$ in the definition of $\epsilon(h)$, guarantee that, for N sufficiently large, the eigenvalue cluster around E_N is well defined and the total multiplicity of the eigenvalues in the cluster is d_N. This is the content of Theorem 3.1 proved in the next section.

3. Spectral analysis of the Zeeman hydrogen atom Hamiltonian and eigenvalue clusters.

The main goal of this section is to show the existence of eigenvalue clusters $\mathcal{C}_N$ for the operator $S_V(\lambda(h, B))$ around the unperturbed eigenvalues $E_N = -1/2(N+1)^2$, taking $h = 1/(N+1)$ with N sufficiently large. We will show that there exist circles Γ_N with centers E_N and radii $r_N \approx N^{-3}$ such that the total number of eigenvalues of $S_V(\lambda(1/(N+1), B))$ inside Γ_N, including multiplicity, is equal to the multiplicity $d_N = (N+1)^2$ of the eigenvalue $E_N = -1/2(N+1)^2$ of S_V. This fact is a consequence of the main technical result of this section showing that the norm of the difference of the spectral projectors P_N and Π_N associated to the spectrum of the operators $S_V(\lambda(h, B))$ and S_V, respectively, inside Γ_N is $O(N^{-\sigma})$, $\sigma > 0$, and therefore smaller than one for N sufficiently large. This will give us the eigenvalue stability that we need in order to have well-defined clusters of eigenvalues.

In subsection 3.1 we describe spectral properties of $S_V(\lambda(h, B))$ by summarizing some of the results of Avron, Herbst, and Simon in their papers [1, 2]. As we are only concerned with the Coulomb potential, we state their results for this case.

The eigenvalue stability $\|P_N - \Pi_N\| \to 0$ as $N \to \infty$ would be immediate if we had norm resolvent convergence of $S_V(\lambda(1/(1+N), B))$ to S_V when $N \to \infty$. However, this is not the case as it was shown in [1]. Avron, Herbst, and Simon [1] showed that we still can have eigenvalue stability due to the fact that for $\mathbf{z} \notin [0, \infty)$ we have the norm convergence $V(S_0(\lambda) - \mathbf{z})^{-1} \to V(S_0 - \mathbf{z})^{-1}$ as $\lambda \to 0$ (see Lemma 3.1) with S_0 and $S_0(\lambda)$ given in Eq. (7). In subsection 3.2, we describe the work of Avron, Herbst and Simon about this point by refining some of their estimates in order to make the dependance on $\lambda(h, B)$ explicit. We prove eigenvalue stability in subsection 3.3 by following reference [1] and prove both suitable and finer estimates required for our purposes.

3.1. **The spectrum.** The Hamiltonian obtained from the scaled Zeeman hydrogen Hamiltonian (14) by setting the Coulomb potential equal to zero is denoted by $S_0(\lambda(h, B))$ with $S_0(\lambda)$ given by Eq.(7) and $\lambda(h, B) = h^3\epsilon(h)B$. For $\lambda > 0$, the spectrum of $S_0(\lambda)$ is purely absolutely continuous and equal to the half line $[\lambda/2, \infty)$. We note that the operator $S_0(\lambda)$ may be represented as a tensor product on the space $L^2(\mathbb{R}^3) = L^2(\mathbb{R}^2_{x_1,x_2}) \otimes L^2(\mathbb{R}_{x_3})$. For this purpose, we recall the two-dimensional Landau Hamiltonian $S_L(\lambda) = -\frac{1}{2}\Delta_{x_1,x_2} + \frac{\lambda^2}{8}(x_1^2+x_2^2) - \frac{\lambda}{2}L_3$. This operator has pure point spectrum $E_n(\lambda) = \frac{\lambda}{2}(n+1)$ with $n \in \mathbb{N}^*$. Each Landau level $E_n(\lambda)$ is an eigenvalue of infinite multiplicity. Then, the Hamiltonian $S_0(\lambda)$ may be written as $S_0(\lambda) = S_L(\lambda) \otimes I_1 + I_2 \otimes \frac{1}{2}(-d^2/dx_3{}^2)$, where I_j is the identity operator on $L^2(\mathbb{R}^j)$, $j = 1, 2$, respectively. The Landau levels appear as thresholds of the operator $S_0(\lambda)$. The spectrum of $S_0(\lambda)$ can then be computed using a well-known result on the spectra of tensor products [17, section XIII.9, Theorem XIII.35]. It follows directly that $\sigma(S_0(\lambda) = \{E \in E_n(\lambda) + [0, \infty) \mid n \in \mathbb{N}^*\} = [\lambda/2, \infty)$, since $\inf \sigma(S_L(\lambda)) = \lambda/2$ and the spectrum of $\frac{1}{2}\left(-d^2/dx_3{}^2\right)$ is the closed half-line $[0, \infty)$.

We now consider $S_V(\lambda(h, B))$ defined via the operator $S_V(\lambda)$ given in Eq. (14). The operator $S_V(\lambda)$ is best understood by studying its restriction to the eigenspaces of L_3. These subspaces are $S_V(\lambda)$-invariant since $S_V(\lambda)$ commutes with L_3. The eigenfunctions of the azimuthal angular momentum operator L_3, as an operator on the circle, are $\varphi_m(\phi) = e^{im\phi}, m \in \mathbb{Z}$. We write $\mathcal{H}_m$, $m \in \mathbb{Z}$, for the subspace of $L^2(\mathbb{R}^3)$ consisting of functions whose angular momentum decomposition contain only $\varphi_m(\phi)$. We then have the direct sum decomposition $L^2(\mathbb{R}^3) = \bigoplus_{m\in\mathbb{Z}} \mathcal{H}_m$. The restriction $S^{(m)}(\lambda) \equiv S_V(\lambda)|\mathcal{H}_m$ of $S_V(\lambda)$ to infinite-dimensional subspaces $\mathcal{H}_m$, $m \in \mathbb{Z}$, of constant azimuthal angular momentum $m \in \mathbb{Z}$, has the form

$$S^{(m)}(\lambda) = \left(-\frac{1}{2}\Delta - 1/|\mathbf{x}| + \frac{\lambda^2}{8}(x_1^2 + x_2^2) - \frac{\lambda}{2}m\right)\Big|_{\mathcal{H}_m}. \tag{16}$$

We let $E^{(m)}(\lambda) \equiv \inf \sigma(S^{(m)}(\lambda))$. This number is a simple isolated eigenvalue of $S^{(m)}(\lambda)$. We refer to $E^{(m)}(\lambda)$ as the ground state of $S^{(m)}(\lambda)$. For negative indices $m < 0$, these eigenvalues satisfy the relation

$$E^{(-m)}(\lambda) = E^{(m)}(\lambda) + m\lambda, \text{ for } m \geq 0. \tag{17}$$

Each operator $S^{(m)}(\lambda)$ has discrete spectra consisting of *simple* eigenvalues accumulating at the bottom of the essential spectrum (see [8], page 5, Main

Results, part b). The essential spectrum of $S^{(m)}(\lambda)$ consists of half-lines

$$\begin{array}{ll} m<0 & \sigma_{\text{ess}}(S^{(m)}(\lambda)) = [(2|m|+1)\frac{\lambda}{2},\infty), \\ m\geq 0 & \sigma_{\text{ess}}(S^{(m)}(\lambda)) = [\frac{\lambda}{2},\infty). \end{array} \tag{18}$$

The spectrum of $S_V(\lambda)$ is the union of the spectra of $S^{(m)}(\lambda)$, for $m \in \mathbb{Z}$. It follows from (18) that $\frac{\lambda}{2} = \inf \sigma_{\text{ess}}(S_V(\lambda))$. The ground state eigenvalues of the operators $S^{(m)}(\lambda)$, for $m \geq 0$, are strictly ordered:

$$E^{(0)}(\lambda) < E^{(1)}(\lambda) < E^{(2)}(\lambda) < \ldots \leq \frac{\lambda}{2} = \inf \sigma_{\text{ess}}(S_V(\lambda)). \tag{19}$$

Because of this ordering (19) for $m \geq 0$ and the relation (17), the ground state of $S_V(\lambda)$ is $E^{(0)}(\lambda) = \inf \sigma(S_V(\lambda))$. It is an isolated eigenvalue satisfying $E^{(0)}(\lambda) = -1/2 + O(\lambda)$. From (19), the discrete spectrum of $S_V(\lambda)$ consists of infinitely-many discrete eigenvalues $\{E^{(m)}(\lambda) \mid m \geq 0\} \cup \{E^{(-m)}(\lambda) \mid E^{(m)}(\lambda) < (1-2m)\frac{\lambda}{2}, m > 0\}$, less than $\frac{\lambda}{2}$, accumulating at $\frac{\lambda}{2} = \inf \sigma_{\text{ess}}(S_V(\lambda))$. There are infinitely-many embedded eigenvalues of finite multiplicity in the essential spectrum $[\frac{\lambda}{2},\infty)$ since, by (17), for $m > 0$ large enough, $E^{(-m)}(\lambda) >> \frac{\lambda}{2}$.

3.2. **Norm resolvent estimates and the key lemma.** We present a refined version of Lemma 6.6 of Avron, Herbst, and Simon [1] on the norm convergence $V(S_0(\lambda) - \mathbf{z})^{-1} \to V(S_0 - \mathbf{z})^{-1}$ as $\lambda \to 0$ for $\mathbf{z} \notin [0,\infty)$ that gives the rate of the convergence. We will specialize to the case of the Coulomb potential $V(x) = -1/|\mathbf{x}|$ and obtain finer estimates when $\mathbf{z}$ is close to an eigenvalue E_N of the hydrogen atom Hamiltonian S_V. We denote the resolvent of S_0 by $R_0(\mathbf{z}) = (S_0 - \mathbf{z})^{-1}$, of $S_V(\lambda)$ by $R_{V,\lambda}(\mathbf{z}) \equiv (S_V(\lambda) - \mathbf{z})^{-1}$, so that for $V = 0$, we have $R_{0,\lambda}(\mathbf{z}) = (S_0(\lambda) - \mathbf{z})^{-1}$. The spectra of S_0 and $S_0(\lambda)$ lie in the positive half-line, so both resolvents $R_0(\mathbf{z})$ and $R_{0,\lambda}(\mathbf{z})$ exist as bounded operators for $\mathbf{z} \notin [0,\infty)$. We have the basic bounds of their norms:

$$\begin{aligned} \|R_0(\mathbf{z})\| &\leq [\text{dist}(\mathbf{z},[0,\infty))]^{-1}, \\ \|R_{0,\lambda}(\mathbf{z})\| &\leq [\text{dist}(\mathbf{z},[\lambda/2,\infty))]^{-1}. \end{aligned} \tag{20}$$

Avron, Herbst, and Simon [1, Lemma 6.4] proved that for $\mathbf{z} \notin [0,\infty)$, $R_{0,\lambda}(\mathbf{z})$ converges strongly to $R_0(\mathbf{z})$ ar $\lambda \to 0$. Moreover, in [1, Theorem 6.3], they showed that $S_V(\lambda) = S_0(\lambda) + V$ does not converge in the norm resolvent sense to $S_V = S_0 + V$ as $\lambda \to 0$, which includes the fact that $R_{0,\lambda}(\mathbf{z})$ does not converge to $R_0(\mathbf{z})$ in norm as $\lambda \to 0$. However, they show [1, Lemma 6.6] the norm convergence $V(S_0(\lambda) - \mathbf{z})^{-1} \to V(S_0 - \mathbf{z})^{-1}$ as $\lambda \to 0$ for $\mathbf{z} \notin [0,\infty)$, which plays the key role in the proof of eigenvalue stability. We prove this last result in Lemma 3.1 and obtain an estimate on the rate of convergence necessary in the proof of the eigenvalue stability theorem, Theorem 3.1.

In order to prove this last result, we introduce the cut-off function χ_R as the characteristic function of the unit $B_R(0)$ of radius $R > 0$ centered at the origin. In the sequel, the symbol C will denote a constant whose value may differ from line-to-line but is independent of N. The first part of the following lemma is effectively [1, Lemma 6.6] and the second part gives the rate of convergence. The following notation will be used in the sequel: a bounded operator whose norm is $O(N^\alpha)$, for some $\alpha \in \mathbb{R}$, will be denoted by $O(N^\alpha)$ as well.

Lemma 3.1. *(Key Lemma) Consider* $\mathbf{z} \notin [0, \infty)$.

(1) *We have the following convergence in norm:*
$$V(S_0(\lambda) - \mathbf{z})^{-1} \to V(S_0 - \mathbf{z})^{-1}, \tag{21}$$
as $\lambda \to 0$.

(2) *Consider* $\lambda = \lambda(h)$ *with* $h = 1/(N+1)$ *and* $\epsilon(h) = h^q$, $q > 3/2$. *For* $|\mathbf{z} - E_N| = O(N^{-3})$ *we have*
$$V(S_0(\lambda(h)) - \mathbf{z})^{-1} - V(S_0 - \mathbf{z})^{-1} = O\left(N^{-\left(\frac{2q-3}{5}\right)}\right), \tag{22}$$
as $N \to \infty$.

Proof. 1. For any fixed $R > 0$, we decompose $V = -1/|\mathbf{x}|$ as $V = V_1 + V_2$, with $V_1 = V\chi_R$ and $V_2 = V(1 - \chi_R)$, so that V_1 has compact support and V_2 is bounded. We choose $R > 0$ below. The contribution of V_2 to (21) is easy to treat. For $\mathbf{z} \notin [0, \infty)$, both $(S_0(\lambda) - \mathbf{z})^{-1}$ and $(S_0 - \mathbf{z})^{-1}$ are bounded by $1/d(\mathbf{z})$ with $d(\mathbf{z}) \equiv \text{dist}(\mathbf{z}, [0, \infty))$. Thus the contribution to (21) from V_2 is bounded by
$$\| V_2 \left[(S_0(\lambda) - \mathbf{z})^{-1} - (S_0 - \mathbf{z})^{-1} \right] \| \leq \|V_2\|_\infty \frac{2}{d(\mathbf{z})} = \frac{2}{R d(\mathbf{z})}. \tag{23}$$
We note that the contribution (23) vanishes as $R \to \infty$ for $d(\mathbf{z})$ fixed.
2. As for the contribution of V_1 to (21), we write the difference of the resolvents using (7) as
$$\begin{aligned} V_1 \left[(S_0(\lambda) - \mathbf{z})^{-1} - (S_0 - \mathbf{z})^{-1} \right] &= \lambda V_1 (S_0 - \mathbf{z})^{-1} \boldsymbol{\Lambda} \cdot (\hat{\mathbf{p}} - \lambda \boldsymbol{\Lambda}) (S_0(\lambda) - \mathbf{z})^{-1} \\ &\quad + \frac{\lambda^2}{2} V_1 (S_0 - \mathbf{z})^{-1} |\boldsymbol{\Lambda}|^2 (S_0(\lambda) - \mathbf{z})^{-1} \end{aligned} \tag{24}$$
where $\boldsymbol{\Lambda} = \frac{1}{2}(-x_2, x_1, 0)$ and $\hat{\mathbf{p}} = (\hat{p}_1, \hat{p}_2, \hat{p}_3) = -\imath \nabla$. Since the spectrum of $S_0(\lambda) = \frac{1}{2} (\hat{\mathbf{p}} - \lambda \boldsymbol{\Lambda})^2$ lies in the interval $[0, \infty)$, the operators $(\hat{\mathbf{p}} - \lambda \boldsymbol{\Lambda}) (S_0(\lambda) - \mathbf{z})^{-1}$ and $(S_0(\lambda) - \mathbf{z})^{-1}$ are uniformly bounded for $\lambda \geq 0$ and $\mathbf{z} \notin [0, \infty)$:
$$\begin{aligned} \| (\hat{\mathbf{p}} - \lambda \boldsymbol{\Lambda}) (S_0(\lambda) - \mathbf{z})^{-1} \| &\leq \max\{ s / |s^2/2 - \mathbf{z}| \mid s \in [0, \infty) \} \\ &= 1/\sqrt{G(\mathbf{z})}, \end{aligned} \tag{25}$$
$$\| (S_0(\lambda) - \mathbf{z})^{-1} \| \leq 1/d(\mathbf{z}) \tag{26}$$
with $G(\mathbf{z}) \equiv |\mathbf{z}| - \Re(\mathbf{z})$.
3. We show that $V_1 (S_0 - \mathbf{z})^{-1} \boldsymbol{\Lambda}$ and $V_1 (S_0 - \mathbf{z})^{-1} |\boldsymbol{\Lambda}|^2$ are bounded operators in order to prove that the norm of the left hand side of (24) goes to zero as $\lambda \to 0$ with R fixed. We also estimate the rate of convergence. We use the following estimate [5] that is a consequence of the bound $\|\Psi\|_\infty \leq C \|\Psi\|_{H^2}$, for all $\Psi \in H^2(\mathbb{R}^3)$. For $\beta > 0$, there exist a constant C such that for $\Psi \in H^2(\mathbb{R}^3)$ we have
$$\|\Psi\|_\infty \leq C \left[\frac{1}{\beta^{1/2}} \|\Delta \Psi\|_2 + \beta^{3/2} \|\Psi\|_2 \right]. \tag{27}$$
We use this inequality together with the simple bound
$$\|f \Psi\|_2 \leq \|f\|_2 \|\Psi\|_\infty, \tag{28}$$
for $f \in L^2(\mathbb{R}^3)$ and $\Psi \in H^2(\mathbb{R}^3)$. Since $V_1 \boldsymbol{\Lambda}$ and $V_1 |\boldsymbol{\Lambda}|^2$ are in $L^2(\mathbb{R}^3)$, estimate (27) with $\Psi = (S_0 - \mathbf{z})^{-1} \phi$, $\phi \in L^2(\mathbb{R}^3)$, suggests to write both operators

$V_1(S_0-\mathbf{z})^{-1}\mathbf{\Lambda}$ and $V_1(S_0-\mathbf{z})^{-1}|\mathbf{\Lambda}|^2$ with the resolvent $(S_0-\mathbf{z})^{-1}$ shifted to the right side by using commutator properties. Thus we consider the following expressions:

$$\begin{aligned} V_1(S_0-\mathbf{z})^{-1}\mathbf{\Lambda} &= V_1\mathbf{\Lambda}(S_0-\mathbf{z})^{-1} \\ &\quad +\frac{\imath}{2}V_1(S_0-\mathbf{z})^{-1}(-\hat{p}_2,\hat{p}_1,0)(S_0-\mathbf{z})^{-1} \end{aligned} \tag{29}$$

$$\begin{aligned} V_1 S_0-\mathbf{z})^{-1}|\mathbf{\Lambda}|^2 &= V_1|\mathbf{\Lambda}|^2(S_0-\mathbf{z})^{-1} \\ &+\frac{\imath}{2}V_1\left[x_1(S_0-\mathbf{z})^{-1}\hat{p}_1(S_0-\mathbf{z})^{-1}+x_2(S_0-\mathbf{z})^{-1}\hat{p}_2(S_0-\mathbf{z})^{-1}\right] \\ &-\frac{1}{2}V_1(S_0-\mathbf{z})^{-1}\left(\hat{p}_1^2+\hat{p}_2^2\right)(S_0-\mathbf{z})^{-2}+\frac{1}{2}V_1(S_0-\mathbf{z})^{-2} \end{aligned} \tag{30}$$

4. We next estimate the right sides of (29) and (30). We first note that for $q=0,1,2$, there exist a constant C such that, for $j=1,2,3$, $\|V_1\Lambda_j^q\|_2\leq CR^{(2q+1)/2}$, with Λ_j denoting the j^{th}-component of the operator $\mathbf{\Lambda}$. Thus, from estimates (27)-(28), we have for $\beta>0$

$$\|V_1\Lambda_j^q(S_0-\mathbf{z})^{-1}\|\leq CR^{\frac{(2q+1)}{2}}\left[\frac{1}{\beta^{1/2}}\|\Delta(S_0-\mathbf{z})^{-1}\|+\beta^{3/2}\|(S_0-\mathbf{z})^{-1}\|\right], \qquad j=1,2,3 \text{ and } q=0,1,2. \tag{31}$$

Since $\|\frac{1}{2}\Delta(S_0-\mathbf{z})^{-1}\|\leq\max\{s/\,|s-\mathbf{z}|\ \mid s\in[0,\infty)\}\leq\eta(\mathbf{z})$, with $\eta(\mathbf{z})=1$, if $\Re(\mathbf{z})\leq 0$ and $\eta(\mathbf{z})=|\mathbf{z}|/|\Im(\mathbf{z})|$ if $\Re(\mathbf{z})>0$, we obtain from (25)-(26) (with $\lambda=0$) together with (31):

$$\|V_1(S_0-\mathbf{z})^{-1}\mathbf{\Lambda}\| \leq C\left[R^{3/2}+\frac{R^{1/2}}{\sqrt{G(\mathbf{z})}}\right]\left[\frac{2\eta(\mathbf{z})}{\beta^{1/2}}+\frac{\beta^{3/2}}{d(\mathbf{z})}\right], \tag{32}$$

$$\begin{aligned}\|V_1(S_0-\mathbf{z})^{-1}|\mathbf{\Lambda}|^2\| &\leq C\left[R^{5/2}+\frac{R^{3/2}}{\sqrt{G(\mathbf{z})}}+\frac{R^{1/2}}{G(\mathbf{z})}+\frac{R^{1/2}}{d(\mathbf{z})}\right] \\ &\quad\cdot\left[\frac{2\eta(\mathbf{z})}{\beta^{1/2}}+\frac{\beta^{3/2}}{d(\mathbf{z})}\right].\end{aligned} \tag{33}$$

Therefore, we get from (24)-(26), and (32)-(33) that for $\beta>0$:

$$\begin{aligned}\|V_1\left[(S_0(\lambda)-\mathbf{z})^{-1}-(S_0-\mathbf{z})^{-1}\right]\| &\leq C\left[\lambda\left(R^{3/2}+\frac{R^{1/2}}{\sqrt{G(\mathbf{z})}}\right)\frac{1}{\sqrt{G(\mathbf{z})}}\right. \\ &\left.+\lambda^2\left(R^{5/2}+\frac{R^{3/2}}{\sqrt{G(\mathbf{z})}}+\frac{R^{1/2}}{G(\mathbf{z})}+\frac{R^{1/2}}{d(\mathbf{z})}\right)\frac{1}{d(\mathbf{z})}\right]\left[\frac{2\eta(\mathbf{z})}{\beta^{1/2}}+\frac{\beta^{3/2}}{d(\mathbf{z})}\right].\end{aligned} \tag{34}$$

We conclude the proof of part (1) of Lemma 3.1 from (34) and (23) by first taking the limit $\lambda\to 0$ with R fixed and then letting $R\to\infty$.
5. For the proof of part (2), let us consider $\lambda=\lambda(h=1/(N+1))$, with $N\in\mathbb{N}$, in (34) and (23). Let us take $R=N^\gamma/d(\mathbf{z})$, $\gamma>0$, in equation (23) in order to have

$$\|V_2\left[(S_0(\lambda(h))-\mathbf{z})^{-1}-(S_0-\mathbf{z})^{-1}\right]\|=O(N^{-\gamma}). \tag{35}$$

We will choose γ below. Since $|\mathbf{z}-E_N| = O(N^{-3})$ then $1/d(\mathbf{z}) = |\mathbf{z}|^{-1} = O(N^2)$, and $\Re(\mathbf{z}) < 0$ for N sufficiently large, which implies $\eta(\mathbf{z}) = 1$. Whence $R = O(N^{2+\gamma})$. Thus we can estimate the two terms appearing in the first factor in square brackets in (34) by using both estimates $\lambda = h^3\epsilon(h)B = O(N^{-3-q})$ and $1/G(\mathbf{z}) \leq 1/|\mathbf{z}|$:

$$\lambda\left(R^{3/2} + \frac{R^{1/2}}{\sqrt{G(\mathbf{z})}}\right)\frac{1}{\sqrt{G(\mathbf{z})}} = O\left(N^{1-q+\frac{3\gamma}{2}}\right), \tag{36}$$

$$\lambda^2\left(R^{5/2} + \frac{R^{3/2}}{\sqrt{G(\mathbf{z})}} + \frac{R^{1/2}}{G(\mathbf{z})} + \frac{R^{1/2}}{d(\mathbf{z})}\right)\frac{1}{d(\mathbf{z})} = O\left(N^{1-2q+\frac{5\gamma}{2}}\right). \tag{37}$$

Now we replace the factor $\left[\frac{2\eta(\mathbf{z})}{\beta^{1/2}} + \frac{\beta^{3/2}}{d(\mathbf{z})}\right]$ appearing in (34) by its minimum value $C(d(\mathbf{z}))^{-1/4} = O(N^{1/2})$. Thus we have

$$\|V\left[(S_0(\lambda)-\mathbf{z})^{-1} - (S_0-\mathbf{z})^{-1}\right]\| = O\left(N^{\frac{3}{2}-q+\frac{3\gamma}{2}}\right) + O(N^{\frac{3}{2}-2q+\frac{5\gamma}{2}}) + O(N^{-\gamma}). \tag{38}$$

6. If we take $q > 3/2$ given then there exist $0 < \gamma < \frac{2}{3}q - 1$ such that both exponents $\frac{3}{2} - 2q + \frac{5\gamma}{2}$ and $\frac{3}{2} - q + \frac{3\gamma}{2}$ are negative. Moreover, since $\gamma < \frac{2}{3}q - 1 < q$ then $\frac{3}{2} - 2q + \frac{5\gamma}{2} < \frac{3}{2} - q + \frac{3\gamma}{2}$, which implies that in the regime $q > 3/2$ and $0 < \gamma < \frac{2}{3}q - 1$ the contribution from the linear term in λ dominates the quadratic one in equation (34). From equations (38) and (35)

$$\|V\left[(S_0(\lambda(h))-\mathbf{z})^{-1} - (S_0-\mathbf{z})^{-1}\right]\| = O\left(N^{3/2-q+\frac{3\gamma}{2}}\right) + O\left(N^{-\gamma}\right) \tag{39}$$

Let us write the right hand side of equation (39) as $O(N^{-E_q(\gamma)})$ with $E_q(\gamma) = \min\{q - 3/2 - \frac{3\gamma}{2}, \gamma\}$. Working in the regime specified above, we actually have that the maximum value of $E_q(\gamma)$ is $E_q(\frac{2}{5}q - \frac{3}{5}) = \frac{2}{5}q - \frac{3}{5}$. Hence we finally have

$$\|V\left[(S_0(\lambda(h))-\mathbf{z})^{-1} - (S_0-\mathbf{z})^{-1}\right]\| = O\left(N^{-\frac{2q-3}{5}}\right). \tag{40}$$

This completes the proof of part (2). □

We prove some resolvent estimates that are needed in the proof of the stability theorem in the next section. For an eigenvalue E_N of S_V, let Γ_N be a circle with center E_N and radius $r_N = cN^{-3}$, with c a suitable constant independent of N in such a way that r_N is smaller than half the distance to the nearest eigenvalue, which is $O(N^{-3})$.

Lemma 3.2. *Uniformly for all $\mathbf{z} \in \Gamma_N$, we have*

(1) $\| V(S_0 - \mathbf{z})^{-1}\| = O(N)$
(2) $\| V(S_V - \mathbf{z})^{-1}\| = O(N^3)$

Proof. 1. for $R > 0$, we decompose $V = V\chi_R + V(1-\chi_R) = V_1 + V_2$, as in the proof of Lemma 3.1, with $V_1 \in L^2(\mathbb{R}^3)$, $V_2 \in L^\infty(\mathbb{R}^3)$, $\|V_1\|_2 = 2\sqrt{\pi}R^{1/2}$ and

$\|V_2\|_\infty = 1/R$. Using estimate (27), we have for all $\beta > 0$

$$\begin{aligned}
\|V\,(S_0-\mathbf{z})^{-1}\,\| &\le \frac{2C\|V_1\|_2}{\beta^{1/2}} \\
&\quad + \left[\frac{2C\|V_1\|_2|\mathbf{z}|}{\beta^{1/2}} + C\|V_1\|_2\beta^{3/2} + \|V_2\|_\infty\right] \|\,(S_0-\mathbf{z})^{-1}\,\| \\
&\le \frac{2CR^{1/2}}{\beta^{1/2}} + \left[\frac{2CR^{1/2}|\mathbf{z}|}{\beta^{1/2}} + CR^{1/2}\beta^{3/2} + \frac{1}{R}\right] \|\,(S_0-\mathbf{z})^{-1}\,\| \\
&\le 2CN^\mu + \left[2CN^\mu|\mathbf{z}| + CN^\mu\beta^2 + \frac{1}{N^{2\mu}\beta}\right] \|\,(S_0-\mathbf{z})^{-1}\,\|, \qquad (41)
\end{aligned}$$

where we have written $R = \beta N^{2\mu}$, with $\mu \in \mathbb{R}$. Then we optimize the function $g(\beta) = CN^\mu\beta^2 + \frac{1}{N^{2\mu}\beta}$ by its minimium value, with N^μ fixed, and use the estimates $|\mathbf{z}| = O(N^{-2})$ and $\|\,(S_0-\mathbf{z})^{-1}\,\| = O(N^2)$, in order to get the estimate $\|V\,(S_0-\mathbf{z})^{-1}\,\| = O(N^\mu) + O(N^{2-\mu})$, which is optimal when $\mu = 1$.
2. As for part (2), from the estimate (27) with $C > 0$ as there, we obtain for all $\beta > 0$:

$$\begin{aligned}
&\|V\,(S_V-\mathbf{z})^{-1}\,\| \le \gamma^{-1}(V_1,\beta)\,\{C\|V_1\|_2 \\
&\quad \cdot \left[\frac{2}{\beta^{1/2}} + \left(\frac{2|\mathbf{z}|}{\beta^{1/2}} + \beta^{3/2}\right)\|\,(S_V-\mathbf{z})^{-1}\,\|\right] + \|V_2\|_\infty\|\,(S_V-\mathbf{z})^{-1}\,\|\Bigg\}, \qquad (42)
\end{aligned}$$

as long as $\gamma(V_1,\beta) := 1 - \frac{2C\|V_1\|_2}{\beta^{1/2}}$ is strictly positive. In order to optimize the upper bound in equation (42), we take $R = \frac{\beta}{(8\sqrt{\pi}C)^2}$. With this choice, the factor satisfies $\gamma(V_1, \beta \ge 1/2$. Thus we have:

$$\|V\,(S_V-\mathbf{z})^{-1}\,\| \le 2\left\{E + F\beta^2 + \frac{G}{\beta}\right\} \qquad (43)$$

with the coefficients $E = \left(1 + |\mathbf{z}|\|\,(S_V-\mathbf{z})^{-1}\,\|\right)/2$, $F = \|\,(S_V-\mathbf{z})^{-1}\,\|/4$ and $G = (8\sqrt{\pi}C)^2\|\,(S_V-\mathbf{z})^{-1}\,\|$. Since the minimum value of the function $g(\beta) := E + F\beta^2 + \frac{G}{\beta}$ on the interval $(0,\infty)$ is $E + \left(G^2F\right)^{1/3}\left(\frac{1}{2^{2/3}} + 2^{1/3}\right)$ then using the estimates $|\mathbf{z}| = O(N^{-2})$ and $\|\,(S_V-z)^{-1}\,\| = O(N^3)$ we conclude the proof. □

3.3. **Eigenvalue stability.** We next prove the main result on eigenvalue stability by following [1] adapted to our setting.

Let us first recall from Kato [14, chapter VIII, section 1, part 4] that an isolated eigenvalue E_o of a closed operator T_o with finite multiplicity N_o is stable with respect to a family of closed perturbations $\{T_n \mid n \in \mathbb{N}\}$ if

(1) There exists an $\epsilon > 0$, so that any $\mathbf{z}$ with $0 < |\mathbf{z} - E_o| < \epsilon$ is not in the spectrum of T_n, for all n large (depending on $\mathbf{z}$), and for such a $\mathbf{z}$, we have $(T_n - \mathbf{z})^{-1} \to (T_o - \mathbf{z})^{-1}$, $n \to \infty$, strongly;
(2) The total multiplicity of the eigenvalues of T_n in a neighborhood of E_o given by $\{\mathbf{z} \mid 0 \le |\mathbf{z} - E_o| < \mu\}$, with $0 < \mu < \epsilon$, is precisely N_o for all n large.

It is proven in [14, chapter VIII, section 1, part 4, Lemma 1.24] that if E_o is stable with respect to the family T_n, and all the operators are self-adjoint, then, in fact, the spectral projectors converge in norm. That is, by part 1 of the definition and $0 < \mu < \epsilon$, the contour $\Gamma_{E_o,\mu} = \{\mathbf{z} \mid |\mathbf{z} - E_o| = \mu\}$ is in the resolvent sets of T_n, for all n large. We can then define the projectors

$$P_n = -\frac{1}{2\pi i} \int_{\Gamma_{E_o,\mu}} (T_n - \mathbf{z})^{-1} \, d\mathbf{z}, \tag{44}$$

and, similarly, we define the projector P_o for T_o using the same contour $\Gamma_{E_o,\mu}$. The self-adjointness of T_n and T_o imply that these are orthogonal projectors. By part 1, we have $P_n \to P_o$ strongly, and by part 2, $\dim \mathrm{Ran} P_n = N_o$, for all n large. Under these conditions, Kato proves that $\|P_n - P_o\| \to 0$, as $n \to \infty$.

We are interested in studying a situation that is not exactly the one described in the above definition by Kato but very much in the same spirit. Namely, given $N \in \mathbb{N}$, let us consider the operator $S_V(\lambda(h = 1/(N+1), B)) = S_V + W(\lambda(h = 1/(N+1), B))$ (see equation (14)). Here we have the fixed (N-independent) operator $S_V = -\frac{1}{2}\Delta - \frac{1}{|\mathbf{x}|}$ plus a perturbation $W(\lambda(h = 1/(N+1), B)) = \frac{(\lambda(h=1/(N+1),B))^2}{8}(x_1^2 + x_2^2) - \frac{\lambda(h=1/(N+1),B)}{2} L_3$ indexed by N. We want to look at the eigenvalues $E_N = -1/2(N+1)^2$ of the hydrogen atom Hamiltonian S_V (remember that each eigenvalue E_N has multiplicity $d_N = (N+1)^2$). We want to show that, for N sufficiently large, the spectrum of $S_V(\lambda(h = 1/(N+1), B))$ inside some neighborhood around E_N consists of a cluster $\mathcal{C}_N$ of d_N eigenvalues (including multiplicity). The size r_N of such a neighborhood should decrease with N. Notice that in this situation, both the eigenvalue E_N and r_N change with N, which is not the case in the definition of stability by Kato where the eigenvalue E_o is fixed and the size ϵ of the neighborhood around E_o can be kept fixed as well. Since the cluster $\mathcal{C}_N$ can be thought of as splitting off of the unperturbed eigenvalue E_N into several eigenvalues of total multiplicity d_N, we will refer to the existence of $\mathcal{C}_N$ as a stability property.

In order to show the existence of the cluster $\mathcal{C}_N$, we first regard E_N as an element of the discrete spectrum of S_V and notice that the distance $\rho(N)$ between E_N and its nearest neighbors is $O(N^{-3})$. Thus we want to consider a circle Γ_N with center E_N and radius $r_N = cN^{-3}$, with c a suitable constant independent of N in such a way that r_N is smaller than $\rho(N)/2$. Then we have the following:

Theorem 3.1 (Stability theorem)**.** *Given $B \geq 0$ and suppose that the constant q in part 2 of Lemma 3.1 satisfies $q > 9$. The following spectral projectors are well-defined for N sufficiently large:*

$$P_N = -\frac{1}{2\pi \imath} \int_{\Gamma_N} (S_V(\lambda(h = 1/(N+1), B)) - \mathbf{z})^{-1} \, d\mathbf{z}, \tag{45}$$

$$\Pi_N = -\frac{1}{2\pi \imath} \int_{\Gamma_N} (S_V - \mathbf{z})^{-1} \, d\mathbf{z}. \tag{46}$$

Moreover, these projectors are orthogonal and satisfy

$$\|P_N - \Pi_N\| = O(N^{-\frac{2q-33}{5}}). \tag{47}$$

For $q > 33/2$, the difference of the orthogonal projectors $P_N - \Pi_N$ converges in norm to zero. Consequently, the spectrum of $S_V(\lambda(h = 1/(N+1), B))$ inside the circle Γ_N consist of a cluster $\mathcal{C}_N$ of eigenvalues with total multiplicity d_N provided N is sufficiently large.

Proof. We follow Avron, Herbst and Simon [1] in obtaining specific upper bounds on the difference $P_N - \Pi_N$. For the purpose of the proof of Theorem 3.1, we will only write λ to actually specify $\lambda(h = 1/(N+1), B)$, assuming $B > 0$.

1. We first establish the existence of the resolvent operator $(S_V(\lambda) - \mathbf{z})^{-1}$ for $\mathbf{z} \in \Gamma_N$. Since both resolvents $(S_V - \mathbf{z})^{-1}$ and $(S_0 - \mathbf{z})^{-1}$ exist for $\mathbf{z} \in \Gamma_N$, the equality $S_V - \mathbf{z} = \left[I + V\,(S_0 - \mathbf{z})^{-1}\right](S_0 - \mathbf{z})$ implies that the operator $I + V\,(S_0 - \mathbf{z})^{-1}$ is invertible. Thus for λ small, we expect from Lemma 3.1 that the operator $I + V\,(S_0(\lambda) - \mathbf{z})^{-1}$ is invertible as well. This, and the invertibility of $S_0(\lambda) - \mathbf{z}$ for $\mathbf{z} \in \Gamma_N$, imply that $S_V(\lambda) - \mathbf{z}$ is invertible for $\mathbf{z} \in \Gamma_N$ since

$$S_V(\lambda) - \mathbf{z} = S_0(\lambda) + V - \mathbf{z} = \left[I + V\,(S_0(\lambda) - \mathbf{z})^{-1}\right](S_0(\lambda) - \mathbf{z}).$$

2. To establish the invertibility $I + V\,(S_0(\lambda) - \mathbf{z})^{-1}$, we write

$$\begin{aligned} I + V\,(S_0(\lambda) - \mathbf{z})^{-1} \;&=\; \Big\{I + V\left[(S_0(\lambda) - \mathbf{z})^{-1} - (S_0 - \mathbf{z})^{-1}\right] \\ &\quad \cdot \left[I + V\,(S_0 - \mathbf{z})^{-1}\right]^{-1}\Big\}\left[I + V\,(S_0 - \mathbf{z})^{-1}\right]. \end{aligned} \tag{48}$$

Because of the estimate in part (2) of Lemma 3.1, we need to estimate

$$\left\|\left[I + V\,(S_0 - \mathbf{z})^{-1}\right]^{-1}\right\| \tag{49}$$

in order to have

$$\left\|V\left[(S_0(\lambda) - \mathbf{z})^{-1} - (S_0 - \mathbf{z})^{-1}\right]\left[I + V\,(S_0 - \mathbf{z})^{-1}\right]^{-1}\right\| < 1, \tag{50}$$

for $\mathbf{z} \in \Gamma_N$, which would imply the invertibility of $I + V\,(S_0(\lambda) - \mathbf{z})^{-1}$ for N large.

We write

$$\begin{aligned} \left[I + V\,(S_0 - \mathbf{z})^{-1}\right]^{-1} \;&=\; \left[(S_0 - \mathbf{z} + V)\,(S_0 - \mathbf{z})^{-1}\right]^{-1} \\ &=\; (S_V - \mathbf{z} - V)(S_V - \mathbf{z})^{-1} = I - V\,(S_V - \mathbf{z})^{-1}. \end{aligned} \tag{51}$$

From part (2) of Lemma 3.2, we have

$$\left\|\left[I + V\,(S_0 - \mathbf{z})^{-1}\right]^{-1}\right\| = O(N^3). \tag{52}$$

Using Lemma 3.1 and (52), we obtain

$$\left\|V\left[(S_0(\lambda) - \mathbf{z})^{-1} - (S_0 - \mathbf{z})^{-1}\right]\left[I + V\,(S_0 - \mathbf{z})^{-1}\right]^{-1}\right\| = O(N^{-\frac{2q-18}{5}}). \tag{53}$$

Thus, in order to satisfy condition (50), and then to have the existence of the resolvent $(S_V(\lambda) - \mathbf{z})^{-1}$ with $|\mathbf{z} - E_N| = r_N$, we need to take $q > 9$.

3. We next apply these estimates to bound the difference of the projectors from above. As the resolvents have been shown to exist on the contour Γ_N, we have

$$P_N - \Pi_N = -\frac{1}{2\pi\imath}\int_{\Gamma_N} \left[(S_V(\lambda)-\mathbf{z})^{-1} - (S_V-\mathbf{z})^{-1}\right] d\mathbf{z}. \tag{54}$$

We know the operator $S_V(\lambda)$ does not converge to S_V in the norm resolvent sense as $\lambda \to 0$ [1]. The key ideas necessary to obtain norm convergence of the left hand side of (54) consist in **(i)** inserting in the right hand side of equation (54) the integrals $\frac{1}{2\pi\imath}\int_{\Gamma_N}(S_0(\lambda)-\mathbf{z}))^{-1}\,d\mathbf{z}$ and $-\frac{1}{2\pi\imath}\int_{\Gamma_N}(S_0-\mathbf{z}))^{-1}\,d\mathbf{z}$ which are zero due to the analyticity of the resolvents $(S_0(\lambda)-\mathbf{z})^{-1}$ and $(S_0-\mathbf{z})^{-1}$ on $\mathbb{C}\backslash[0,\infty)$, and then **(ii)** using the convergence of $(S_V(\lambda)-\mathbf{z})^{-1}-(S_0(\lambda)-\mathbf{z})^{-1}$ to $(S_V-\mathbf{z})^{-1}-(S_0-\mathbf{z})^{-1}$ as $\lambda\to 0$. In order to estimate this last convergence, we write

$$\begin{aligned}
&\left\|\left[(S_V(\lambda)-\mathbf{z})^{-1}-(S_0(\lambda)-\mathbf{z})^{-1}\right]-\left[(S_V-\mathbf{z})^{-1}-(S_0-\mathbf{z})^{-1}\right]\right\| \\
&= \left\| (S_0(\lambda)-\mathbf{z})^{-1}\, V\,(S_V(\lambda)-\mathbf{z})^{-1} - (S_0-\mathbf{z})^{-1}\, V\,(S_V-\mathbf{z})^{-1}\right\| \\
&= \left\| (S_0(\lambda)-\mathbf{z})^{-1}\left[V\,(S_V(\lambda)-\mathbf{z})^{-1} - V\,(S_V-\mathbf{z})^{-1}\right]\right. \\
&\quad \left. + \left[(S_0(\lambda)-\mathbf{z})^{-1}\, V - (S_0-\mathbf{z})^{-1}\, V\right](S_V-\mathbf{z})^{-1}\right\| \\
&\leq \left\|(S_0(\lambda)-\mathbf{z})^{-1}\right\|\left\|V\,(S_V(\lambda)-\mathbf{z})^{-1} - V\,(S_V-\mathbf{z})^{-1}\right\| \\
&\quad + \left\| (S_0(\lambda)-\mathbf{z})^{-1}\, V - (S_0-\mathbf{z})^{-1}\, V\right\|\left\| (S_V-\mathbf{z})^{-1}\right\|.
\end{aligned} \tag{55}$$

In light of resolvent estimates (20), and the estimate (22), we can control the norm of the difference of the resolvents in (55) provided we can estimate

$$\left\| V\,(S_V(\lambda)-\mathbf{z})^{-1} - V\,(S_V-\mathbf{z})^{-1}\right\|. \tag{56}$$

4. To obtain an upper bound on the norm in (56), we write

$$V\,(S_V(\lambda)-\mathbf{z})^{-1} = V\,(S_0(\lambda)-\mathbf{z})^{-1}\left[I+V\,(S_0(\lambda)-\mathbf{z})^{-1}\right]^{-1}, \tag{57}$$

$$V\,(S_V-\mathbf{z})^{-1} = V\,(S_0-\mathbf{z})^{-1}\left[I+V\,(S_0-\mathbf{z})^{-1}\right]^{-1}. \tag{58}$$

The invertibility of $I+V\,(S_0-\mathbf{z})^{-1}$, appearing in (58), was established in (52). We prove that $I+V\,(S_0(\lambda)-\mathbf{z})^{-1}$ in (57) is invertible as follows. We write this factor as

$$\begin{aligned}
\left[I+V\,(S_0(\lambda)-\mathbf{z})^{-1}\right] &= \left[I+V\,(S_0-\mathbf{z})^{-1}\right]\left[I+\left(I+V\,(S_0-\mathbf{z})^{-1}\right)^{-1}\right. \\
&\quad \left.\times\left\{V\,(S_0(\lambda)-\mathbf{z})^{-1} - V\,(S_0-\mathbf{z})^{-1}\right\}\right].
\end{aligned} \tag{59}$$

It follows from (52) and part (2) of Lemma 3.1 that

$$\|\left(I+V\,(S_0-\mathbf{z})^{-1}\right)^{-1}\left\{V\,(S_0(\lambda)-\mathbf{z})^{-1} - V\,(S_0-\mathbf{z})^{-1}\right\}\| = O(N^{-(\frac{2q-18}{5})}), \tag{60}$$

so each factor in square brackets on the right side of (59) is invertible. Furthermore, it follows from (59)–(60) that

$$\left\| \left[I + V\left(S_0(\lambda) - \mathbf{z}\right)^{-1} \right]^{-1} \right\| = O(N^3). \tag{61}$$

Returning to (57)–(58), we have

$$\begin{aligned} &\|V(S_V(\lambda) - \mathbf{z})^{-1} - V(S_V - \mathbf{z})^{-1}\| \\ &\quad \leq \ \|V(S_0(\lambda) - \mathbf{z})^{-1} - V(S_0 - \mathbf{z})^{-1}\| \|[1 + V(S_0(\lambda) - \mathbf{z})^{-1}]^{-1}\| \\ &\qquad + \|V(S_0 - \mathbf{z})^{-1}\| \|[1 + V(S_0(\lambda) - \mathbf{z})^{-1}]^{-1} - [1 + V(S_0 - \mathbf{z})^{-1}]^{-1}\|. \end{aligned} \tag{62}$$

The first term on the right in (62) is bounded from part (2) of Lemma 3.1 and (61). As for the second term on the right, we note that from equations (52)-(53) we obtain

$$\left\| \left[I + V\left(S_0(\lambda) - \mathbf{z}\right)^{-1} \right]^{-1} - \left[I + V\left(S_0 - \mathbf{z}\right)^{-1} \right]^{-1} \right\| = O\left(N^{-\frac{2q-33}{5}}\right). \tag{63}$$

and $\|V(S_0 - \mathbf{z})^{-1}\| = O(N)$ from part (1) of Lemma 3.2. Consequently, we have the bound

$$\|V\left(S_V(\lambda) - \mathbf{z}\right)^{-1} - V\left(S_V - \mathbf{z}\right)^{-1}\| = O(N^{-\frac{2q-38}{5}}). \tag{64}$$

5. We conclude the convergence of the projectors as follows. From Lemma 3.1, equation (64), and the norm estimates $\left\|(S_0(\lambda) - \mathbf{z})^{-1}\right\| = O(N^2)$ and $\left\| (S_V - \mathbf{z})^{-1}\right\| = O(N^3)$, we finally get the estimate for the difference of the spectral projectors

$$\begin{aligned} \|P_N - \Pi_N\| \ \leq \ & \frac{1}{2\pi} \int_{\Gamma_N} \left\| \left[(S_V(\lambda) - \mathbf{z})^{-1} - (S_0(\lambda) - \mathbf{z})^{-1} \right] \right. \\ & \left. - \left[(S_V - \mathbf{z})^{-1} - (S_0 - \mathbf{z})^{-1} \right] \right\| |d\mathbf{z}| = O(N^{-\frac{2q-33}{5}}). \end{aligned} \tag{65}$$

Thus taking $q > 33/2$ we have, for N sufficiently large, $\|P_N - \Pi_N\| < 1$ and then that the dimension of the range of both projectors P_N and Π_N is the same (see reference [14]) which in turn implies the existence of the cluster $\mathcal{C}_N$. □

4. A semiclassical trace identity for Zeeman eigenvalue clusters.

From Theorem 3.1, we know that for $q > 33/2$ the size of the eigenvalue cluster $\mathcal{C}_N$ around E_N is no larger than $r_N = O(N^{-3})$. We need to get a better estimate on the size of $\mathcal{C}_N$ in order to scale the shifts of eigenvalues within $\mathcal{C}_N$. Let us first consider the case of the eigenvalue cluster formed by the perturbation $S_V(\lambda)$ of S_V, where $\lambda \geq 0$ is the magnetic field strength independent of any other parameters. In this case, Theorem 5.6 in reference [1], when applied to the Coulomb potential, shows that if we take a *fixed* eigenvalue E_M of the scaled hydrogen atom Hamiltonian S_V with multiplicity $d_M = (M+1)^2$, then we have for λ sufficiently small that the operator $S_V(\lambda)$ has a cluster of eigenvalues $E_{M,j}(\lambda)$, $j = 1, \ldots, d_M$ around E_M inside a small but *fixed* circle with center E_M. The eigenvalues in the cluster can be written in the following way: Let

$m = -(M-1), \ldots, M-1$ be the eigenvalues of $\Pi_M L_3 \Pi_M$, where Π_M projects onto the eigenspace of S_V and eigenvalue E_M. Then, for a given j, there exist an index m so that

$$E_{M,j}(\lambda) = E_M - \lambda m + O(\lambda^2). \tag{66}$$

This indicates that the size of the cluster of eigenvalues around E_M is $O(\lambda)$, with M fixed.

In our setting, the parameter N controls both the strength of the effective magnetic field $\lambda = \lambda(h, B) = h^3 \epsilon(h) B$, $h = 1/(N+1)$, and the radius r_N of the circles $\mathcal{C}_N$ where our clusters of eigenvalues are well defined. Thus neither the center E_N nor the radius r_N stay fixed as it is the case of the mentioned result of reference [1]. So we need to get estimates considering that fact. We begin with norm estimates of the operators $\Pi_N L_3 \Pi_N$ and $\Pi_N (x_1^2 + x_2^2) \Pi_N$:

Lemma 4.1. *Let Π_N be the projector to the eigenspace associated to the eigenvalue E_N of the scaled hydrogen atom Hamiltonian S_V as above. Then for $N \to \infty$ and $k \in \mathbb{N}$ fixed we have*

$$\begin{aligned} \Pi_N L_3 \Pi_N &= O(N), & (67)\\ \Pi_N (x_1^2 + x_2^2)^k \Pi_N &= O(N^{4k}). & (68) \end{aligned}$$

Remark 1. The physical intuition for equation (68) comes from the Kepler problem. In that case, the maximum apogee distance $r_{\max}(E)$ for an orbit in configuration space of negative energy E is $1/|E|$ (including collision and non-collision orbits). So, $r_{\max}(E = -1/2) = 2$ and $r_{\max}(E = -1/(2N^2)) = 2N^2$. Thus we expect, semiclassically speaking , that for a Kepler orbit in configuration space, $x_1^2 + x_2^2 = O(N^4)$. This property is implemented via coherent states $\Psi_{\boldsymbol{\alpha},N}$ with N large.

Before presenting the proof of Lemma 4.1, we briefly recall some facts about the coherent states $\Psi_{\boldsymbol{\alpha},N}$, complete details are presented in Appendix 2, section 9. The index $\boldsymbol{\alpha} \in \mathbb{C}^4$ is an element of $\mathcal{A} = \{\boldsymbol{\alpha} \in \mathbb{C}^4 \mid |\Re(\boldsymbol{\alpha})| = |\Im(\boldsymbol{\alpha})| = 1,\ \Re(\boldsymbol{\alpha}) \cdot \Im(\boldsymbol{\alpha}) = 0\}$. The set $\mathcal{A}$ can be thought of as the unit cotangent bundle $T_1^*\mathbb{S}^3$ of the 3-sphere $\mathbb{S}^3$ with $\Re\boldsymbol{\alpha} \in \mathbb{S}^3$ and $\Im\boldsymbol{\alpha}$ an element of the cotangent space to $\mathbb{S}^3$ at the point $\Re\alpha$. The inverse of the Moser map (see Appendix 1, section 8) then relates $T_1^*\mathbb{S}_o^3$ (the unit cotangent bundle $T_1^*\mathbb{S}^3$ minus the north pole) with the energy surface $\Sigma(-1/2)$ of the Kepler problem. The states $\Psi_{\boldsymbol{\alpha},N}$ belong to the range of Π_N and provide a resolution of the identity giving an expression for the projector Π_N in terms of them, see equation (146) in Appendix 2, section 9.

Proof. 1. Equation (67) comes from the well known fact that the eigenvalues of L_3 restricted to the range of Π_N are $-N, \ldots, N$.
2. We use the coherent states $\Psi_{\boldsymbol{\alpha},N}$, for $\boldsymbol{\alpha} \in \mathcal{A}$ in the proof of (68). In [18], it is shown that the dilated coherent state $D_{(N+1)^2}\Psi_{\boldsymbol{\alpha},N}$ has a fast decay outside of a ball of radius $r_0 > 2$. Specifically, we have the following result shown in [18, 4.19]:

Lemma 4.2. *Let $\tilde{V} : \mathbb{R}^3 \to \mathbb{R}$ be a polynomially bounded continuous function. Then for $r_0 > 2$ we have*

$$\Pi_N D_{(N+1)^{-2}} \tilde{V} D_{(N+1)^2} \Pi_N = \Pi_N D_{(N+1)^{-2}} \tilde{V} \chi_{|\mathbf{x}| \le r_0} D_{(N+1)^2} \Pi_N + O(N^{-\infty}) \tag{69}$$

where $\chi_{|\mathbf{x}| \le r_0}$ is the characteristic function of the ball $|\mathbf{x}| \le r_0$ and the dilation operator D_α is defined in (12)*.*

The proof of equation (68) is then a consequence of Lemma 4.2 and the following equalities:

$$\begin{aligned} D_{(N+1)^{-2}} (x_1^2 + x_2^2)^k D_{(N+1)^2} &= \frac{1}{(N+1)^{4k}} (x_1^2 + x_2^2)^k \\ \Pi_N (x_1^2 + x_2^2)^k \Pi_N &= (N+1)^{4k} \Pi_N D_{(N+1)^{-2}} (x_1^2 + x_2^2)^k D_{(N+1)^2} \Pi_N. \end{aligned} \tag{70}$$

Thus we finally have $\|\Pi_N D_{(N+1)^{-2}} (x_1^2 + x_2^2)^k D_{(N+1)^2} \Pi_N\| = O(1)$ and then the proof of (68). $\square$

Remark 2. We can actually say more about the coherent states $D_{(N+1)^2} \Psi_{\boldsymbol{\alpha},N}$ in terms of concentration. It can be shown that for $\boldsymbol{\alpha} \in \mathcal{A}$ given, the state $D_{(N+1)^2} \Psi_{\boldsymbol{\alpha},N}$ is highly concentrated along the classical orbit in configuration space associated to α by the inverse of the Moser map and the classical flow of the Kepler problem on the energy surface $\Sigma(-1/2)$. See references [18] and [20] for details.

Let us denote by $\tilde{E}_{N,j}$, $j = 1, \dots, d_N$, the eigenvalues of $S_V(\lambda)$ inside the circle Γ_N (this notion is well defined for N sufficiently large). Now we consider the eigenvalue shifts $\tilde{\nu}_{N,j} = \tilde{E}_{N,j} - E_N$ thinking of them as the eigenvalues of the operator $P_N (S_V(\lambda) - E_N) P_N$.

We write

$$\begin{aligned} P_N (S_V(\lambda) - E_N) P_N &= P_N (S_V(\lambda) - E_N) P_N \Pi_N \\ &\quad + P_N (S_V(\lambda) - E_N) P_N \, (P_N - \Pi_N) \end{aligned} \tag{71}$$

which in turn implies

$$\begin{aligned} &P_N (S_V(\lambda) - E_N) P_N \, [I - (P_N - \Pi_N)] \\ &\qquad = P_N (S_V(\lambda) - E_N) \Pi_N = P_N W(\lambda) \Pi_N. \end{aligned} \tag{72}$$

For $q > 33/2$, we have from Theorem 3.1 that $I - (P_N - \Pi_N)$ is invertible for N sufficiently large. Moreover $\| [I - (P_N - \Pi_N)]^{-1} - I \| = O(N^{-\sigma})$ with $\|P_N - \Pi_N\| = O(N^{-\sigma})$ and $\sigma = \frac{2q-33}{5} > 0$. Thus we have

$$\begin{aligned} P_N (S_V(\lambda) - E_N) P_N &= \Pi_N W(\lambda) \Pi_N + (P_N - \Pi_N) \, W(\lambda) \Pi_N \\ &\quad + P_N W(\lambda) \Pi_N \left\{ [I - (P_N - \Pi_N)]^{-1} - I \right\}, \\ &= \Pi_N W(\lambda) \Pi_N + O(N^{-\sigma}) W(\lambda) \Pi_N \\ &\quad + P_N W(\lambda) \Pi_N O(N^{-\sigma}). \end{aligned} \tag{73}$$

From Lemma 4.1, we have

$$\begin{aligned} \|L_3\Pi_N\| &= \|\Pi_N L_3 \Pi_N\| = O(N), \\ \| \left(x_1^2+x_2^2\right)\Pi_N\| &= \| \left(\left(x_1^2+x_2^2\right)\Pi_N\right)^* \left(x_1^2+x_2^2\right)\Pi_N\|^{1/2} \\ &= \|\Pi_N \left(x_1^2+x_2^2\right)^2 \Pi_N\|^{1/2} = O(N^4) \end{aligned} \tag{74}$$

which implies $\|W(\lambda)\Pi_N\| = O\left(h^2\epsilon(h)\right)$. Hence, we have from equation (73)

$$\begin{aligned} \frac{P_N(S_V(\lambda)-E_N)P_N}{h^2\epsilon(h)} &= \frac{\Pi_N W(\lambda)\Pi_N}{h^2\epsilon(h)} + O(N^{-\sigma}) = \Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N \\ &+ O(\epsilon(h)) + O(N^{-\sigma}) = \Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N + O(N^{-\sigma}). \end{aligned} \tag{75}$$

Since $\|\Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N\| = O(1)$ then $\left\|\frac{P_N(S_V(\lambda)-E_N)P_N}{h^2\epsilon(h)}\right\| = O(1)$. Due to the self-adjointness of $\frac{P_N(S_V(\lambda)-E_N)P_N}{h^2\epsilon(h)}$, then the spectral radius of the operator $\frac{P_N(S_V(\lambda)-E_N)P_N}{h^2\epsilon(h)}$ is $O(1)$ as well. Thus we see that the size of the eigenvalue shifts $\tilde{\nu}_{N,j}$ is $O(h^2\epsilon(h))$. Moreover, equation (75) is the basis to establish the following theorem:

Theorem 4.1. *Let $h = 1/(N+1)$ and $\sigma = (2q-33)/5$. For any polynomial Q, we have*

$$\frac{1}{d_N}\sum_{j=1}^{d_N} Q\left(\frac{\tilde{\nu}_{N,j}}{h^2\epsilon(h)}\right) = \frac{1}{d_N}\mathrm{Tr}\, Q\left(\Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N\right) + O(N^{-\sigma}). \tag{76}$$

So for $q > 33/2$, the remainder term in (76) vanishes as $N \to \infty$.

Proof. For N sufficiently large, there exist a fixed interval $[-A, A]$ containing both $\frac{\tilde{\nu}_{N,j}}{h^2\epsilon(h)}$, $j = 1, \dots, d_N$, and the eigenvalues of the operator $\Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N$. Since a polynomial is a finite linear combination of monomials, then we only need to show equation (76) for a monomial. We consider a monomial of degree $k \in \mathbb{N}$ and write

$$\frac{1}{d_N}\sum_{j=1}^{d_N}\left(\frac{\tilde{\nu}_{N,j}}{h^2\epsilon(h)}\right)^k = \frac{1}{d_N}\mathrm{Tr}\left(\frac{P_N\left(S_V(\lambda)-E_N\right)P_N}{h^2\epsilon(h)}\right)^k. \tag{77}$$

To simplify notation, let $A_N := \Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N$. From equation (75), we have

$$\begin{aligned} \left(\frac{P_N(S_V(\lambda)-E_N)P_N}{h^2\epsilon(h)}\right)^k &= P_N\left(A_N\right)^k + P_N O(N^{-\sigma}), \\ &= \left(A_N\right)^k + \left(P_N - \Pi_N\right)\left(A_N\right)^k + P_N O(N^{-\sigma}). \end{aligned} \tag{78}$$

To evaluate the trace of the second term on the right of the last line of (78), consider an orthonormal basis $\{\phi_j\}_{j=1}^{d_N}$ for the range of Π_N and extend it to an orthonormal basis $\{\phi_j\}_{j=1}^{\infty}$ of $L^2(\mathbb{R}^3)$. Then, we have

$$\begin{aligned}\left|\frac{1}{d_N}\text{Tr }\left(P_N-\Pi_N\right)A_N^k\right| &= \left|\frac{1}{d_N}\sum_{j=1}^{\infty}\langle\phi_j,\left(P_N-\Pi_N\right)A_N^k\phi_j\rangle\right|, \\ &= \left|\frac{1}{d_N}\sum_{j=1}^{d_N}\langle\phi_j,\left(P_N-\Pi_N\right)A_N^k\phi_j\rangle\right| \leq \|P_N-\Pi_N\| = O(N^{-\sigma}). \quad (79)\end{aligned}$$

To evaluate the trace of the third term on the right of the last line of (78), consider an orthonormal basis $\{\Psi_j\}_{j=1}^{d_N}$ for the range of P_N and extend it to an orthonormal basis $\{\Psi_j\}_{j=1}^{\infty}$ of $L^2(\mathbb{R}^3)$. Thus, we have

$$\begin{aligned}\left|\frac{1}{d_N}\text{Tr }\big(P_N O(N^{-\sigma})\big)\right| &= \left|\frac{1}{d_N}\sum_{j=1}^{\infty}\langle O(N^{-\sigma})\Psi_j, P_N\Psi_j\rangle\right|, \\ &= \left|\frac{1}{d_N}\sum_{j=1}^{d_N}\langle O(N^{-\sigma})\Psi_j, P_N\Psi_j\rangle\right| \leq O(N^{-\sigma}). \quad (80)\end{aligned}$$

From equations (77)-(80), the theorem follows for a monomial and hence for any polynomial. □

5. A trace estimate for the Zeeman perturbation of the hydrogen atom.

In this section, we calculate the large N limit of the trace in the right hand side of (76) involving a continuous function $\rho : \mathbb{R} \mapsto \mathbb{R}$ (not only a polynomial Q) and the component L_3 of the angular momentum operator along the direction of the magnetic field $\mathbf{B}(h)$. This extends previous results to a family of perturbations that are first-order differential operators. In section 5.1, we prove Proposition 5.1 that presents a large N estimate for the expected value of powers of the operator $h\frac{B}{2}L_3$, $h = 1/(N+1)$, on a coherent state $\Psi_{\boldsymbol{\alpha},N}$. This key technical result is used in section 5.2 to prove the Szegö-type theorem for the angular momentum operator, Theorem 5.1. Finally, the proofs of the main theorems are given in section 5.3. We remark that, although we only use the result of Theorem 5.1 for polynomials, it is interesting on its own to establish such a theorem for continuous functions.

5.1. **The angular momentum perturbation term.** In this section, we prove a Szegö-type theorem for the operator $h\frac{B}{2}L_3$, theorem 5.1, which describes the limit $N \to \infty$ of the normalized trace indicated in the right-hand side of equation (76) in Theorem 4.1. As in section 4, it is enough to consider the case $\rho(x) = x^k$, $k \in \mathbb{N}^*$, on a compact interval (see proof of Theorem 5.1 below).

The key idea in the proof of Theorem 5.1 is to use, for each N, the system of coherent states $\{\Psi_{\boldsymbol{\alpha},N}\}_{\boldsymbol{\alpha}\in\mathcal{A}}$ (see section 9, Appendix 2). Such a system gives a resolution of the identity on the range of Π_N (see equation (146)) and, as a consequence, one can express the trace in equation (76), with $\rho(x) = x^k$, as an integral involving the inner products $\left\langle \Psi_{\boldsymbol{\alpha},N}, ((-hB/2)L_3)^k\, \Psi_{\boldsymbol{\alpha},N} \right\rangle$ with respect to the measure $d\mu(\alpha)$ (see equation (102)).

We estimate that inner product in Proposition 5.1. This result goes beyond our work with the Stark hydrogen atom Hamiltonian [12] as we must estimate the derivatives of the coherent states. We first state the proposition but defer its proof until after the key technical Lemma 5.1.

Proposition 5.1. *For $\boldsymbol{\alpha} \in \mathcal{A}$, an integer $k > 0$, and $h = 1/(N+1)$, we have for $N \to \infty$,*

$$\left\langle \Psi_{\boldsymbol{\alpha},N}, \left(h\tilde{B}L_3\right)^k \Psi_{\boldsymbol{\alpha},N} \right\rangle = \left(\tilde{B}\ell_3(\boldsymbol{\alpha})\right)^k + O(N^{-1}), \tag{81}$$

where $\ell_3(\boldsymbol{\alpha}) = \Re(\alpha)_2\Im(\alpha)_1 - \Re(\alpha)_1\Im(\alpha)_2$ and $\tilde{B} = -B/2$.

Before presenting the proof, we present the lemma on the decay properties of the derivatives of the coherent states as $N \to \infty$. We recall some notation from Appendix 2, section 9. For $\boldsymbol{\alpha} \in \mathcal{A}$, a coherent state is defined by

$$\Psi_{\boldsymbol{\alpha},N} = \mathcal{F}^{-1} D_{r_N} J^{1/2} K \Phi_{\boldsymbol{\alpha},N}, \tag{82}$$

with $\Phi_{\boldsymbol{\alpha},N}(\boldsymbol{\omega}) = a(N)(\boldsymbol{\alpha}\cdot\boldsymbol{\omega})^N$, where $\mathcal{F}$ is the Fourier transform (see Eq. (141)), the operator K is the unitary operator defined in Eq. (144) and the operator J is the self-adjoint operator defined in Eq. (145), the operator D_σ is the dilation operator defined in (12), and $\boldsymbol{\omega} \in \mathbb{S}^3$. We also define $\tilde{L}_3 = \mathcal{F}L_3\mathcal{F}^{-1} = \imath \left[p_2\frac{\partial}{\partial p_1} - p_1\frac{\partial}{\partial p_2}\right]$.

Lemma 5.1. *Let $k \geq 1$ be an integer and $\boldsymbol{\alpha} \in \mathcal{A}$. Then for $h = 1/(N+1)$ we have*

$$\begin{aligned}&\left(h\tilde{B}\tilde{L}_3\right)^k J^{1/2} K \Phi_{\boldsymbol{\alpha},N}(\mathbf{p}) = \\ &\qquad \frac{\left(\imath\tilde{B}\right)^k \left\{ [\alpha_1 p_2 - \alpha_2 p_1]^k + Q_{\alpha,k}(\mathbf{p};N) \right\}}{\left(\frac{|\mathbf{p}|^2+1}{2}\right)^{k+2}} \left[\frac{\Phi_{\boldsymbol{\alpha},N}(\boldsymbol{\omega}(\mathbf{p}))}{(\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p}))^k}\right],\end{aligned} \tag{83}$$

where the functions $Q_{\alpha,k}$ are given by

$$Q_{\alpha,k}(\mathbf{p};N) = \sum_{\ell=0}^{k-1} P_{\alpha,k-\ell}(p_1,p_2;N)\left(\frac{|\mathbf{p}|^2+1}{2}\right)^\ell (\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p}))^\ell \tag{84}$$

with $P_{\alpha,r}$, $1 \leq r \leq k$, having the following structure:

$$P_{\alpha,r}(p_1,p_2;N) = \sum_{j=0}^{r} C_{r,j}(N)\,[\alpha_1p_2 - \alpha_2p_1]^j\,[\alpha_1p_1 + \alpha_2p_2]^{r-j} \tag{85}$$

and all the real coefficients $C_{r,j}(N)$ are $O(N^{-1})$.

The specific expression for the coefficients $C_{r,j}(N)$ is not relevant for us. The important property is that they are $O(N^{-1})$. So, for k given, we will speak generically saying that a function $F(\mathbf{p};N)$ is a $Q_{\alpha,k}$-type function meaning that $F(\mathbf{p};N)$ can be written as in equation (84) for some coefficients $C_{r,j}(N)$ as indicated in equation (85). Similarly, we will refer to $P_{\alpha,r}$-type functions.

Proof of lemma 5.1. **Step 1**. The following equalities hold for all integer $q \geq 1$:

$$
\begin{aligned}
&\tilde{L}_3 \left(\frac{2}{|\mathbf{p}|^2+1} \right)^q = 0, \\
&\tilde{L}_3 \left(\boldsymbol{\alpha} \cdot \boldsymbol{\omega}(\mathbf{p}) \right)^q = \imath q \left(\boldsymbol{\alpha} \cdot \boldsymbol{\omega}(\mathbf{p}) \right)^{q-1} \left(\frac{2}{|\mathbf{p}|^2+1} \right) \left(\alpha_1 p_2 - \alpha_2 p_1 \right), \\
&\tilde{L}_3 \left(\alpha_1 p_2 - \alpha_2 p_1 \right) = -\imath \left(\alpha_1 p_1 + \alpha_2 p_2 \right), \\
&\tilde{L}_3 \left(\alpha_1 p_1 + \alpha_2 p_2 \right) = \imath \left(\alpha_1 p_2 - \alpha_2 p_1 \right).
\end{aligned} \tag{86}
$$

We also note that $\tilde{L}_3$ is dilation invariant.
Step 2. We prove Lemma 5.1 by induction. We write (see Appendix 2, section 9),

$$
J^{1/2} K \Phi_{\boldsymbol{\alpha},N}(\mathbf{p}) = a(N) \left(\frac{2}{|\mathbf{p}|^2+1} \right)^2 \left(\boldsymbol{\alpha} \cdot \boldsymbol{\omega}(\mathbf{p}) \right)^N. \tag{87}
$$

First note that for $k = 1$

$$
\begin{aligned}
&\left(h \tilde{B} \tilde{L}_3 \right) J^{1/2} K \Phi_{\boldsymbol{\alpha},N}(\mathbf{p}) = \\
&\qquad \frac{\left(\imath \tilde{B} \right) \left(\, [\alpha_1 p_2 - \alpha_2 p_1] - \frac{1}{N+1} [\alpha_1 p_2 - \alpha_2 p_1] \, \right)}{\left(\frac{|\mathbf{p}|^2+1}{2} \right)^3} \; \frac{\Phi_{\boldsymbol{\alpha},N}(\boldsymbol{\omega}(\mathbf{p}))}{(\boldsymbol{\alpha} \cdot \boldsymbol{\omega}(\mathbf{p}))}.
\end{aligned} \tag{88}
$$

Since $-\frac{1}{N+1} [\alpha_1 p_2 - \alpha_2 p_1]$ is a $Q_{\alpha,1}$-type function (take $\ell = 0$ in equation (84) and $C_{1,0}(N) = 0$, $C_{1,1}(N) = -\frac{1}{N+1}$ in equation (85)) then Lemma 5.1 is valid for $k = 1$.
Step 3. Let us assume that equation (83) holds for an integer $k > 1$. Using equations in (86) we have:

$$
\begin{aligned}
\left(h \tilde{B} \tilde{L}_3 \right)^{k+1} J^{1/2} K \Phi_{\boldsymbol{\alpha},N}(\mathbf{p}) = {} & \frac{\left(\imath \tilde{B} \right)^{k+1}}{\left(\frac{|\mathbf{p}|^2+1}{2} \right)^{k+3}} \frac{\Phi_{\boldsymbol{\alpha},N}(\boldsymbol{\omega}(\mathbf{p}))}{(\boldsymbol{\alpha} \cdot \boldsymbol{\omega}(\mathbf{p}))^{k+1}} \\
\cdot \Bigg\{ [\alpha_1 p_2 - \alpha_2 p_1]^{k+1} & - \left(\frac{k+1}{N+1} \right) [\alpha_1 p_2 - \alpha_2 p_1]^{k+1} \\
- \left(\frac{k}{N+1} \right) & [\alpha_1 p_2 - \alpha_2 p_1]^{k-1} [\alpha_1 p_1 + \alpha_2 p_2] \left(\frac{|\mathbf{p}|^2+1}{2} \right) (\boldsymbol{\alpha} \cdot \boldsymbol{\omega}(\mathbf{p})) \\
+ \frac{1}{N+1} \sum_{\ell=0}^{k-1} & \left(-\imath \tilde{L}_3 P_{\alpha,k-\ell}(p_1, p_2; N) \right) \left(\frac{|\mathbf{p}|^2+1}{2} \right)^{\ell+1} (\boldsymbol{\alpha} \cdot \boldsymbol{\omega}(\mathbf{p}))^{\ell+1} \\
+ \sum_{\ell=0}^{k-1} \frac{N-k+\ell}{N+1} & P_{\alpha,k-\ell}(p_1, p_2; N) [\alpha_1 p_2 - \alpha_2 p_1] \left(\frac{|\mathbf{p}|^2+1}{2} \right)^{\ell} (\boldsymbol{\alpha} \cdot \boldsymbol{\omega}(\mathbf{p}))^{\ell} \Bigg\}.
\end{aligned} \tag{89}
$$

One can check that the second and third terms inside the curl brakets in equation (89) are $Q_{\alpha,k+1}$-type functions. Regading the fourth term, we write

$$
\begin{aligned}
-\imath\tilde{L}_3 P_{\alpha,k-\ell}(p_1,p_2;N) = \\
&- \sum_{j=0}^{k-\ell-1} (j+1) C_{k-\ell,j+1}(N) \left[\alpha_1 p_2 - \alpha_2 p_1\right]^j \left[\alpha_1 p_1 + \alpha_2 p_2\right]^{k-\ell-j} \\
&+ \sum_{j=1}^{k-\ell} (k-\ell-j+1) C_{k-\ell,j-1}(N) \left[\alpha_1 p_2 - \alpha_2 p_1\right]^j \left[\alpha_1 p_1 + \alpha_2 p_2\right]^{k-\ell-j} \quad (90)
\end{aligned}
$$

Thus $-\imath\tilde{L}_3 P_{\alpha,k-\ell}(p_1,p_2;N)$ can be written as a $P_{\alpha,k+1-(\ell+1)}(p_1,p_2;N)$-type function and then the fourth term is a $Q_{\alpha,k+1}$-type function. For the last term, we write

$$
\begin{aligned}
P_{\alpha,k-\ell}(p_1,p_2;N) \left[\alpha_1 p_2 - \alpha_2 p_1\right] = \\
&\sum_{j=1}^{k+1-\ell} C_{k-\ell,j-1}(N) \left[\alpha_1 p_2 - \alpha_2 p_1\right]^j \left[\alpha_1 p_1 + \alpha_2 p_2\right]^{k+1-\ell-j} \quad (91)
\end{aligned}
$$

which is a $P_{\alpha,k+1-\ell}$-type function. Thus the last term is a $Q_{\alpha,k+1}$-type function as well. We conclude the proof. □

We finish this section with the proof of Proposition 5.1.

Proof of Proposition 5.1. **Step 1**. First note that Proposition 5.1 is obviously valid for $k = 0$, so we assume $k \geq 1$. Using the definition of $\Psi_{\boldsymbol{\alpha},N}$ in (82), the inner product is

$$
\begin{aligned}
&\left\langle \Psi_{\boldsymbol{\alpha},N}, \left(h\tilde{B}L_3\right)^k \Psi_{\boldsymbol{\alpha},N} \right\rangle_{L^2(\mathbb{R}^3)} \\
&\qquad = \left\langle \Phi_{\boldsymbol{\alpha},N}, K^{-1} J^{1/2} \left(h\tilde{B}\tilde{L}_3\right)^k J^{1/2} K \Phi_{\alpha,N} \right\rangle_{L^2(\mathbb{S}^3)}, \quad (92)
\end{aligned}
$$

where $\tilde{L}_3 = \mathcal{F} L_3 \mathcal{F}^{-1} = \imath \left[p_2 \frac{\partial}{\partial p_1} - p_1 \frac{\partial}{\partial p_2}\right]$ and $D_{r_N}^{-1} \tilde{L}_3 D_{r_N} = \tilde{L}_3$.
Step 2. Using Lemma 5.1, we have

$$
\begin{aligned}
&K^{-1} J^{1/2} \left(h\tilde{B}\tilde{L}_3\right)^k J^{1/2} K \Phi_{\boldsymbol{\alpha},N}(\boldsymbol{\omega}) = \\
&\qquad \frac{\left(\imath\tilde{B}\right)^k \left\{ \left[\alpha_1 p_2(\boldsymbol{\omega}) - \alpha_2 p_1(\boldsymbol{\omega})\right]^k + Q_{\alpha,k}(\mathbf{p}(\boldsymbol{\omega});N) \right\}}{\left(\frac{|\mathbf{p}|^2(\boldsymbol{\omega})+1}{2}\right)^{k+1}} \left(\frac{\Phi_{\boldsymbol{\alpha},N}(\boldsymbol{\omega})}{(\boldsymbol{\alpha}\cdot\boldsymbol{\omega})^k}\right), \quad (93)
\end{aligned}
$$

where $Q_{\alpha,k}(p;N)$ is defined in (84) and $P_{\alpha,r}(p_1,p_2;N)$ is defined in (85).
Step 3. Since $|\alpha| = \sqrt{2}$ then, for N sufficiently large, there exist a constant C such that $|P_{\alpha,k-\ell}(p_1,p_2;N)| \leq C|p|^{k-\ell}/N$ uniformly in α. Since $|\left(\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p})\right)| \leq 1$ for all $\boldsymbol{\alpha} \in \mathcal{A}$ and $p \in \mathbb{R}^3$ then we have $|Q_{\alpha,k}(p;N)| \leq C|p|^{2k-1}/N$ uniformly

in $\boldsymbol{\alpha} \in \mathcal{A}$ which in turn implies

$$\frac{Q_{\alpha,k}(\mathbf{p}(\boldsymbol{\omega});N)}{\left(\frac{|\mathbf{p}|^2(\boldsymbol{\omega})+1}{2}\right)^{k+1}} = O(N^{-1}) \qquad \text{uniformly in } \boldsymbol{\omega} \in \mathbb{S}^3 \text{ and } \boldsymbol{\alpha} \in \mathcal{A}. \tag{94}$$

Now notice that for k fixed and $d\Omega$ denoting the surface measure on the 3-sphere:

$$\int \frac{|\Phi_{\boldsymbol{\alpha},N}(\boldsymbol{\omega})|^2}{|\boldsymbol{\alpha}\cdot\boldsymbol{\omega}|^k} d\Omega(\boldsymbol{\omega}) \leq a^2(N) \int |\boldsymbol{\alpha}\cdot\boldsymbol{\omega}|^{2(N-k)} d\Omega(\boldsymbol{\omega}) = \frac{a^2(N)}{a^2(N-k)}. \tag{95}$$

Step 4. From Proposition 9.1 in Appendix 2, we have that the integral $\int |\Phi_{\alpha,N}(\boldsymbol{\omega})|^2 / |\left(\boldsymbol{\alpha}\cdot\boldsymbol{\omega}\right)^k| d\Omega(\boldsymbol{\omega}) = O(1)$ for k fixed and $N \to \infty$. Thus using the expression for the inverse of the stereographic projection $p = \mathbf{p}(\boldsymbol{\omega})$ (see equation (130)) and equation (94) we obtain

$$\begin{aligned}
\left\langle \Psi_{\boldsymbol{\alpha},N}, \left(h\tilde{B}L_3\right)^k \Psi_{\boldsymbol{\alpha},N} \right\rangle_{L^2(\mathbb{R}^3)} &= \left(\imath\tilde{B}\right)^k a^2(N) \\
&\cdot \int \exp\left(\imath N \phi_{\boldsymbol{\alpha}}(\boldsymbol{\omega})\right) \frac{\left[\alpha_1 p_2(\boldsymbol{\omega}) - \alpha_2 p_1(\boldsymbol{\omega})\right]^k}{\left(\frac{(|\mathbf{p}|^2(\boldsymbol{\omega})+1)}{2}\right)^{k+1} (\boldsymbol{\alpha}\cdot\boldsymbol{\omega})^k} d\Omega(\boldsymbol{\omega}) + O(N^{-1}), \\
&= \left(\imath\tilde{B}\right)^k a^2(N) \\
&\cdot \int \exp\left(\imath N \phi_{\boldsymbol{\alpha}}(\boldsymbol{\omega})\right) (1-\omega_4) \frac{\left[\alpha_1\omega_2 - \alpha_2\omega_1\right]^k}{(\boldsymbol{\alpha}\cdot\boldsymbol{\omega})^k} d\Omega(\boldsymbol{\omega}) + O(N^{-1}), \qquad (96)
\end{aligned}$$

where the phase function is given by $\phi_{\boldsymbol{\alpha}}(\boldsymbol{\omega}) = -\imath \ln\left(|\boldsymbol{\alpha}\cdot\boldsymbol{\omega}|^2\right)$.

Step 5. Let us denote by $\mathbf{a} = \Re\boldsymbol{\alpha}$ and $\mathbf{b} = -\Im\boldsymbol{\alpha}$. In order to evaluate the integral in (96), we introduce the following coordinates for $\mathbb{S}^3$. Consider two orthonormal vectors $\mathbf{e}_3$ and $\mathbf{e}_4$ such that $\{\mathbf{a},\mathbf{b},\mathbf{e}_3,\mathbf{e}_4\}$ is an orthonormal basis of $\mathbb{R}^4$. Except for a set of measure zero, any element $\boldsymbol{\omega} \in \mathbb{S}^3$ can be written as

$$\boldsymbol{\omega} = \sqrt{1-z_3^2-z_4^2}\cos(\theta)\mathbf{a} + \sqrt{1-z_3^2-z_4^2}\sin(\theta)\mathbf{b} + z_3\mathbf{e}_3 + z_4\mathbf{e}_4 \tag{97}$$

with $\theta \in [0, 2\pi]$ and $z = (z_3, z_4)$ in the unit disk $z_3^2 + z_4^2 < 1$.

6. The surface measure is given by $d\Omega(\boldsymbol{\omega}) = d\theta dz_3 dz_4$. Now we write the integral in (96) as an iterated integral estimating the integration with respect to the variable z by using the stationary phase method. Note that $\phi_{\boldsymbol{\alpha}}(\boldsymbol{\omega}) = -\imath\ln(1-z_1^2-z_2^2)$ is independent of θ. Since $z = 0$ is a non-degenerate critical point of the function $\phi_{\boldsymbol{\alpha}}$ and $\left[\det\left(\frac{N\phi''_{\boldsymbol{\alpha}}(0)}{2\pi\imath}\right)\right]^{-1/2} = \frac{\pi}{N}$, with $\phi''_{\boldsymbol{\alpha}}$ denoting the Hessian matrix of the function $\phi_{\boldsymbol{\alpha}}$ with respect to the variable z, then

$$\begin{aligned}
\left\langle \Psi_{\alpha,N}, \left(h\tilde{B}L_3\right)^k \Psi_{\boldsymbol{\alpha},N} \right\rangle_{L^2(\mathbb{R}^3)} &= \frac{\left(\imath\tilde{B}\right)^k}{2\pi} \int_0^{2\pi} \frac{[1 - a_4\cos(\theta) - b_4\sin(\theta)]}{\exp(\imath k\theta)} \\
&\times \left[\alpha_1\{a_2\cos(\theta) + b_2\sin(\theta)\} - \alpha_2\{a_1\cos(\theta) + b_1\sin(\theta)\}\right]^k d\theta + O(N^{-1}) \\
&= \tilde{B}^k \left[a_1 b_2 - b_1 a_2\right]^k + O(N^{-1}), \qquad (98)
\end{aligned}$$

where we have used the estimate $a^2(N) = \frac{N}{\pi}\left[\frac{1}{2\pi} + O(N^{-1})\right]$ (see Appendix 2, section 9) and the equality $\alpha_1\{a_2\cos(\theta)+b_2\sin(\theta)\} - \alpha_2\{a_1\cos(\theta)+b_1\sin(\theta)\} = \imath[b_1a_2 - a_1b_2]\exp(\imath\theta)$. This leads to the expression on the right side of (81). $\square$

5.2. **Szegö-type theorem for the angular momentum operator.** Using the resolution of the identity given by the coherent states $\Psi_{\boldsymbol{\alpha},N}$ (see equation (146)), Proposition 5.1, and the commutativity of L_3 with the scaled hydrogen atom Hamiltonian S_V we have the following Szegö -type theorem:

Theorem 5.1 (Szegö theorem)**.** *Let $\rho : \mathbb{R} \to \mathbb{R}$ be continuous. Then, for $h = 1/(N+1)$ we have*

$$\lim_{N\to\infty} \frac{1}{d_N} Tr\left(\rho\left(\Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N\right)\right) = \int_{\mathcal{A}} \rho\left(-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right)\, d\mu(\boldsymbol{\alpha}) \tag{99}$$

$$= \int_{\Sigma(-1/2)} \rho\left(-\frac{B}{2}\ell_3(\mathbf{x},\mathbf{p})\right)\, d\mu_L(\mathbf{x},\mathbf{p}) \tag{100}$$

where $\ell_3(\mathbf{x},\mathbf{p}) = x_1p_2 - x_2p_1$ is the component of the classical angular momentum along the direction of the magnetic field $\mathbf{B}(h)$ assigned to the point $(\mathbf{x},\mathbf{p}) \in \Sigma(-1/2)$.

Proof. **Step 1**. As in the proof of Theorem 4.1, we first prove (100) for a polynomial. Consequently, it is enough to show Theorem 5.1 for a monomial $\rho(x) = x^k$. Since L_3 commutes with the Hamiltonian H_V, then L_3 commutes with the projections Π_N which in turn implies $\left(\Pi_N\left(-\frac{B}{2}h\right)L_3\Pi_N\right)^k = \Pi_N\left(-\frac{B}{2}hL_3\right)^k\Pi_N$. Thus we have from Proposition 5.1

$$\begin{aligned}\frac{1}{d_N}Tr\left(\left(\Pi_N\left(-\frac{B}{2}h\right)L_3\Pi_N\right)^k\right) &= \frac{1}{d_N}Tr\left(\Pi_N\left(-\frac{B}{2}hL_3\right)^k\Pi_N\right)\\ &= \int_{\boldsymbol{\alpha}\in\mathcal{A}}\left\langle\Psi_{\boldsymbol{\alpha},N}, \left(-\frac{B}{2}hL_3\right)^k\Psi_{\boldsymbol{\alpha},N}\right\rangle_{L^2(\mathbb{R}^3)} d\mu(\alpha)\\ &= \int_{\boldsymbol{\alpha}\in\mathcal{A}}\left(-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right)^k d\mu(\boldsymbol{\alpha}) + O(N^{-1}),\end{aligned} \tag{101}$$

where we have used that the measure $\int_{\mathcal{A}} d\mu = 1$ and that for any linear operator $T : \mathcal{E}_N \to \mathcal{E}_N$, with $\mathcal{E}_N$ denoting the range of Π_N, we have

$$Tr(T) = d_N \int_{\boldsymbol{\alpha}\in\mathcal{A}} \langle\Psi_{\boldsymbol{\alpha},N}, T\Psi_{\boldsymbol{\alpha},N}\rangle\, d\mu(\boldsymbol{\alpha}). \tag{102}$$

Taking the limit $N \to \infty$ we get the first equality in Theorem 5.1 for monomials and hence for polynomials Q.

Step 2. To extend the result to continuous functions ρ, we note that the operators $A_N =: \Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N$ satisfy $\|A_N\| \leq B/2$, so they are uniformly bounded in N. Similarly, for $(\mathbf{x},\mathbf{p}) \in \Sigma(-1/2)$, we have $|\ell_3(\mathbf{x},\mathbf{p})| \leq 1$, so that $\left|-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right| \leq \frac{B}{2}$. Consequently, we only need to consider continuous functions on the interval $[-B/2, B/2]$. Given $\epsilon > 0$, there exists a polynomial Q_ϵ so that

$$|\rho(x) - Q_\epsilon(x)| \leq \frac{2\epsilon}{B},\ \forall x \in \left[-\frac{B}{2}, \frac{B}{2}\right]. \tag{103}$$

This implies that for all N:

$$\|\rho(A_N) - Q_\epsilon(A_N)\| \leq \epsilon, \tag{104}$$

which in turn implies that for all N:

$$\left| \frac{1}{d_N} Tr\left(\rho\left(A_N\right)\right) - \frac{1}{d_N} Tr\left(Q_\epsilon\left(A_N\right)\right) \right| \leq \epsilon. \tag{105}$$

It also follows from (103) that

$$\left| \int_{\mathcal{A}} \rho\left(-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right)\, d\mu(\boldsymbol{\alpha}) - \int_{\mathcal{A}} Q_\epsilon\left(-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right)\, d\mu(\boldsymbol{\alpha}) \right| \leq \epsilon, \tag{106}$$

since $\int_{\mathcal{A}}\, d\mu(\boldsymbol{\alpha}) = 1$. By (104)–(105), we have

$$\begin{aligned} &\left| \frac{1}{d_N} Tr\left(\rho\left(A_N\right)\right) - \int_{\mathcal{A}} \rho\left(-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right)\, d\mu(\boldsymbol{\alpha}) \right| \\ &\qquad \leq 2\epsilon + \left| \frac{1}{d_N} Tr\left(Q_\epsilon\left(A_N\right)\right) - \int_{\mathcal{A}} Q_\epsilon\left(-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right)\, d\mu(\boldsymbol{\alpha}) \right|. \end{aligned} \tag{107}$$

By step 1 of the proof of Theorem 4.1, the limit as $N \to \infty$ of the second term on the right side of (107) is zero. Since $\epsilon > 0$ is arbitrary, it follows that the limit as $N \to \infty$ of the first term on the left side of (107) is zero establishing the first equality of (100).
Step 3. As for the second equality in (100), we recall that $\mathcal{A}$ can be identified with the unit cotangent bundle $T_1^*(\mathbb{S}^3)$ of the 3-sphere by the map $\sigma(\boldsymbol{\alpha}) = (\Re\boldsymbol{\alpha}, -\Im\boldsymbol{\alpha})$. The inverse of the Moser map $\mathcal{M}^{-1}$ (see Appendix 1) identifies in turn $T_1^*(\mathbb{S}_o^3)$ with the surface of constant energy $\Sigma(-1/2)$ for the Kepler problem. Hence we have $\ell_3(\boldsymbol{\alpha}) = \ell_3(\mathbf{x}, \mathbf{p})$ where $(\mathbf{x}, \mathbf{p}) = \mathcal{M}^{-1} \circ \sigma(\boldsymbol{\alpha})$. Thus the second equality of Theorem 5.1 is consequence of equation (99) and Proposition 5.2 below. □

Proposition 5.2. *The Liouville measure* $d\mu_L$ *on* $\Sigma(-1/2)$ *is the push-forward measure of* $d\tilde{\mu}$ *by the map* $\mathcal{M}^{-1} \circ \sigma$ *with* $d\tilde{\mu}$ *the restriction of* $d\mu$ *to the set* $\tilde{\mathcal{A}} = \{\boldsymbol{\alpha} \in \mathcal{A} \mid \Re\boldsymbol{\alpha} \neq (0,0,0,1)\}$.

Proof. **Step 1**. We have $d\mu$ defined as the normalized SO(4)-invariant measure on $\mathcal{A}$. Note that the push-forward measure $\sigma_*(d\mu)$ is the normalized SO(4)-invariant measure on $T_1^*\mathbb{S}^3$. Let us consider the normalized Liouville measure $d\nu_L$ on $T_1^*\mathbb{S}^3$ obtained from the symplectic form $\sum_{k=1}^4 d\xi_k \wedge d\omega_k \mid_{T^*\mathbb{S}^3}$ that endows $T^*\mathbb{S}^3$ with a symplectic structure. It is given by the restriction to $T^*\mathbb{S}^3$ of the canonical symplectic form $\sum_{k=1}^4 d\xi_k \wedge d\omega_k$ for the ambient $T^*\mathbb{R}^4$. Here $(\boldsymbol{\omega}, \boldsymbol{\xi})$ are canonical coordinates for $T^*\mathbb{R}^4$ and the condition $|\boldsymbol{\omega}| = 1$ specifies the 3-sphere $\mathbb{S}^3$. Note that $d\nu_L$ is SO(4)-invariant. Therefore the measure $\sigma_*(d\mu)$ coincides with $d\nu_L$.
Step 2. On the other hand, the Moser map $\mathcal{M}$ is a canonical transformation (symplectic diffeomorphism) from $T^*\mathbb{R}^3$ onto $T^*\mathbb{S}_o^3$ and $\mathcal{M}(\Sigma(-1/2)) = T_1^*\mathbb{S}_o^3$. Thus the restriction to $T_1^*\mathbb{S}_o^3$ of the measure $d\nu_L$ is actually the push-forward measure of $d\mu_L$ under the Moser map. Since $d\nu_L = \sigma_*(d\mu)$ then the restriction $d\tilde{\mu}$ of $d\mu$ to the set $\tilde{\mathcal{A}}$ must coincide with $(\sigma^{-1} \circ \mathcal{M})_* d\mu_L$. From the equality

$\mu\left(\{\boldsymbol{\alpha} \in \mathcal{A} \mid \Re\boldsymbol{\alpha} = (0,0,0,1)\}\right) = 0$, we have that for any integrable function $f : \Sigma(-1/2) \to \mathbb{R}$:

$$\int_{\Sigma(-1/2)} f(x,p) d\mu_L(x,p) = \int_{\tilde{\mathcal{A}}} f \circ \mathcal{M}^{-1} \circ \sigma(\boldsymbol{\alpha}) d\tilde{\mu} = \int_{\mathcal{A}} \hat{f}(\boldsymbol{\alpha}) d\mu \tag{108}$$

where $\hat{f}$ is an extension of $f \circ \mathcal{M}^{-1} \circ \sigma$ with domain $\tilde{\mathcal{A}}$ to the set $\mathcal{A}$. □

5.3. **Conclusion of the proof of Theorems 1.1 and 1.2.** For any continuous function ρ and $\epsilon > 0$, there is a polynomial Q_ϵ that uniformly approximates ρ on $\left[-\frac{B}{2}, \frac{B}{2}\right]$ as above. It follows from Theorem 4.1 that for any continuous ρ, we have

$$\begin{aligned}
&\left| \frac{1}{d_N} \sum_{j=1}^{d_N} \rho\left(\frac{\tilde{\nu}_{N,j}}{h^2\epsilon(h)}\right) - \frac{1}{d_N} \mathrm{Tr}\rho(A_N) \right| \\
&\quad \leq \frac{1}{d_N} \sum_{j=1}^{d_N} \left| \rho\left(\frac{\tilde{\nu}_{N,j}}{h^2\epsilon(h)}\right) - Q_\epsilon\left(\frac{\tilde{\nu}_{N,j}}{h^2\epsilon(h)}\right) \right| + \frac{1}{d_N} \left|\mathrm{Tr}\rho(A_N) - \mathrm{Tr}Q_\epsilon(A_N)\right| \\
&\qquad + \frac{1}{d_N} \left| \sum_{j=1}^{d_N} Q_\epsilon\left(\frac{\tilde{\nu}_{N,j}}{h^2\epsilon(h)}\right) - \mathrm{Tr}Q_\epsilon(A_N) \right| \leq 2\epsilon + O_{Q_\epsilon}(N^{-\sigma})
\end{aligned} \tag{109}$$

where we are using the notation $O_{Q_\epsilon}(N^{-\sigma})$ to emphasize that the third term $\frac{1}{d_N}\left|\sum_{j=1}^{d_N} Q_\epsilon\left(\frac{\tilde{\nu}_{N,j}}{h^2\epsilon(h)}\right) - \mathrm{Tr}Q_\epsilon(A_N)\right|$ is $O(N^{-\sigma})$ but depends on the polynomial Q_ϵ.

Next ,we keep $\epsilon > 0$ fixed and take $N \to \infty$. Then we use the fact that ϵ is arbitrary to obtain:

$$\lim_{N\to\infty} \frac{1}{d_N} \sum_{j=1}^{d_N} \rho\left(\frac{\tilde{\nu}_{N,j}}{h^2\epsilon(h)}\right) = \lim_{N\to\infty} \frac{1}{d_N} \mathrm{Tr}\rho(A_N) \tag{110}$$

Combining this with Theorem 5.1, we have now proved that for $\epsilon(h) = h^q$, $q > 33/2$ and $h = 1/(N+1)$:

$$\begin{aligned}
\lim_{N\to\infty} \frac{1}{d_N} \sum_{j=1}^{d_N} \rho\left(\frac{\tilde{\nu}_{N,j}}{h^2\epsilon(h)}\right) &= \int_{\mathcal{A}} \rho\left(-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right) d\mu(\boldsymbol{\alpha}) \\
&= \int_{\Sigma(-1/2)} \rho\left(-\frac{B}{2}\ell_3(\mathbf{x},\mathbf{p})\right) d\mu_L(\mathbf{x},\mathbf{p}).
\end{aligned} \tag{111}$$

Since the eigenvalue shifts $E_{N,j}(1/(N+1), B) - E_N(1/(N+1)) = \frac{\tilde{\nu}_{N,j}}{h^2}$ (see (13)), this concludes the proofs of Theorem 1.1 and Theorem 1.2 .

6. Proof of Theorem 1.3.

In order to prove Theorem 1.3, we use an explicit expression for the measure $d\mu$ obtained in [20] in terms of coordinates related to the Kepler problem that we specify below. Then, by doing the integral indicated in equation (5), we obtain equation (6).

We know that the angular momentum vector $\boldsymbol{\ell}$ and the Runge-Lenz vector $\mathbf{a} = \mathbf{p} \times \boldsymbol{\ell} - \frac{\mathbf{x}}{|\mathbf{x}|}$ are integrals of motion for the Kepler problem and satisfy the following relations on the energy surface $\Sigma(-1/2)$:

$$\boldsymbol{\ell}^2 + \mathbf{a}^2 = 1, \tag{112}$$

$$\boldsymbol{\ell} \cdot \mathbf{a} = 0. \tag{113}$$

So we write:

$$\boldsymbol{\ell} = \cos(\psi)\left(\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)\right), \tag{114}$$

$$\mathbf{a} = \sin(\psi)\left(\cos(\gamma)\hat{u} + \sin(\gamma)\hat{v}\right), \tag{115}$$

where $\psi \in (0, \pi/2)$, and (θ, ϕ) are usual spherical coordinates for the two-sphere $\mathbb{S}^2$, with $\phi \in [0, 2\pi]$ and $\theta \in [0, \pi]$. The unit vectors $\hat{\mathbf{u}} = (\sin(\phi), -\cos(\phi), 0)$ and $\hat{\mathbf{v}} = (\cos(\theta)\cos(\phi), \cos(\theta)\sin(\phi), -\sin(\theta))$ generate the orthogonal plane to $\boldsymbol{\ell}$. The parameter $\gamma \in [0, 2\pi]$ takes us around that plane. Note that to cover all possible cases for $|\boldsymbol{\ell}|$ and $|\mathbf{a}|$ we should take $\psi \in [0, \pi/2]$, but we only miss a set of measure zero with the choice $\psi \in (0, \pi/2)$. In this way, the vectors $\boldsymbol{\ell}$ and $\mathbf{a}$ are non-zero. The set $(\psi, \theta, \phi, \gamma)$ gives a parametrization of the set of Kepler orbits on the energy surface $\Sigma(-1/2)$. Then, via the the Moser map $\mathcal{M}$, we obtain a parametrization for the space of oriented geodesics of the 3-sphere $\mathbb{S}^3$ as well.

A parametrization for $\Sigma(-1/2)$, and, consequently, for $\mathcal{A}$ through the Moser map $\mathcal{M}$ and the map σ^{-1} (see (133)), can be obtained by introducing the parameter $\beta \in [0, 2\pi]$ which takes us along the Kepler orbit determined by $\boldsymbol{\ell}$ and $\mathbf{a}$. Namely, consider β such that

$$\frac{\mathbf{x}}{|\mathbf{x}|} = \cos(\beta)\frac{\mathbf{a}}{|\mathbf{a}|} + \sin(\beta)\frac{\boldsymbol{\ell} \times \mathbf{a}}{|\boldsymbol{\ell}||\mathbf{a}|}. \tag{116}$$

Note that $\mathbf{a}/|\mathbf{a}|$ and $\boldsymbol{\ell} \times \mathbf{a}/(|\boldsymbol{\ell}||\mathbf{a}|)$ give an orthonormal basis for the plane of the Kepler orbit in configuration space.

Moreover, it can be shown that, in momentum space $\mathbb{R}^3$, the momentum vector $\mathbf{p}$ is in a circle with center $\frac{\boldsymbol{\ell} \times \mathbf{a}}{|\boldsymbol{\ell}|^2}$ and radius $1/|\boldsymbol{\ell}|$. Namely, the coordinate $\mathbf{p}$ satisfies the following equation

$$\mathbf{p} = \frac{\boldsymbol{\ell} \times \mathbf{a}}{|\boldsymbol{\ell}|^2} + \frac{\boldsymbol{\ell} \times \mathbf{x}}{|\boldsymbol{\ell}|^2|\mathbf{x}|}. \tag{117}$$

Thus from equations (116) and (117) we have

$$\mathbf{p} = -\sin(\beta)\frac{\mathbf{a}}{|\mathbf{a}||\boldsymbol{\ell}|} + \left(|\mathbf{a}| + \cos(\beta)\right). \frac{\boldsymbol{\ell} \times \mathbf{a}}{|\mathbf{a}||\boldsymbol{\ell}|^2} \tag{118}$$

From equations (116), (118), the relation $|\mathbf{x}| = 2/(|\mathbf{p}|^2 + 1)$, the Moser map (see equations (128) and (129)) and the map σ^{-1}, we obtain a parametrization for $\mathcal{A}$ based on the five real parameters $W = (\psi, \theta, \phi, \gamma, \beta)$. Namely, we can obtain $(\boldsymbol{\omega}(W), \boldsymbol{\xi}(W)) \in T^*\mathbb{S}^3_0$ (see equations (4.35), (4.36) and (4.39) in reference [20]) such that $\boldsymbol{\alpha} = \boldsymbol{\omega}(W) - \imath\boldsymbol{\xi}(W)$, with $\boldsymbol{\alpha} \in \tilde{\mathcal{A}}$.

In addition, we can give a parametrization for the elements of the matrix representation by 4×4 matrices of the group $SO(4)$. For $g \in SO(4)$, we construct the matrix

$$\begin{aligned}\mathcal{R}(g) &= (\boldsymbol{\omega}(W), \boldsymbol{\xi}(W), \cos(\delta)\boldsymbol{\eta}(W) + \sin(\delta)\boldsymbol{\chi}(W)\,, \\ &\quad -\sin(\delta)\boldsymbol{\eta}(W) + \cos(\delta)\boldsymbol{\chi}(W))\,, \end{aligned} \tag{119}$$

from column vectors given by the vectors $\boldsymbol{\eta}(W)$ and $\boldsymbol{\chi}(W)$ that are two orthonormal vectors generating the plane orthogonal to the vectors $\boldsymbol{\omega}(W)$ and $\boldsymbol{\xi}(W)$. The parameter $\delta \in [0, 2\pi]$ takes us around the plane generated by $\{\boldsymbol{\eta}(W), \boldsymbol{\chi}(W)\}$.

The normalized Haar measure $d\mu_H$ for the group SO(4) can be computed from the parametrization indicated in equation (119). After a long computation (see reference [20]), we obtain:

$$d\mu_H = \frac{1}{(2\pi)^4} \frac{\cos^2(\psi)\sin(\psi)\sin(\theta)}{1+\sin(\psi)\cos(\beta)} d\psi d\theta d\phi d\gamma d\beta d\delta. \tag{120}$$

Integrating the measure $d\mu_H$ with respect to δ, we obtain a normalized SO(4) invariant measure $d\mu$ parametrized by W:

$$d\mu = \frac{1}{(2\pi)^3} \frac{\cos^2(\psi)\sin(\psi)\sin(\theta)}{1+\sin(\psi)\cos(\beta)} d\psi d\theta d\phi d\gamma d\beta. \tag{121}$$

Moreover, integrating $d\mu$ with respect to β, we obtain the normalized SO(4)-invariant measure $d\mu_\Gamma$ on the space of oriented geodesics:

$$d\mu_\Gamma = \frac{1}{(2\pi)^2} \cos(\psi)\sin(\psi)\sin(\theta) d\psi d\theta d\phi d\gamma. \tag{122}$$

Now we want to do the integral appearing on the right hand side of equation (5). Since the function $\rho\left(-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right) = \rho\left(-\frac{B}{2}\cos(\psi)\cos(\theta)\right)$ depends only on the variables ψ and θ, we integrate out the variables ϕ and γ in $d\mu_\Gamma$ in (122) to obtain the measure $d\tilde{\mu}_\Gamma = \cos(\psi)\sin(\psi)\sin(\theta) d\psi d\theta$. Making the change of variables $u = \cos(\psi)\cos(\theta)$, $v = \cos(\psi)\sin(\theta)$, with (u, v) in the half-disk $u^2 + v^2 \leq 1$, $v \geq 0$, we have

$$\begin{aligned}\int_{\mathcal{A}} \rho\left(-\frac{B}{2}\ell_3(\boldsymbol{\alpha})\right)\, d\mu(\boldsymbol{\alpha}) &= \int_{\psi=0}^{\pi/2}\int_{\theta=0}^{\theta=\pi} \rho\left(-\frac{B}{2}\cos(\psi)\cos(\theta)\right) d\tilde{\mu}_\Gamma(\psi,\theta), \\ &= \int_{u=-1}^{u=1} \rho\left(-\frac{B}{2}u\right)\int_{v=0}^{v=\sqrt{1-u^2}} \frac{v}{\sqrt{u^2+v^2}}\; dvdu, \\ &= \int_{-1}^{1} \rho\left(-\frac{B}{2}u\right)[1-|u|\,]\; du. \end{aligned} \tag{123}$$

This completes the proof of Theorem 1.3.

7. Alternate description of the limit measure in Theorem 1.3.

The proof of Theorem 1.3 presented in section 6 is based on the geometric description of the Kepler orbits on $\Sigma(-1/2)$ afforded by the Moser map. In this section, we present an alternate proof based on a more detailed analysis of the eigenvalue clusters $\mathcal{C}_N$. Although this proof is more direct and shorter, it does not reveal the full geometric content of Theorems 1.1 and 1.2.

7.1. **Eigenvalue approximation.** From equation (75), we know that, for N sufficiently large, the $d_N = (N+1)^2$ eigenvalues of $S_V(\lambda)$ inside the cluster $\mathcal{C}_N$ around E_N are actually in an interval of size $O(h^2\epsilon(h))$. In this section, we prove that if we take $\sigma > 1$ (i.e. $q > 19$), then those eigenvalues are in sub-clusters around the eigenvalues of the operator $\Pi_N \left(-\frac{1}{2}\Delta - \frac{1}{|\mathbf{x}|} - \frac{\lambda(h,B)}{2} L_3\right) \Pi_N$ inside the cluster $\mathcal{C}_N$. That is, the eigenvalues cluster around the numbers $E_N - \frac{\lambda(h,B)}{2} m = E_N - \frac{B}{2} h^3\epsilon(h)m$, with $m \in \mathbb{Z}$ and $|m| \leq N$.

Proposition 7.1. *Assume $\sigma > 1$. Then, for N sufficiently large, the spectrum of $S_V(\lambda)$ inside the cluster $\mathcal{C}_N$ consists of a union of sub-clusters $\mathcal{C}_{N,m}$ of eigenvalues around $E_N - \frac{B}{2}h^3\epsilon(h)m$, with $m \in \mathbb{Z}$ and $|m| \leq N$. Moreover, each sub-cluster $\mathcal{C}_{N,m}$ contains $N+1-|m|$ eigenvalues of $S_V(\lambda)$ and has size $h^{\sigma+2}\epsilon(h)$.*

Proof. 1. The eigenvalues of the operator $\Pi_N \left(-\frac{B}{2}hL_3\right)\Pi_N$ are $-\frac{B}{2}\frac{m}{N+1}$, $m \in \mathbb{Z}$ and $|m| \leq N$, with multiplicity $N+1-|m|$. They are uniformly distributed with a distance $\frac{B}{2}\frac{1}{N+1} = O(N^{-1})$ between consecutive eigenvalues. Since the error term in equation (75) is a bounded operator whose norm is $O(N^{-\sigma})$, $\sigma > 1$, one can show that if the distance between $w \in \mathbb{C}$ and the spectrum of $\Pi_N \left(-\frac{B}{2}hL_3\right)\Pi_N$ is greater than $O(N^{-\sigma})$, then w is in the resolvent set of $\frac{P_N(S_V(\lambda)-E_N)P_N}{h^2\epsilon(h)}$. Namely, the spectrum of $\frac{P_N(S_V(\lambda)-E_N)P_N}{h^2\epsilon(h)}$ is contained in the union of the disjoint closed intervals $[-\frac{B}{2}\frac{m}{N+1} - O(N^{-\sigma}), -\frac{B}{2}\frac{m}{N+1} + O(N^{-\sigma})]$, $|m| \leq N$.
2. Let $\Gamma_{N,m}$ be the circle with center $-\frac{B}{2}\frac{m}{N+1}$ and radius $\frac{B}{8}\frac{1}{N+1}$, $|m| \leq N$. Let us denote by $\Pi_{N,m}$ and $P_{N,m}$ the Riez projectors asociated to the spectrum of $\Pi_N \left(-\frac{B}{2}hL_3\right)\Pi_N$ and $\frac{P_N(S_V(\lambda)-E_N)P_N}{h^2\epsilon(h)}$ inside the circle $\Gamma_{N,m}$, respectively. Then we have

$$\begin{aligned}\|P_{N,m} - \Pi_{N,m}\| = \Bigg\| \frac{1}{2\pi\imath}\int_{\Gamma_{N,m}} &\left[\left(\frac{P_N(S_V(\lambda)-E_N)P_N}{h^2\epsilon(h)} - \mathbf{z}\right)^{-1}\right. \\ &\left. - \left(\Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N - \mathbf{z}\right)^{-1}\right] d\mathbf{z}\Bigg\|. \end{aligned} \tag{124}$$

Note that both $\left\|\left(\frac{P_N(S_V(\lambda)-E_N)P_N}{h^2\epsilon(h)} - \mathbf{z}\right)^{-1}\right\|$ and $\left\|\left(\Pi_N\left(-\frac{B}{2}hL_3\right)\Pi_N - \mathbf{z}\right)^{-1}\right\|$ are $O(N)$. Thus from equations (75) and (124), we obtain that the norm $\|P_{N,m} - \Pi_{N,m}\| = O(N^{1-\sigma})$, which in turn implies that, for N sufficiently large, $\|P_{N,m} - \Pi_{N,m}\| < 1$. Hence the dimension of the range of the projectors $P_{N,m}$ and $\Pi_{N,m}$ is the same, namely equal to $N+1-|m|$. □

Proposition 7.1 implies the following eigenvalue approximation.

Proposition 7.2. *Assume $\sigma > 1$. The eigenvalues of $S_V(\lambda)$ inside the cluster $\mathcal{C}_N$ around E_N can be written in the following way: For N sufficiently large and $m = -N, \ldots, N$, we have*

$$E_{N,m,k} = E_N - \frac{B}{2}\frac{m}{N+1}h^2\epsilon(h) + G(N,m,k) \tag{125}$$

where, given m*, the index* $k = 1, \ldots, N+1-|m|$ *and the error term* $G(N,m,k) = O(N^{-\sigma})h^2\epsilon(h)$.

Remark 3. A similar expansion was obtained by Karasev and Novikova [13] using different methods.

7.2. **Alternate proof of Theorem 1.3.** Using Proposition 7.2, we can prove Theorem 1.3 when ρ is a polynomial on a fixed compact interval. Then Theorem 1.3 can be shown for ρ continuous with a uniform approximation argument.

The averages appearing in the left hand side of equation (6) can be written, for N sufficiently large, as:

$$\begin{aligned}
&\frac{1}{d_N}\sum_{j=1}^{d_N}\rho\left(\frac{E_{N,j}(1/(N+1),B) - E_N(1/(N+1))}{\epsilon(1/(N+1))}\right) \\
&\quad = \frac{1}{d_N}\sum_{m=-N}^{m=N}\sum_{k=1}^{N+1-|m|}\rho\left(-\frac{B}{2}\frac{m}{N+1} + \frac{G(N,m,k)}{h^2\epsilon(h)}\right) \\
&\quad = \frac{1}{d_N}\sum_{m=-N}^{m=N}(N+1-|m|)\,\rho\left(-\frac{B}{2}\frac{m}{N+1}\right) + O(N^{-\sigma}) \\
&\quad = \sum_{m=-(N+1)}^{m=N}\left(1-\frac{|m|}{N+1}\right)\rho\left(-\frac{B}{2}\frac{m}{N+1}\right)\frac{1}{N+1} + O(N^{-\sigma}). \qquad (126)
\end{aligned}$$

To obtain the second equality, we have used the mean value theorem, that ρ' is bounded on a fixed compact interval, and the fact that $\sum_{m=-N}^{m=N}(N+1-|m|) = d_N$. The first term in equation (126) can be thought of as a Riemann sum associated to $\int_{[-1,1]}\rho(-\frac{B}{2}u)\,(1-|u|)\,du$ with the partition $\left\{-1, \frac{-N}{N+1}, \ldots, \frac{N}{N+1}, 1\right\}$ of the interval $[-1,1]$. Taking the limit $N \to \infty$ we conclude the proof of Theorem 1.3.

8. Appendix 1: The Kepler problem and the Moser map.

We review the Moser map as a regularization of the Kepler problem. The Kepler problem in $\mathbb{R}^3 - \{0\}$ is defined as the Hamiltonian $G : T^*(\mathbb{R}^3 - \{0\}) \to \mathbb{R}$ given by

$$G(\mathbf{x},\mathbf{p}) = \frac{|\mathbf{p}|^2}{2} - \frac{1}{|\mathbf{x}|}. \qquad (127)$$

The symmetries of the Kepler problem are given by conservation of the angular momentum vector $\boldsymbol{\ell} = \mathbf{x}\times\mathbf{p}$ and the Runge-Lenz vector $\mathbf{a} = \mathbf{p}\times\boldsymbol{\ell} - \frac{\mathbf{x}}{|\mathbf{x}|}$. For negative energy, they imply that the orbits in configuration space are either ellipses ($|\boldsymbol{\ell}| \neq 0$) or contained in segments of straight lines with the origin $\mathbf{x} = 0$ as an end ($\boldsymbol{\ell} = 0$, collision orbits). The symmetries $\boldsymbol{\ell}$ and $\mathbf{a}$ also imply that the orbits in momentum space are either circles ($|\boldsymbol{\ell}| \neq 0$) or half lines passing through the origin ($\boldsymbol{\ell} = 0$).

We now restrict ourselves to the energy surface $\Sigma(-1/2) = \{(\mathbf{x},\mathbf{p}) \in T^*(\mathbb{R}^3 - \{0\}) \mid G(\mathbf{x},\mathbf{p}) = -1/2\}$. We first note that the vectors $\boldsymbol{\ell}$ and $\mathbf{a}$ satisfy the relation $|\boldsymbol{\ell}|^2 + |\mathbf{a}|^2 = 1$ on $\Sigma(-1/2)$ which, in particular, implies that $|\ell_3| \leq 1$ on $\Sigma(-1/2)$ with $\boldsymbol{\ell} = (\ell_1, \ell_2, \ell_3)$.

Following J. Moser [16], we consider the stereographic projection $S : \mathbb{R}^3 \to \mathbb{S}^3_o$, where $\mathbb{S}^3_o$ denotes the 3-sphere with the north pole removed. The map S is given by the assignment $\mathbf{p} = (p_1, p_2, p_3) \to \boldsymbol{\omega} = (\omega_1, \omega_2, \omega_3, \omega_4)$ with

$$\begin{aligned} \omega_i &= \left(\frac{2}{|\mathbf{p}|^2 + 1}\right) p_i, \quad i = 1, 2, 3, \quad |\mathbf{p}|^2 = p_1^2 + p_2^2 + p_3^2 \\ \omega_4 &= \frac{|\mathbf{p}|^2 - 1}{|\mathbf{p}|^2 + 1}. \end{aligned} \tag{128}$$

The stereographic projection S maps the circles in momentum space mentioned above to great circles on $\mathbb{S}^3$ that do not contain the north pole. The image of a half line passing through the origin in momentum space under the stereographic projection is contained in a great circle passing through the north pole.

Moser [16] extended the stereographic projection S to a map $\mathcal{M} : T^*(\mathbb{R}^3) \to T^*(\mathbb{S}^3_o)$. The Moser map $\mathcal{M}$ maps the point $(\mathbf{x}, \mathbf{p})$ to $(\boldsymbol{\omega}, \boldsymbol{\xi})$ under the requirement that $\mathcal{M}^*(\boldsymbol{\xi} \cdot d\boldsymbol{\omega}) = \mathbf{y} \cdot d\mathbf{p}$ with $\mathbf{y} = -\mathbf{x}$. Thus the Moser map is a canonical transformation $\mathcal{M}^*(d\boldsymbol{\xi} \wedge d\boldsymbol{\omega}) = d\mathbf{p} \wedge d\mathbf{x}$ given explicitly by (128) and the following equations:

$$\begin{aligned} \xi_i &= \frac{|\mathbf{p}|^2 + 1}{2} y_i - (\mathbf{y} \cdot \mathbf{p}) p_i, \quad i = 1, 2, 3 \\ \xi_4 &= \mathbf{y} \cdot \mathbf{p}. \end{aligned} \tag{129}$$

The inverse map $\mathcal{M}^{-1}$ is determined by the equations

$$\begin{aligned} p_i &= \frac{\omega_i}{1 - \omega_4}, \quad i = 1, 2, 3 \\ y_i &= (1 - \omega_4)\xi_i + \xi_4 \omega_i. \quad i = 1, 2, 3 \end{aligned} \tag{130}$$

The Moser map $\mathcal{M}$ transforms the Hamiltonian flow of the Kepler problem on the energy surface $\Sigma(-1/2)$ into the geodesic flow on the 3-sphere under the time re-parametrization $s \mapsto t$ given by the equation

$$\frac{d}{ds} = |\mathbf{x}| \frac{d}{dt}. \tag{131}$$

Considering the geodesic flow on $T^*(\mathbb{S}^3)$ (i.e. including the north pole) corresponds to extending the collision orbits by making the convention that the particle is reflected back to its trajectory after a collision. Thus all of the orbits on the energy surface $\Sigma(-1/2)$ are periodic orbits with period 2π. See reference [16] for details.

9. Appendix 2: Coherent states for the hydrogen atom.

We review the construction and properties of the coherent states that form an over-complete set in the eigenspace $\mathcal{E}_N$ of the hydrogen atom Hamiltonian $S_V = -\frac{1}{2}\Delta - \frac{1}{|\mathbf{x}|}$ corresponding to the eigenvalue $E_N = -1/(2(N+1)^2)$, $N \in \mathbb{N}^*$.

We begin by defining the null quadric $\mathbb{Q}^n$, with $n \geq 1$ a natural number, as the set

$$\begin{aligned}\mathbb{Q}^n &= \left\{\boldsymbol{\alpha} = (\alpha_1 \ldots, \alpha_{n+1}) \in \mathbb{C}^{n+1} \mid \alpha_1^2 + \ldots + \alpha_{n+1}^2 = 0\right\}, \\ &= \left\{\boldsymbol{\alpha} \in \mathbb{C}^{n+1} \mid |\Re\boldsymbol{\alpha}| = |\Im\boldsymbol{\alpha}|, \ \Re\boldsymbol{\alpha} \cdot \Im\boldsymbol{\alpha} = 0\right\}. \end{aligned} \tag{132}$$

The null quadric $\mathbb{Q}^n$ with the origin removed can be identified with the cotangent bundle of the n-sphere $T^*\mathbb{S}^n$ with the zero section removed through the following map :

$$\begin{aligned}\sigma &: \mathbb{Q}^n - \{0\} \to T^*\mathbb{S}^n - \{0\} \\ \sigma(\boldsymbol{\alpha}) &= \left(-\frac{\Re\boldsymbol{\alpha}}{|\Re\boldsymbol{\alpha}|}, \Im\boldsymbol{\alpha}\right). \end{aligned} \tag{133}$$

Let $\mathcal{A}$ be the $2n-1$ real-dimensional subset of $\mathbb{Q}^n$ defined by

$$\mathcal{A} = \{\boldsymbol{\alpha} \in \mathbb{C}^{n+1} \mid |\Re\boldsymbol{\alpha}| = |\Im\boldsymbol{\alpha}| = 1, \ \Re\boldsymbol{\alpha} \cdot \Im\boldsymbol{\alpha} = 0\} \subset \mathbb{Q}^n. \tag{134}$$

This provides a parametrization of the unit cotangent bundle $T_1^*\mathbb{S}^n$ of the n-sphere $\mathbb{S}^n$ under the map $\boldsymbol{\alpha} \to (\Re\boldsymbol{\alpha}, -\Im\boldsymbol{\alpha})$. There is a $SO(n+1)$-rotationally invariant probability measure on $\mathcal{A}$ that we denote by μ.

Coherent states on $\mathbb{S}^n$ have the form

$$\Phi_{\boldsymbol{\alpha},N}(\boldsymbol{\omega}) = a(N)(\boldsymbol{\alpha} \cdot \boldsymbol{\omega})^N, \ \boldsymbol{\omega} \in \mathbb{S}^n, \ \alpha \in \mathcal{A}, \ N \in \mathbb{N}^*. \tag{135}$$

The coefficient $a(N) \sim N^{(n-1)/2}$ is fixed by the requirement that the $L^2(\mathbb{S}^n)$-norm of $\Phi_{\boldsymbol{\alpha},N}$ is equal to one, see [18, (2.11)]. The states $\Phi_{\boldsymbol{\alpha},N}$ are spherical harmonics i.e they are restrictions to the sphere $\mathbb{S}^n$ of harmonic homogeneous polynomilas of degree N in the ambient $\mathbb{R}^{n+1}$. Hence they are eigenstates of the normalized spherical Laplacian $\Delta_{\mathbb{S}^n}$ with eigenvalue $\left(N + \frac{n-1}{2}\right)^2$. Note that $\Delta_{\mathbb{S}^n}$ is the usual positive spherical Laplacian on the n-sphere with eigenvalues $N(N-1) + nN$, $N \in \mathbb{N}^*$, shifted by the constant $(n-1)^2/4$. The entire family $\{\Phi_{\boldsymbol{\alpha},N}(\boldsymbol{\omega}) \mid \boldsymbol{\alpha} \in \mathcal{A}\}$ is over complete and spans the eigenspace $\mathcal{L}_N$ of $\Delta_{\mathbb{S}^n}$ with eigenvalue $(N + \frac{n-1}{2})^2$ in the following sense: Let P_N^S be the projector from $L^2(\mathbb{S}^n)$ onto $\mathcal{L}_N$. Then for all $\Psi \in L^2(\mathbb{S}^n)$

$$P_N^S\Psi = d_n(N) \int_{\mathcal{A}} \langle \Phi_{\boldsymbol{\alpha},N}, \Psi \rangle_{L^2(\mathbb{S}^n)} \ \Phi_{\boldsymbol{\alpha},N} \, d\mu(\boldsymbol{\alpha}). \tag{136}$$

where $d_n(N)$ denotes the dimension of $\mathcal{L}_N$. The following notation for the projector P_N^S in equation (136) is also used:

$$P_N^S = d_n(N) \int_{\mathcal{A}} |\Phi_{\boldsymbol{\alpha},N}\rangle\langle\Phi_{\boldsymbol{\alpha},N}| \, d\mu(\boldsymbol{\alpha}). \tag{137}$$

We note that the state $\Phi_{\boldsymbol{\alpha},N}$ concentrates on the great circle $\{\boldsymbol{\omega} \in \mathbb{S}^n \mid |\boldsymbol{\alpha} \cdot \boldsymbol{\omega}| = 1\}$ generated by $\boldsymbol{\alpha}$ as $N \to \infty$.

The normalization factor $a(N)$ can be estimated by the stationary phase method. Here we show an estimate of the error $O(N^{-1})$ which improves the estimate $O(N^{-1/2})$ obtained in [18, (2.11)].

Proposition 9.1. *For N large, we have*

$$a^2(N) = \left(\frac{N}{\pi}\right)^{\frac{n-1}{2}} \left[\frac{1}{2\pi} + O(N^{-1})\right]. \tag{138}$$

Proof. The proof follows a similar procedure as the one used to show (96). Namely, given α in $\mathcal{A}$, let us consider the following coordinates for the n-sphere. Consider orthonormal vectors $\mathbf{e}_3, \ldots, \mathbf{e}_{n+1}$ such that $\{\Re\boldsymbol{\alpha}, \Im\boldsymbol{\alpha}, \mathbf{e}_3, \ldots \mathbf{e}_{n+1}\}$ is an orthonormal basis of $\mathbb{R}^{n+1}$. Then for almost every element $\boldsymbol{\omega} \in \mathbb{S}^n$ we can write $\boldsymbol{\omega} = \sqrt{1-|\mathbf{z}|^2}\cos(\theta)\Re\boldsymbol{\alpha} + \sqrt{1-|\mathbf{z}|^2}\sin(\theta)\Im\boldsymbol{\alpha} + z_3\mathbf{e}_3 + \ldots + z_{n+1}\mathbf{e}_{n+1}$ with $\theta \in [0, 2\pi]$ and $\mathbf{z} = (z_3, \ldots, z_{n+1})$ such that $|\mathbf{z}|^2 < 1$. The volume form in these coordinates is $d\Omega(\boldsymbol{\omega}) = dz_3 \cdots dz_{n+1} d\theta$. Thus

$$\int |\alpha \cdot \boldsymbol{\omega}|^{2N}\, d\Omega(\boldsymbol{\omega}) = \int_0^{2\pi} \int_{\mathbf{z}} \exp\left(\imath N \phi_{\boldsymbol{\alpha}}(\mathbf{z})\right) dz_3 \cdots dz_{n+1} d\theta$$
$$= 2\pi \left[\det\left(\frac{\phi''_{\boldsymbol{\alpha}}(0)N}{2\pi\imath}\right)\right]^{-1/2} + O(N^{-\frac{n+1}{2}}) = \left(\frac{\pi}{N}\right)^{\frac{n-1}{2}} \left[2\pi + O(N^{-1})\right] \quad (139)$$

where $\phi_{\boldsymbol{\alpha}}(\mathbf{z}) = -\imath \ln(1-|\mathbf{z}|^2)$ and $\phi''_{\boldsymbol{\alpha}}(0)$ denotes the $(n-1) \times (n-1)$ Hessian matrix of $\phi_{\boldsymbol{\alpha}}$ evaluated at the critical point $\mathbf{z} = 0$ such that $\det\left(\frac{\phi''_{\boldsymbol{\alpha}}(0)N}{2\pi\imath}\right) = \left(\frac{N}{\pi}\right)^{n-1}$. $\square$

Let us now restrict ourselves to the $n = 3$ case. The coherent states functions in both momentum and configuration space, constructed from the coherent states for the 3-sphere defined in equation (135), were considered by Thomas and Villegas-Blas [18]. The construction uses a transformation due to V. Fock [7] and described in reference [3].

The coherent states functions in momentum space $\hat{\Psi}_{\alpha,N}$ are defined as a suitable dilation of $\Phi_{\boldsymbol{\alpha},N}(\boldsymbol{\omega}(\mathbf{p}))$, where $\boldsymbol{\omega}(\mathbf{p})$ is given by the stereographic projection map S defined in equations (128), times a factor that involves not only the square root of the corresponding Jacobian but also a factor $2/(|\mathbf{p}|^2+1)$, which is precisely $|\mathbf{x}|$ on the energy surface $\Sigma(-1/2)$ of the Kepler problem. In addition, the factor $|\mathbf{x}|$ is exactly the factor used in the time reparametrization for the regularization of the Kepler problem. We still have the isometry property $\|\hat{\Psi}_{\alpha,N}(\mathbf{p})\| = 1$ due to the Virial Theorem. See reference [3] for details.

The coherent states $\hat{\Psi}_{\alpha,N}$ have the following explicit form. For any $\alpha \in \mathcal{A}$, we define

$$\hat{\Psi}_{\alpha,N}(\mathbf{p}) = a(N)(N+1)^{3/2}\left(\frac{2}{(N+1)^2|\mathbf{p}|^2+1}\right)^2 (\boldsymbol{\alpha} \cdot \boldsymbol{\omega}((N+1)\mathbf{p}))^N,\ p \in \mathbb{R}^3. \quad (140)$$

The coherent states $\hat{\Psi}_{\boldsymbol{\alpha},N}$ are in $L^2(\mathbb{R}^3)$.

To obtain the formula for the coherent states in configuration space, we use the Fourier transform given by

$$\mathcal{F}(g)(\mathbf{p}) = \frac{1}{(2\pi)^{3/2}} \int e^{-\imath \mathbf{p}\cdot\mathbf{x}}\, g(\mathbf{x})\, d\mathbf{x}, \quad (141)$$

that is a unitary operator on $L^2(\mathbb{R}^3)$. The inverse Fourier transforms $\Psi_{\boldsymbol{\alpha},N}$ of the coherent states $\hat{\Psi}_{\boldsymbol{\alpha},N}$ are eigenfunctions of S_V with eigenvalue $E_N = -\frac{1}{2(N+1)^2}$. For fixed N and $\boldsymbol{\alpha} \in \mathcal{A}$, they form a normalized (but not orthogonal) overdetermined basis of the $(N+1)^2$-dimensional eigenspace $\mathcal{E}_N \subset L^2(\mathbb{R}^3)$ of the hydrogen atom Hamiltonian with eigenvalue E_N. These coherent states functions in configuration space have the form

$$\begin{aligned}\Psi_{\boldsymbol{\alpha},N}(\mathbf{x}) &= \frac{a(N)(N+1)^{3/2}}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d\mathbf{p}\; e^{i\mathbf{x}\cdot\mathbf{p}} \left\{ \left(\frac{2}{(N+1)^2|\mathbf{p}|^2+1} \right)^2 \right. \\ &\quad \left. \times \left(\boldsymbol{\alpha}\cdot\boldsymbol{\omega}((N+1)\mathbf{p})\right)^N \right\}. \end{aligned} \tag{142}$$

Note that the coherent states $\Psi_{\boldsymbol{\alpha},N}$ can be written as

$$\Psi_{\boldsymbol{\alpha},N} = \mathcal{F}^{-1} D_{r_N} J^{1/2} K \Phi_{\boldsymbol{\alpha},N} \tag{143}$$

where $r_N = N+1$, $K : L^2(S^3) \to L^2(\mathbb{R}^3)$ is the unitary operator

$$K(f)(\mathbf{p}) = \left(\frac{2}{|\mathbf{p}|^2+1} \right)^{3/2} f(\boldsymbol{\omega}(\mathbf{p})) \tag{144}$$

and J is the self-adjoint multiplicative operator acting in momentum space $J : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ given by

$$J(\hat{\Psi})(\mathbf{p}) = \frac{2}{|\mathbf{p}|^2+1} \hat{\Psi}.(\mathbf{p}) \tag{145}$$

We remark that $d\Omega(\boldsymbol{\omega}) = \left(\frac{2}{|\mathbf{p}|^2+1}\right)^3 d\mathbf{p}$ under the stereographic projection (128). Thus the factor $\left(\frac{2}{|\mathbf{p}|^2+1}\right)^{3/2}$ defining the operator K is the square root of the Jacobian $\left(\frac{2}{|\mathbf{p}|^2+1}\right)^3$.

Let μ be the normalized SO(4)-invariant measure on $\mathcal{A}$. The orthogonal projector Π_N onto the eigenspace $\mathcal{E}_N$ can be written as

$$\Pi_N = (N+1)^2 \int_{\mathcal{A}} |\Psi_{\boldsymbol{\alpha},N}\rangle\langle\Psi_{\boldsymbol{\alpha},N}|\; d\mu(\boldsymbol{\alpha}). \tag{146}$$

Equation (146) expresses the fact that the system of coherent states $\{\Psi_{\boldsymbol{\alpha},N}\}_{\boldsymbol{\alpha}\in\mathcal{A}}$ gives a resolution of the identity for the eigenspace $\mathcal{E}_N$.

In reference [18], it is shown that the coherent state $\Psi_{\boldsymbol{\alpha},N}$ concentrates on the Kepler orbit determined by $\boldsymbol{\alpha}$ as $N \to \infty$ in the case when such an orbit is an ellipse.

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CONACYT Research Fellow - Departamento de Matemáticas, Universidad de Sonora,
E-mail address: misaelave@mat.uson.mx

Department of Mathematics, University of Kentucky, Lexington, Kentucky 40506-0027, USA
E-mail address: peter.hislop@uky.edu

Universidad Nacional Autónoma de México, Instituto de Matemáticas, Unidad Cuernavaca, Mexico and Unidad Mixta Internacional (UMI) del CNRS, "Laboratorio Solomon Lefschetz".
E-mail address: villegas@matcuer.unam.mx