Asymptotics of Rydberg States for the Hydrogen Atom

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ABSTRACT

The asymptotics of Rydberg states, i.e., highly excited bound states of the hydrogen atom Hamiltonian, and various expectations involving these states are investigated. We show that suitable linear combinations of these states, appropriately rescaled and regarded as functions either in momentum space or configuration space, are highly concentrated on classical momentum space or configuration space Kepler orbits respectively, for large quantum numbers. Expectations of momentum space or configuration space functions with respect to these states are related to time-averages of these functions over Kepler orbits.

Section I. Introduction

Let H be the hydrogen atom Hamiltonian $H = -\frac{1}{2}\Delta - |\mathbf{x}|^{-1}$ acting in $L^2(\mathbf{R}^3)$, with Δ the 3-dimensional Laplacian. The purpose of this article is to investigate the asymptotics of Rydberg states of the Hamiltonian H, i.e., states with large principal quantum number k, and to investigate the asymptotics of various expectations involving these states, as k goes to infinity.

We begin by indicating the sort of asymptotics that suitable linear combinations of these Rydberg states might exhibit. The eigenvalues of H are given in terms of the principal quantum number k by $E_k = -\frac{1}{2}(k+1)^{-2}$, $k = 0, 1, 2, \ldots$; the eigenvalue E_k has degeneracy $(k+1)^2$. By the virial theorem, one knows that for an eigenstate of energy E, the expected value for the kinetic energy is $-E$, and the expected value of the potential energy $-|\mathbf{x}|^{-1}$ is $2E$. The same is true for classical Kepler bounded orbits (excluding collision orbits), if expected values are replaced by time averages. These facts suggest that in the momentum space representation, the eigenfunctions corresponding to $E = E_k$ have most of their mass within a distance $\sim 1/(k+1)$ of the origin and in configuration space, the eigenfunctions have most of their mass at a distance $\sim (k+1)^2$ from the origin. Thus to see interesting asymptotics, an eigenfunction $\hat{\Psi}_k$ corresponding to the eigenvalue E_k and in the momentum representation should be rescaled by a factor $O(k^{-1})$, i.e., $\hat{\Psi}_k(\mathbf{p}) \mapsto (k+1)k^{-3/2}\hat{\Psi}(\mathbf{p}/(k+1))$. In configuration space, the inverse Fourier transform of $\hat{\Psi}_k$, Ψ_k, should be rescaled by a factor $O(k^2)$, $\Psi_k(\mathbf{x}) \mapsto (k+1)^3\Psi_k((k+1)^2\mathbf{x})$. The precise scaling we employ is given in Sections 2 and 3.

Indeed, we show for a set of eigenfunctions spanning the bound states, $\{\hat{\Psi}_{\alpha,k}\}$ in momentum space, $\{\Psi_{\alpha,k}\}$ in configuration space, and parametrized by k and another continuous variable α taking values in a five dimensional manifold–in fact the unit cotangent space of the three dimensional sphere $\mathcal{S}^3$– that for fixed α, the states $k^{-3/2}\hat{\Psi}_{\alpha,k}(\mathbf{p}/k)$ become concentrated on a classical Kepler *circle* in momentum space, with classical energy $E = -1/2$, as $k \to \infty$, at least in a weak sense. Similarly in configuration space, their rescaled inverse Fourier transforms $k^3\Psi_{\alpha,k}(k^2\mathbf{x})$ become concentrated on a classical Kepler ellipse, $k \to \infty$. These states are not in general eigenfunctions of angular momentum or of the quantum Runge-Lenz vectors. The densities associated with these states are proportional to the local time that a classical particle spends in a given region as it travels its Kepler orbit. This is part of the content of theorems (3.1) and (4.2) in sections 3 and 4.

We refer to these states $\{\hat{\Psi}_{\alpha,k}\}$ in momentum space, or their inverse Fourier transforms $\{\Psi_{\alpha,k}\}$ in configuration space as *coherent* states because of their localization properties in both momentum and configuration space. They are over-complete, but the projection onto the eigenspace of the quantum operator H corresponding to E_k, $\hat{\mathbf{P}}_k$ in the momentum representation (or $\mathbf{P}_k$ in the configuration space representation), is simply expressed as an integral over α of the states $\{\hat{\Psi}_{\alpha,k}\}$ (resp. $\{\Psi_{\alpha,k}\}$) with fixed k in analogy with the resolution of the identity using coherent states for the quantum mechanical harmonic oscillator. There is another reason for referring to our states as coherent: Recall that there is an isometry mapping the hyperspherical harmonics on the 3-dimensional sphere $\mathcal{S}^3$ onto the bound states of the hydrogen atom Hamiltonian which is constructed via a stereographic transformation mapping the $\mathcal{S}^3$ to momentum space $\mathbf{R}^3$ [2]. In particular, k^{th}-order hyperspherical harmonics are mapped to eigenstates having eigenvalue E_k. Our states, in the momentum representation, are nothing more than the images of spherical coherent states, which have been considered by Radcliffe [13], Arecchi et al. [1] and many others in the physics literature, and more recently Uribe [17] and others in the mathematics literature, and which, in Lie algebra terms, are maximal rank vectors of the Lie algebra $so(4)$.

The question of coherent states for the hydrogen is by no means new. Gay et al. [5] consider special cases of the coherent states we use, and show that they are highly concentrated on the classical orbits in both configuration space and momentum space. They do no relate the state density to the local time density nor do they discuss a completeness relation for them, as we need for our work here. Nauenberg [12] also constructs eigenstates highly peaked along Kepler orbits in configuration space, and considers the time-evolution of superpositions of these states. Gaeta and Stroud [4] discuss the evolution of minimal uncertainty Gaussian-like wave packets along a Kepler orbit. Most recently Klauder [9] identifies a class of coherent state families, depending only on continuous variables. These states in these families are not eigenstates of H, but do have a simple evolution under the group $exp(-itH)$ and provide a resolution of the projection onto the bound states. He does not investigate the support properties of the states.

Coherent states are, in general, useful for investigating the semi- classical limit, either Planck's constant $\hbar \to 0$ or the high quantum number limit. Here, we use our states to prove limiting distribution theorems for the Rydberg states, the main content of theorems (3.1) and (4.2). These theorems are of the following sort: Let $\hat{\mathbf{P}}_k$ be the projection onto states of energy E_k as above, and consider the limit

$$\lim_{k\to\infty}\frac{1}{(k+1)^2}tr\hat{\mathbf{P}}_kW_k, \tag{1.1}$$

where W_k is a multiplication operator W in momentum space, suitably rescaled. More complicated expectations with W_k in the above trace replaced by functions of $\hat{\mathbf{P}}_kW_k\hat{\mathbf{P}}_k$ are also considered. (The factor $1/(k+1)^2$ is simply to normalize the trace.) Then the above limit is equal to an integral over all possible classical bound orbits of a standard energy, $E = -1/2$–an integral over the space of α's–with integrand given by an expression involving a path integral of W over a given classical orbit in momentum space. A similar theorem holds in the configuration space representation. These theorems are analogous to a theorem of Szegö [6] who considered limits of traces as above, but with W_k taken to be a function of P_kVP_k with V a function on the circle and P_k the $(k+1)$-dimensional projection onto the subspace spanned by 1, $e^{\imath x}$, $e^{2\imath x}$, $\cdots$, $e^{\imath kx}$. The above limits should also be compared with Weyl-Szegö type limits in which the projections $\mathbf{P}_k$ or $\hat{\mathbf{P}}_k$ appearing above are replaced by $\mathbf{P}_{E\leq E_0}$, that is, a projection onto the subspace corresponding to energies $E\leq E_0$; such limits can be related to integrals of W over phase space. For a further discussion of the distinction of these kinds of limits, see the introductory remarks in [16]. For a recent discussion of Weyl-Szegö limits, see [10] and for classical results on the large k limit of orthogonal functions see of course the work of Szegö, [15].

We remark that the trace in the above limit expression (1.1) can be thought of as a quantum mechanical microcanonical state for the hydrogen atom. The theorems then relate this state, in the large k limit to a classical microcanonical state involving integrals over classical Kepler orbits. Also note that were one doing first order perturbation theory, the trace expression gives, by the Feynman-Hellman formula, the average of the first order shifts in the eigenvalues from E_k, for the operator $H+\epsilon W_k$, i.e., $\sum_{1\leq j\leq k^2}\partial E_{k,j}/\partial\epsilon$, where $E_{k,j}$ is the j^{th} eigenvalue about E_k.

In section 2 we revisit coherent states on spheres $\mathcal{S}^n$ of any dimension n, and prove a Szegö theorem and, as a corollary, a limiting distribution theorem, Corollary (2.5). This limiting distribution theorem, first proved by Kac-Spencer[8], Weinstein [19] and Widom [20], (see also Guillemin and Sternberg [7]), describes the asymptotic distribution of eigenvalues $k\to\infty$ for $-\Delta_n+V$, with Δ_n the spherical Laplacian on $\mathcal{S}^n$, and with V multiplication by a continuous function $V(\boldsymbol{\omega})$ on $\mathcal{S}^n$. These theorems were originally proved using either properties of special functions [8] , or pseudo- differential operator techniques

[19, 20]. Here we wish to emphasize the use of coherent states to provide simple, self-contained proofs of these theorems. Transformed to momentum space, these states become our coherent states for the hydrogen atom problem; conversely, analysis of the Rydberg states in the momentum representation can be carried out by transforming back to the spherical problem setting.

Section 3 contains the definition of the hydrogen atom coherent states in the momentum representation, a review of some aspects of the classical Kepler orbits, and a proof of a Szegö theorem for the Rydberg states in the momentum representation. Its proof is almost immediate from the results of section 2 with one caveat: The mapping taking states $\Phi_{\alpha,k}$ on the sphere to states $\hat{\Psi}_{\alpha,k}$ is composition with a (rescaled) stereographic transformation, times an appropriate Jacobian factor maintaining unitarity, *times another factor which is a function of momentum* $\mathbf{p}$. Again, the Szegö theorem relates certain quantum expectations to averages over classical Kepler orbits in momentum space. This extra multiplicative factor is seen to account for the (generally non-uniform) speed of a classical particle, as it travels along a classical orbit in momentum space.

Section 4 contains a Szegö theorem for the Rydberg states in the configuration space representation which relates a Rydberg expectation of a multiplication operator $V(\mathbf{x})$ to an integral over orbits of an integrand involving V integrated over a classical (elliptical) orbit. The proof is to a large extent carried out in momentum space, where V is approximated by a differential operator. Its effect on the coherent states is easily calculated and gives rise to an effective multiplication operator (a symbol) to which we can apply the results of the previous section in order to complete the proof of the theorem.

In the appendix, we provide a parametrization of the space of Kepler orbits in terms of the angular momentum and Runge-Lenz vectors. We also provide an explicit differential measure in terms of this parametrization suitable for computing the needed orbit space integrals.

Section II. Limiting Distribution Theorem for the Laplacian Δ_n on the n-sphere $\mathcal{S}^n$.

2.1 *Coherent States* $\Phi_{\alpha,k}$ *on* $\mathcal{S}^n$

In this section we introduce coherent states defined on $\mathcal{S}^n$. Following A. Uribe [17], we Let $\boldsymbol{\alpha} = \Re\boldsymbol{\alpha} + \imath\Im\boldsymbol{\alpha}$ be an $n+1$-dimensional complex vector with $\Re\boldsymbol{\alpha}$ and $\Im\boldsymbol{\alpha}$ both real vectors of unit length and orthogonal to each other, $\Re\boldsymbol{\alpha}\cdot\Im\boldsymbol{\alpha} = 0$. For convenience, we shall usually denote such a vector $\boldsymbol{\alpha}$ by α unless we are emphasizing its vector nature in which case we will use the boldface notation. Let $\mathcal{A}$ denote the set of such α's satisfying these conditions. Given an α, let $\Phi_{\alpha,k}$ be the function defined on $\mathcal{S}^n$,

$$\Phi_{\alpha,k}(\boldsymbol{\omega}) = a(k)(\boldsymbol{\alpha}\cdot\boldsymbol{\omega})^k, \qquad \boldsymbol{\omega}\in\mathcal{S}^n. \tag{2.1}$$

Here, $a(k)$ is a normalization constant chosen so that the $L^2(\mathcal{S}^n)$-norm of $\Phi_{\alpha,k}$ is one; $a(k)$ is $O(k^{(n-1)/4})$ as will be seen below.

The function $\Phi_{\alpha,k}$ is a (hyper)-spherical harmonic of order k, i.e., an eigenfunction of the spherical Laplacian Δ_n on $\mathcal{S}^n$ with eigenvalues $-\lambda_k = -(k^2 + (n-1)k)$. The collection of functions $\{\Phi_{\alpha,k}\}$, $\alpha \in \mathcal{A}$ is (over)-complete in that they span the k^{th}-order spherical harmonics. In particular, the orthogonal projection $\mathbf{P}_{\mathbf{S}k}$ onto these harmonics is given by

$$\mathbf{P}_{\mathbf{S}k} = d(k)\int_{\alpha\in\mathcal{A}} |\Phi_{\alpha,k}\rangle\langle\Phi_{\alpha,k}|d\mu(\alpha). \tag{2.2}$$

Here $d(k)$ is the dimension of the space spanned by the k^{th} order spherical harmonics, and $d\mu$ is a probability measure on $\mathcal{A}$ which is rotationally invariant; $\mu(\mathcal{R}A) = \mu(A)$ for any measurable subset A of $\mathcal{A}$ and rotation $\mathcal{R}\in SO(n+1)$. Note that, as a function of $\boldsymbol{\omega}$, $\Phi_{\alpha,k}$ becomes more and more concentrated on the geodesic circle $\gamma(\alpha)$ defined by $|\boldsymbol{\alpha}\cdot\boldsymbol{\omega}| = 1$, as $k\to\infty$.

2.2 *Estimation of the matrix elements* $\langle\Phi_{\alpha,k} \mid V \mid \Phi_{\beta,k}\rangle$.

The point of this paragraph is to obtain an asymptotic formula for matrix elements of the form $\langle\Phi_{\alpha,k} \mid V \mid \Phi_{\beta,k}\rangle$ for $k\to\infty$ with V a multiplication operator analytic in a neighborhood of each point on the sphere $\mathcal{S}^n$. Since for k large the states $\Phi_{\alpha,k}$ and $\Phi_{\beta,k}$ are concentrated on geodesics $\gamma(\alpha)$ and $\gamma(\beta)$ respectively, we expect that when $\gamma(\alpha)$ and $\gamma(\beta)$ are nearly the same geodesic, the main contribution to the matrix element comes from the values of V along this geodesic; otherwise, we expect the matrix element to be very small. The lemma below makes this intuition more precise. Let $(\theta_1,\theta_2,\ldots,\theta_n)$ be spherical coordinates for $\mathcal{S}^n$ so that for rectangular coordinates, $\boldsymbol{\omega} = (\omega_1,\omega_2,\ldots,\omega_{n+1})$,

$$\begin{aligned}\omega_1 &= \cos(\theta_1)\prod_{j=2}^{n}\sin(\theta_j)\\ \omega_2 &= \sin(\theta_1)\prod_{j=2}^{n}\sin(\theta_j)\\ \omega_i &= \cos(\theta_{i-1})\prod_{j=i}^{n}\sin(\theta_j) \qquad i = 3,4,\ldots,n+1.\end{aligned} \tag{2.3}$$

Lemma 2.1 *Let V be analytic in the variables $(\theta_1, \theta_2, \ldots \theta_n)$ of $\mathcal{S}^n$. Then for any $\delta > 0$,*

$$\langle \Phi_{\alpha,k} \mid V \mid \Phi_{\beta,k} \rangle = (\frac{1}{2}\boldsymbol{\alpha}^* \cdot \boldsymbol{\beta})^k \times \left(\frac{1}{2\pi} \int_{\gamma(\alpha)} V ds + O(k^{\delta - \frac{1}{2}}) \right) + O(k^{-\infty}) \quad (2.4)$$

where the integral $\int_{\gamma(\alpha)} V ds = \int_0^{2\pi} V(\boldsymbol{\omega}(s,\alpha)) ds$ with $\boldsymbol{\omega}(s,\alpha)$ a parametrization of the geodesic $\gamma(\alpha)$ by arclength s. Equivalently, the line integral of V may be taken over $\gamma(\beta)$.

Proof: Because of rotational invariance we can assume that $\alpha, \beta \in \mathcal{A}$ are given as vector expressions by the equations

$$\boldsymbol{\alpha} = \mathbf{e}_1 + \imath \mathbf{e}_2 \quad (2.5)$$

with $\mathbf{e}_j$ a unit vector along the j^{th}-coordinate axis, and

$$\boldsymbol{\beta} = \exp(\imath\phi) \exp(\imath \boldsymbol{\mu} \cdot \mathbf{J}) \boldsymbol{\alpha}, \quad (2.6)$$

with

$$\boldsymbol{\mu} \cdot \mathbf{J} = \sum_{k=3}^{n+1} \mu_{1,k} J(1,k) + \mu_{2,k} J(2,k). \quad (2.7)$$

In this equation, for $i < j$, $J(i,j)$ is an $(n+1) \times (n+1)$ self-adjoint matrix equal to $\imath$ in the $(i,j)^{th}$ entry, $-\imath$ in the $(j,i)^{th}$ entry, and all other entries zero. Thus $J(i,j)$ generates rotations leaving the $(i,j)^{th}$ coordinate plane invariant. Note that $\mathcal{A}$ is $(2n-1)$-dimensional; $\boldsymbol{\mu}$ and ϕ are local coordinates (Euler angles) for this space.

Now if $\boldsymbol{\beta}$ undergoes the transformation $\boldsymbol{\beta} \to \exp(\imath\phi)\boldsymbol{\beta}$, then $\Phi_{\beta,k}$ undergoes just a phase change by a factor $\exp(\imath k \phi)$, as does the right side of the statement in the lemma Eq.(2.4), so it suffices to prove the lemma for $\phi = 0$.

By expanding Eq.(2.6) in powers of $(\imath \boldsymbol{\mu} \cdot \mathbf{J})$, we obtain:

$$\boldsymbol{\beta} = \begin{bmatrix} 1 + \left(\frac{-1}{2}\right) \sum_{j=3}^{n+1} \mu_{1,j}(\mu_{1,j} + \imath \mu_{2,j}) + O(\mu^4) \\ \imath + \left(\frac{-1}{2}\right) \sum_{j=3}^{n+1} \mu_{2,j}(\mu_{1,j} + \imath \mu_{2,j}) + O(\mu^4) \\ -(\mu_{1,3} + \imath \mu_{2,3}) + O(\mu^3) \\ \vdots \\ -(\mu_{1,n+1} + \imath \mu_{2,n+1}) + O(\mu^3) \end{bmatrix}. \quad (2.8)$$

Here and below, $\mu^2 = |\boldsymbol{\mu}|^2$ is just the squared Euclidean length of $\boldsymbol{\mu}$, and $O(\mu^n) = O(|\boldsymbol{\mu}|^n)$. By using this equation Eq.(2.8) and by expanding the functions $\sin(\theta_j)$ and $\cos(\theta_j)$ $j = 2, 3, \ldots n$ about $\frac{\pi}{2}$, we obtain:

$$\begin{aligned}\ln((\boldsymbol{\alpha}^* \cdot \boldsymbol{\omega})(\boldsymbol{\beta} \cdot \boldsymbol{\beta})) &= -\sum_{j=2}^{n}(\theta_j - \frac{1}{2}(\pi + (\mu_{1,j+1} + \imath\mu_{2,j+1})\exp(-\imath\theta_1)))^2 \\ &\quad -\frac{1}{4}\sum_{j=3}^{n+1}(\mu_{1,j}^2 + \mu_{2,j}^2) + O((\theta - \frac{\pi}{2})^4) + O(\mu^4). \qquad (2.9)\end{aligned}$$

where $O((\theta - \frac{\pi}{2})^4)$ is actually bounded by fourth powers of $\theta_j - \frac{\pi}{2}$, $j = 2, \ldots, n$ only.

The above equation Eq.(2.9), the fact that both $\Phi_{\alpha,k}$ and $\Phi_{\beta,k}$ are $O(k^{-\infty})$ away from $|\boldsymbol{\alpha} \cdot \boldsymbol{\omega}| = 1$ and $|\boldsymbol{\beta} \cdot \boldsymbol{\omega}| = 1$ respectively, and the analyticity allow the matrix element $\langle \Phi_{\alpha,k} \mid V \mid \Phi_{\beta,k} \rangle$ to be estimated by the saddle point method. Doing the $(\theta_2, \ldots \theta_n)$-integration first in the matrix element, we find that

$$\begin{aligned}&\langle \Phi_{\alpha,k} \mid V \mid \Phi_{\beta,k} \rangle = a(k)^2 \int V(\boldsymbol{\omega}) \exp\left[k \ln((\boldsymbol{\alpha}^* \cdot \boldsymbol{\omega})(\boldsymbol{\beta} \cdot \boldsymbol{\omega}))\right] d\boldsymbol{\omega} \\ &= a(k)^2 \left(\frac{\pi}{k}\right)^{\frac{n-1}{2}} \exp\left[-k(\mu^2 + O(\mu^4))\right] \times \\ &\quad \left[\int_0^{2\pi} (V(\Theta(\theta_1, \boldsymbol{\mu})) \prod_{j=2}^{n} \sin^{j-1}(\Theta_j(\theta_1, \boldsymbol{\mu})) + O(k^{-1/2})) d\theta_1\right] + O(k^{-\infty}) \\ &= a(k)^2 \left(\frac{\pi}{k}\right)^{\frac{n-1}{2}} \exp\left[-k(\mu^2 + O(\mu^4))\right] \times \\ &\quad \left[\int_0^{2\pi} V(\theta_1, \frac{\pi}{2}, \cdots, \frac{\pi}{2}) d\theta_1 + O(\mu) + \ O(k^{-1/2})\right] + O(k^{-\infty}) \qquad (2.10)\end{aligned}$$

where $\Theta(\theta_1, \boldsymbol{\mu}) = (\Theta_1, \Theta_2, \cdots, \Theta_n)$ with $\Theta_1(\theta_1, \boldsymbol{\mu}) = \theta_1$, and $\Theta_j(\theta_1, \boldsymbol{\mu}) = \frac{1}{2}[\pi + (\mu_{1,j+1} + \imath\mu_{2,j+1})\exp(-\imath\theta_1)]$, $j = 2, \cdots, n$.

Note that the integral involving V in the last line of Eq.(2.10) is precisely the line integral of V over $\gamma(\alpha)$. In the special case of $V \equiv 1$ and $\boldsymbol{\mu} = 0$, we infer that

$$a(k)^2 \left(\frac{\pi}{k}\right)^{\frac{n-1}{2}} = \frac{1}{2\pi} + O(k^{-1/2}). \qquad (2.11)$$

With these remarks, it follows that Eq.(2.10) can be written,

$$\langle \Phi_{\alpha,k} \mid V \mid \Phi_{\beta,k} \rangle \qquad (2.12)$$

$$= \exp\left[-k(\mu^2 + O(\mu^4))\right]\left[\frac{1}{2\pi}\int_{\gamma(\alpha)} V ds + O(\mu) + O(k^{-1/2})\right] + O(k^{-\infty}).$$

In this last equation, we note that if $0 \le |\boldsymbol{\mu}| < k^{\delta-1/2}$, then the exponential factor $\exp(-kO(\mu^4)) = 1 + O(k^{4\delta-1})$ with the exponent $4\delta - 1 < \delta - 1/2$ (at least if $\delta < 1/6$). If $k^{\delta-1/2} \le |\boldsymbol{\mu}| < \mu_0$, with μ_0 sufficiently small so that the $O(\mu^4)$-term in the exponent is strictly less than μ^2, then the first term on the right side of Eq.(2.12) is $O(k^{-\infty})$. Thus in both of these cases, the $O(\mu)$-term after the integral in Eq.(2.12) can be replaced by $O(k^{\delta-1/2})$ and the $kO(\mu^4)$ in the exponential factor can be absorbed into this term as well. Since, from Eqs.(2.5,2.8),

$$\ln\frac{1}{2}(\boldsymbol{\alpha}^* \cdot \boldsymbol{\beta}) = -\frac{1}{4}\mu^2 + O(\mu^4), \tag{2.13}$$

and so the exponential factor in the previous equation, Eq.(2.12) can be replaced by $(\frac{1}{2}\boldsymbol{\alpha}^* \cdot \boldsymbol{\beta})^k$, again absorbing the $kO(\mu^4)$ error into the $O(k^{\delta-1/2})$-term, still with $0 \le |\boldsymbol{\mu}| < \mu_0$. With all of these replacements,we obtain the statement of the lemma, Eq.(2.4), for the case of small $|\boldsymbol{\mu}|$.

It remains to consider the case when β is bounded away from α with $|\mu| > 0$. Now the right side of the statement of the lemma, Eq.(2.4), is certainly $O(k^{-\infty})$ in this case so the problem is to show that the matrix element itself is of this order. Suppose then, that α and β are such that

$$\boldsymbol{\beta} = \boldsymbol{\beta}^0 + \boldsymbol{\beta}^\perp \tag{2.14}$$

where the real and imaginary components of $\boldsymbol{\beta}^0$ are in the plane spanned by the real and imaginary parts of $\boldsymbol{\alpha}$, and the real and imaginary parts of $\boldsymbol{\beta}^\perp \ne 0$ are orthogonal to these parts. Let $\boldsymbol{\omega}_0$ be a critical point where $\Re\ln((\boldsymbol{\alpha}^* \cdot \boldsymbol{\omega})(\boldsymbol{\beta} \cdot \boldsymbol{\omega})) \le 0$ is maximum. (The maximum must be zero, otherwise, the integrand in the integral for the matrix element is clearly of $O(k^{-\infty})$ and so is the matrix element.)

Let ξ be the directional derivative of $\ln(\boldsymbol{\alpha}^* \cdot \boldsymbol{\omega}\boldsymbol{\beta} \cdot \boldsymbol{\omega})$ in the direction of $\boldsymbol{\beta}^\perp$ at this critical point:

$$\xi = \frac{\boldsymbol{\beta} \cdot D\boldsymbol{\omega}}{\boldsymbol{\beta} \cdot \boldsymbol{\omega}_0}. \tag{2.15}$$

Evidently, ξ must be pure imaginary, since if it had a real part, then the real part of the logarithm expression would not be maximized. Moreover, $\|\xi\| = \|\boldsymbol{\beta}^\perp\| = \sqrt{\boldsymbol{\beta}^{\perp *} \cdot \boldsymbol{\beta}^\perp} \ne 0$. Making a C^∞- partition of unity for the sphere $\mathcal{S}^n$, we reduce the problem of computing the matrix element integral to computing the integral over a small neighborhood of each critical point. The integrand of such an integral contains a factor of a C^∞-function supported in that neighborhood coming from the partition of unity. The integral is of course n-dimensional, but it necessarily involves a one-dimensional integral having a highly oscillatory integrand and of the following sort:

$$\int \exp\left(\imath k\xi\theta + kb(\theta)\right)\chi(\theta)d\theta \tag{2.16}$$

where $b(\theta)$ is analytic in θ and is such that its real part is of the form

$$\Re b(\theta) = -c_0\theta^{2p} + O(\theta^{2p+1}) \tag{2.17}$$

with $c_0 > 0$ and where χ is C^∞ and compactly supported. But such an integral is $O(k^{-\infty})$ which we argue below, hence the matrix element itself, which again is a finite sum of integrals over these small neighborhoods, must be $O(k^{-\infty})$. Finally we remark that in the special case that $\boldsymbol{\beta} = \boldsymbol{\alpha}^*$, i.e., that $\boldsymbol{\beta}$ lies in the same plane as $\boldsymbol{\alpha}$ but has the opposite orientation, this same argument applies but with the integrand highly oscillatory in the azimuthal variable. This completes the proof of the lemma, except for estimating the above integral Eq.(2.16).

The first step in estimating Eq.(2.16) is to make the *real* change of variables $\theta' = \theta + \Im b(\theta)$. With such a change of variables one obtains an integral of precisely the same form as that of Eq.(2.16), but with $b(\theta)$ real. Integrating by parts m times, Eq.(2.16) becomes

$$\left(\frac{\imath}{\|\xi\|k}\right)^m \int \exp\left(\imath k\xi\theta\right)\frac{d^m}{d\theta^m}(exp(kb(\theta))\chi(\theta))d\theta. \tag{2.18}$$

Note that if $\Re b \equiv 0$ one immediately sees that the integral is $O(k^{-m})$. Computing the derivative in the integrand, one obtains powers of $k\frac{db}{d\theta}(\theta)$ and derivatives of this quantity, times the exponential of $kb(\theta)$, times innocuous derivatives of χ. The trick is then to split the resulting integral Eq.(2.18) into two pieces, a part where the integration takes place over $|\theta| \leq (c_0k)^{-1/2p}$, and a part where $|\theta| > (c_0k)^{-1/2p}$. In the former case, one simply takes advantage of the smallness of θ to estimate the integrand; in the latter case one uses the exponential to control the powers, for example,

$$\begin{aligned}\left|(k\frac{db}{d\theta})^m \exp\left(kb\right)(\theta)\right| &= \left|(kb)^m \exp\left(kb\right)\left(\frac{1}{b}\frac{db}{d\theta}(\theta)\right)^m\right| \\ &\leq \text{constant}\left|\frac{1}{\theta}\right|^m \leq \text{constant}(c_0k)^{m/2p},\end{aligned} \tag{2.19}$$

using the fact that $x^m \exp(-x)$ is bounded, $x \geq 0$. In both cases, one finds that the integrals are $O(k^{-m(1-\frac{1}{2p})})$. Thus Eq.(2.16) is of this order, for any m, and hence is $O(k^{-\infty})$. This completes the proof of the lemma. $\square$

The lemma implies, with the choice $V \equiv 1$, that

$$\langle \Phi_{\alpha,k} \mid \Phi_{\beta,k} \rangle = (\frac{1}{2}\boldsymbol{\alpha}^* \cdot \boldsymbol{\beta})^k (1 + O(k^{\delta-\frac{1}{2}})) + O(k^{-\infty}), \tag{2.20}$$

and substituting this relation back into the equation of the lemma, we obtain for arbitrary V satisfying the hypotheses of the lemma that

$$\langle \Phi_{\alpha,k} \mid V \mid \Phi_{\beta,k} \rangle = \langle \Phi_{\alpha,k} \mid \Phi_{\beta,k} \rangle \left(\frac{1}{2\pi} \int_{\gamma(\alpha)} V\, ds + O(k^{\delta-\frac{1}{2}}) \right) + O(k^{-\infty}). \tag{2.21}$$

Also, an immediate consequence of the lemma is the following estimate:

Lemma 2.2 *There exists a constant $M > 0$ independent of k such that for all $q \geq 0$,*

$$d(k)^{q-1} \left[\int \int \cdots \int \mid \langle \Phi_{\alpha_1,k} \mid \Phi_{\alpha_2,k} \rangle \langle \Phi_{\alpha_2,k} \mid \Phi_{\alpha_3,k} \rangle \cdots \langle \Phi_{\alpha_q,k} \mid \Phi_{\alpha_1,k} \rangle \mid \right.$$
$$\left. \times\, d\mu(\alpha_1) d\mu(\alpha_2) \cdots d\mu(\alpha_q) \right] \leq M^q. \tag{2.22}$$

Proof: Since $\mid \langle \Phi_{\alpha_q,k} \mid \Phi_{\alpha_1,k} \rangle \mid \leq 1$, we just omit this factor in the above integral, therefore bounding it by

$$d(k)^{q-1} \left[\int \int \cdots \int \mid \langle \Phi_{\alpha_1,k} \mid \Phi_{\alpha_2,k} \rangle \langle \Phi_{\alpha_2,k} \mid \Phi_{\alpha_3,k} \rangle \cdots \langle \Phi_{\alpha_{q-1},k} \mid \Phi_{\alpha_q,k} \rangle \mid \right.$$
$$\left. \times\, d\mu(\alpha_1) d\mu(\alpha_2) \cdots d\mu(\alpha_q) \right]$$
$$= \left[d(k) \int \mid \langle \Phi_{\alpha_1,k} \mid \Phi_{\alpha_2,k} \rangle \mid d\mu(\alpha_2) \right]^{q-1} \tag{2.23}$$

by the facts that $d\mu$ is rotation invariant and is a probability measure. Now the degeneracy $d(k) = O(k^{n-1})$ for the n-dimensional sphere, $\mathcal{S}^n$, and, by the previous lemma (2.1), Eq.(2.4), the integral in the last line of Eq.(2.23), is essentially a Gaussian integral of order $O(k^{-(n-1)})$, noting that $\boldsymbol{\mu}$ is a $2n-2$-dimensional vector. $\square$

We can now proceed to the proof of a Szegö's theorem for the sphere. The heart of the proof is the following lemma:

Lemma 2.3 *Let $G(\gamma(\alpha_1),\gamma(\alpha_2),\cdots,\gamma(\alpha_q))$ be a continuous function of the orbits $\{\gamma(\alpha_i)\}$, $i=1,\ldots,q$. Then*

$$\lim_{k\to\infty} d(k)^{q-1}\left[\int\int\cdots\int \langle\Phi_{\alpha_1,k}\mid\Phi_{\alpha_2,k}\rangle\langle\Phi_{\alpha_2,k}\mid\Phi_{\alpha_3,k}\rangle\cdots\langle\Phi_{\alpha_q,k}\mid\Phi_{\alpha_1,k}\rangle)\right.$$
$$\left.\times\, G(\gamma(\alpha_1),\gamma(\alpha_2),\cdots,\gamma(\alpha_q))d\mu(\alpha_1)d\mu(\alpha_2)\cdots d\mu(\alpha_q)\right]$$
$$=\int G(\gamma(\alpha),\gamma(\alpha),\cdots,\gamma(\alpha))d\mu(\alpha). \tag{2.24}$$

Proof: The proof is a standard approximate identity argument. In order to fix some coordinates, let the geodesic $\gamma(\alpha_q)$ be obtained from $\gamma(\alpha_1)$ by the rotation $\exp(\imath\boldsymbol{\mu}\cdot\mathbf{J})$ where $\boldsymbol{\mu}$ is chosen as above in Eq.(2.6,2.7). Then, given ϵ, there exists a δ, such that if $|\boldsymbol{\mu}|<\delta$ the difference

$$G(\gamma(\alpha_1),\gamma(\alpha_2),\cdots,\gamma(\alpha_q))-G(\gamma(\alpha_1),\gamma(\alpha_2),\cdots,\gamma(\alpha_{q-1}),\gamma(\alpha_1)) \tag{2.25}$$

is, in magnitude, less than ϵ. If we replace G in the integral on the left side of Eq.(2.24) by this difference, and split the integral into two pieces, one over the region where $|\boldsymbol{\mu}|<\delta$, the other where $|\boldsymbol{\mu}|\geq\delta$, then the first integral is bounded by $M^q\epsilon$ by the previous lemma, and the second integral is $O(k^{-\infty})$ since $\langle\Phi_{\alpha_q,k}\mid\Phi_{\alpha_1,k}\rangle$ is $O(k^{-\infty})$. It follows that the integral in the left side of Eq.(2.24) differs by $O(\epsilon)+O(k^{-\infty})$ from

$$d(k)^{q-1}\left[\int\int\cdots\int\langle\Phi_{\alpha_1,k}\mid\Phi_{\alpha_2,k}\rangle\langle\Phi_{\alpha_2,k}\mid\Phi_{\alpha_3,k}\rangle\cdots\langle\Phi_{\alpha_q,k}\mid\Phi_{\alpha_1,k}\rangle)\right.$$
$$\left.\times\, G(\gamma(\alpha_1),\cdots,\gamma(\alpha_{q-1}),\gamma(\alpha_1))d\mu(\alpha_1)d\mu(\alpha_2)\cdots d\mu(\alpha_q)\right]$$
$$=d(k)^{q-2}\left[\int\int\cdots\int\langle\Phi_{\alpha_1,k}\mid\Phi_{\alpha_2,k}\rangle\langle\Phi_{\alpha_2,k}\mid\Phi_{\alpha_3,k}\rangle\cdots\langle\Phi_{\alpha_{q-1},k}\mid\Phi_{\alpha_1,k}\rangle)\right.$$
$$\left.\times\, G(\gamma(\alpha_1),\cdots,\gamma(\alpha_{q-1}),\gamma(\alpha_1))d\mu(\alpha_1)d\mu(\alpha_2)\cdots d\mu(\alpha_{q-1})\right]\quad, \tag{2.26}$$

since the α_q can be integrated out, using Eq.(2.2) defining the projection $\mathbf{P}_{\mathbf{S}k}$ as an integral over the coherent states. The argument is then repeated, reducing q by one at each step, until the right side of Eq.(2.24) is obtained. Taking $k\to\infty$, and letting $\epsilon\to 0$ gives the result of the lemma. □

2.3 *Szegö Theorem for $\mathcal{S}^n$*

In this section we use the lemmas of section 2.2 to prove a Szegö Theorem for $\mathcal{S}^n$. As in the introduction, we define the Radon transform of a function V on the sphere by

$$\hat{V}(\alpha) = \frac{1}{2\pi}\int_0^{2\pi} V(\boldsymbol{\omega}(s,\alpha))ds, \tag{2.27}$$

for $\alpha \in \mathcal{A}$.

Theorem 2.4 Szegö Theorem for the $n-$sphere $\mathcal{S}^n$. *Let V a multiplication operator by a continuous function on the sphere $\mathcal{S}^n$. Let $F : \mathbf{R} \mapsto \mathbf{R}$ be a continuous function. Then*

$$\lim_{k\to\infty} \frac{1}{d(k)} tr\mathbf{P}_{\mathbf{S}^k}(F(\mathbf{P}_{\mathbf{S}^k} V \mathbf{P}_{\mathbf{S}^k})) = \int_{\alpha\in\mathcal{A}} F(\hat{V}(\alpha))d\mu(\alpha) \tag{2.28}$$

Proof: The operator $\mathbf{P}_{\mathbf{S}^k} V \mathbf{P}_{\mathbf{S}^k}$ is self-adjoint with spectrum in the interval $[-\|V\|_\infty, \|V\|_\infty]$ which permits us to approximate F uniformly by a polynomial on this interval. Also, V itself can be approximated by a polynomial in the rectangular coordinate functions $\omega_1, \omega_2, \ldots, \omega_{n+1}$ (see Eq.(2.3)) by Stone-Weierstrass, hence by an analytic function. In particular it suffices to prove the theorem for F a monomial and V analytic.

Now for $F(x) = x^q$ the left side of Eq.(2.28) is equal to

$$\begin{aligned} & d(k)^{q-1} \int\int\cdots\int \langle \Phi_{\alpha_1,k} \mid V \mid \Phi_{\alpha_2,k}\rangle\langle \Phi_{\alpha_2,k} \mid V \mid \Phi_{\alpha_3,k}\rangle \cdots \\ & \qquad \times \langle \Phi_{\alpha_q,k} \mid V \mid \Phi_{\alpha_1,k}\rangle d\mu(\alpha_1)d\mu(\alpha_2)\cdots d\mu(\alpha_q) \\ = \;& d(k)^{q-1} \int\int\cdots\int \langle \Phi_{\alpha_1,k} \mid \Phi_{\alpha_2,k}\rangle\langle \Phi_{\alpha_2,k} \mid \Phi_{\alpha_3,k}\rangle \cdots \langle \Phi_{\alpha_q,k} \mid \Phi_{\alpha_1,k}\rangle) \\ & \qquad \times \prod_{i=1}^{q} \hat{V}(\alpha_i) d\mu(\alpha_1)d\mu(\alpha_2)\cdots d\mu(\alpha_q) + O(k^{\delta-1/2}), \end{aligned} \tag{2.29}$$

by lemmas(2.1,2.2). But this last expression converges for $k \to \infty$ to

$$\int_{\alpha\in\mathcal{A}} (\hat{V}(\alpha))^q d\mu(\alpha) \tag{2.30}$$

by the previous lemma (2.3), and this completes the proof of the theorem. □

2.4 *Limiting Distribution Theorem for the Laplacian on $\mathcal{S}^n$*

An immediate corollary of Theorem (2.4) is the limiting distribution theorem, due to Weinstein [19], Widom [20] and Kac and Spencer [8].

Corollary 2.5 Limiting Distribution Theorem for the Laplacian on $\mathcal{S}^n$. *Let V be a multiplication operator by a continuous function on the sphere $\mathcal{S}^n$, and F a function in the Schwartz space of the real line $S(\mathbf{R})$. Then:*

$$\lim_{k\to\infty} \frac{1}{d(k)} tr F(-\Delta_n + V - \lambda_k) = \int_{\alpha\in\mathcal{A}} F(\hat{V}(\alpha)) d\mu(\alpha). \tag{2.31}$$

A proof of this corollary can be found in [18], see also [16]. We will restrict ourselves to mentioning the following main ideas. For k sufficiently large, the cluster of eigenvalues of the operator $H = -\Delta_n + V$ around the unperturbed eigenvalue λ_k is well defined. Denote by $\mathbf{Q}_k$ the projector onto the eigenspace of $-\Delta_n + V$ associated with that cluster. Since the function F decays very rapidly, the trace of the operator $F(-\Delta_n + V - \lambda_k)$ can be approximated by $tr(\mathbf{Q}_k F(\mathbf{Q}_k(-\Delta_n + V - \lambda_k)\mathbf{Q}_k)$, making an error of order $O(k^{-\infty})$. Next, from the integral representation for the projector $\mathbf{Q}_k$:

$$\mathbf{Q}_k = \frac{1}{2\pi\imath} \oint_{\mathcal{C}} \frac{dz}{z - H} \tag{2.32}$$

where $\mathcal{C}$ is a circle of radius $k/2$ and center λ_k and the resolvent identity for a perturbation of $-\Delta_n$, one shows that the norm of $\mathbf{Q}_k - \mathbf{P}_{\mathbf{S}k}$ is of order $O(k^{-1})$. Here, as above, $\mathbf{P}_{\mathbf{S}k}$ denotes the projector onto the eigenspace of $-\Delta_n$ with eigenvalue λ_k. Thus we have

$$\frac{1}{d(k)} tr \mathbf{Q}_k F(\mathbf{Q}_k(-\Delta_n + V - \lambda_k)\mathbf{Q}_k) = \frac{1}{d(k)} tr(\mathbf{P}_{\mathbf{S}k} F(\mathbf{P}_{\mathbf{S}k} V \mathbf{P}_{\mathbf{S}k})) + O(k^{-1}) \tag{2.33}$$

where we have used the fact that the norm of the operator $F(\mathbf{Q}_k(-\Delta_n + V - \lambda_k)\mathbf{Q}_k) - F(\mathbf{P}_{\mathbf{S}k} V \mathbf{P}_{\mathbf{S}k})$ is of order $O(k^{-1})$ since $\mathbf{Q}_k(-\Delta_n + V - \lambda_k)\mathbf{Q}_k - \mathbf{P}_{\mathbf{S}k} V \mathbf{P}_{\mathbf{S}k}$ is $O(k^{-1})$ and F is smooth. Now the right side of Eq.(2.33) converges to the right side of Eq.(2.31) by the Szegö theorem (2.4), and this concludes the proof of the corollary. □

Section III. Szegö-type Theorem for the Hydrogen Bound States in the Momentum Representation

In this section we define eigenstates of the hydrogen Hamiltonian which serve as coherent states, review some aspects of the classical elliptical Kepler orbits, and give a Szegö theorem for functions of momentum.

3.1 *Coherent States in Momentum Representation*

Our eigenstates for the hydrogen Hamiltonian are obtained by mapping the coherent states on $\mathcal{S}^3$ to momentum space via a stereographic transformation from $\mathcal{S}^3$ to $\mathbf{R}^3$. For the stereographic transformation, the momentum variables $\mathbf{p} = (p_1, p_2, p_3)$ and the rectangular coordinates $\boldsymbol{\omega} = (\omega_1, \cdots, \omega_4)$ are related by the equations

$$\begin{aligned} \omega_i &= \frac{2p_i}{\mathbf{p}^2+1}, \quad i = 1,2,3 \\ \omega_4 &= \frac{\mathbf{p}^2-1}{\mathbf{p}^2+1}, \end{aligned} \tag{3.1}$$

where $\mathbf{p}^2 = \mathbf{p}\cdot\mathbf{p}$. For later purposes we note that differential arclengths ds on the sphere and dp in momentum space are related by

$$ds = \frac{2dp}{\mathbf{p}^2+1}. \tag{3.2}$$

and that the surface differential on the sphere and volume differential in momentum space satisfy

$$d^3\boldsymbol{\omega} = \left(\frac{2}{\mathbf{p}^2+1}\right)^3 d^3\mathbf{p}. \tag{3.3}$$

For any $r > 0$ define the unitary dilation operator D_r acting on functions in the momentum space representation by the equation

$$D_r\hat{\Psi}(\mathbf{p}) = r^{3/2}\hat{\Psi}(r\mathbf{p}) \tag{3.4}$$

for any function $\hat{\Psi} \in L^2(\mathbf{R}^3)$.) Let J be the multiplication operator acting in momentum space,

$$J\hat{\Psi}(\mathbf{p}) = \frac{2}{\mathbf{p}^2+1}\hat{\Psi}(\mathbf{p}), \tag{3.5}$$

and let $K : L^2(\mathcal{S}^3) \mapsto L^2(\mathbf{R}^3)$ be the unitary transformation defined by

$$K\Phi(\mathbf{p}) = \left(\frac{2}{\mathbf{p}^2+1}\right)^{3/2} \Phi(\boldsymbol{\omega}(\mathbf{p})), \tag{3.6}$$

with $\omega(\mathbf{p})$ defined above.

For k a non-negative integer, $\alpha \in \mathcal{A}$ and a coherent state $\Phi_{\alpha,k}$ as defined in the previous section, set

$$\hat{\Psi}_{\alpha,k}(\mathbf{p}) = D_{k+1}J^{1/2}K\Phi_{\alpha,k}(\mathbf{p}). \tag{3.7}$$

(The "hat" over Ψ emphasizes that the function is in the momentum space representation.) The function $\hat{\Psi}_{\alpha,k}$ is an eigenfunction of the hydrogen atom Hamiltonian with eigenvalue $E_k = -\frac{1}{2}(k+1)^{-2}$, [2]. Moreover, $\hat{\Psi}_{\alpha,k}$ is normalized and

$$\langle \hat{\Psi}_{\alpha,k} \mid \hat{\Psi}_{\beta,k} \rangle_{L^2(\mathbf{R}^3)} = \langle \Phi_{\alpha,k} \mid \Phi_{\beta,k} \rangle_{L^2(\mathcal{S}^3)}. \tag{3.8}$$

Were it not for the factor $J^{1/2}$, this last equation would be obvious from the unitarity of the operators D_{k+1} and K. That it is still true with this factor follows from the virial theorem which implies that

$$\langle \hat{\Psi}_{\alpha,k} \mid \mathbf{p}^2 \mid \hat{\Psi}_{\beta,k} \rangle = \frac{1}{(k+1)^2} \langle \hat{\Psi}_{\alpha,k} \mid \hat{\Psi}_{\beta,k} \rangle \tag{3.9}$$

which can be used to show Eq.(3.8).

Let $U : L^2(\mathcal{S}^3) \mapsto L^2(\mathbf{R}^3)$ be the isometry defined by $U\Phi_{\alpha,k} = \hat{\Psi}_{\alpha,k}$. Then the projection $\hat{\mathbf{P}}_k$ onto the subspace of bound states of the hydrogen atom with energy E_k in the momentum representation is given by

$$\hat{\mathbf{P}}_k = U\mathbf{P}_{\mathbf{S}^k}U^{-1} = (k+1)^2 \int_{\alpha \in \mathcal{A}} \mid \hat{\Psi}_{\alpha,k} \rangle \langle \hat{\Psi}_{\alpha,k} \mid d\mu(\alpha) \tag{3.10}$$

where the factor $(k+1)^2$ is the dimension of this subspace.

3.2 *Classical Kepler Orbits*

We will have need for a parametrization of the Kepler orbits in both classical configuration space as well as momentum space and which we label by points $\alpha \in \mathcal{A}$. Recall that α is actually a complex vector, here a 4-vector, defined at the beginning of the previous section, with real and imaginary parts $\Re\boldsymbol{\alpha}$ and $\Im\boldsymbol{\alpha}$. Given such an α, let

$$\begin{aligned} \mathbf{x}(s,\alpha) &= \Re\vec{\alpha}(\sin(s) - \Im\alpha_4) + \Im\vec{\alpha}(-\cos(s) + \Re\alpha_4) \\ \mathbf{p}(s,\alpha) &= \frac{\Re\vec{\alpha}\cos(s) + \Im\vec{\alpha}\sin(s)}{1 - \Re\alpha_4\cos(s) - \Im\alpha_4\sin(s)}. \end{aligned} \tag{3.11}$$

In these equations, $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$, and α_4 is just the fourth component of $\boldsymbol{\alpha}$. Here, $\mathbf{p}(s,\alpha)$ is just the image of the great circle lying in the plane spanned by the real and imaginary parts of α, i.e., $\omega(s,\alpha) = \Re\boldsymbol{\alpha}\cos(s) + \Im\boldsymbol{\alpha}\sin(s)$, under the stereographic map; $\mathbf{p}(s,\alpha)$ thus traces out a circle in momentum space, except in the degenerate case of a collision orbit. The significance of the function $\mathbf{x}(s,\alpha)$ will become clearer in the last section, but here we note that it traces out an ellipse, again except for the case of a collision orbit. Most important, under a time-change defined by

$$\begin{aligned} dt &= |\mathbf{x}|ds = \left(\frac{2}{\mathbf{p}^2+1}\right) ds \\ &= (1 - \Re\alpha_4 \cos(s) - \Im\alpha_4 \sin(s))ds, \end{aligned} \tag{3.12}$$

$\{\mathbf{x}(s(t),\alpha), \mathbf{p}(s(t),\alpha)\}$ together constitute a solution to Hamilton's equations for the classical Kepler problem with Hamiltonian $H = \frac{1}{2}\mathbf{p}^2 - |\mathbf{x}|^{-1}$, and having energy $E = -1/2$. Eq.(3.12) is a regularization of the time variable, for example discussed by Moser in his analysis of the classical Kepler problem via a stereographic mapping to $\mathcal{S}^3$, [11].

3.3 *Szegö Theorem in Momentum Representation*

Let $W : \mathbf{R}^3 \mapsto \mathbf{R}$ be a continuous function. We define a kind of Radon transform $\tilde{W}$ of W. For $\alpha \in \mathcal{A}$ set

$$\begin{aligned} \tilde{W}(\alpha) &\equiv \frac{1}{2\pi}\int_0^{2\pi} W(\mathbf{p}(s,\alpha)) \left(\frac{2}{(\mathbf{p}(s,\alpha))^2+1}\right) ds \\ &= \frac{1}{2\pi}\int_0^{2\pi} W(\mathbf{p}(s(t),\alpha))dt, \end{aligned} \tag{3.13}$$

by Eq.(3.12) above. Thus $\tilde{W}$ is just the time average of W over the momentum space orbit determined by α. (The periods of these orbits are all 2π.) Note that by Eq.(3.2), $\tilde{W}(\alpha)$ is also just the line integral

$$\frac{1}{2\pi}\int W(\mathbf{p}) \left(\frac{2}{\mathbf{p}^2+1}\right)^2 dp, \tag{3.14}$$

over the curve traced out by $\mathbf{p}(s,\alpha)$.

Theorem 3.1 Szegö Theorem in Momentum Representation
Let $W : \mathbf{R}^3 \mapsto \mathbf{R}$ be a bounded continuous function and let $F : \mathbf{R} \mapsto \mathbf{R}$ be continuous. Then for $W = W(\mathbf{p})$ regarded as a multiplication operator of the momentum $\mathbf{p}$,

$$\lim_{k\to\infty} \langle \hat{\Psi}_{\alpha,k} \mid D_{k+1} W D_{k+1}^{-1} \mid \hat{\Psi}_{\alpha,k}\rangle = \tilde{W}(\alpha) \tag{3.15}$$

and

$$\lim_{k\to\infty} \frac{1}{(k+1)^2} tr \hat{\mathbf{P}}_k F(\hat{\mathbf{P}}_k D_{k+1} W D_{k+1}^{-1} \hat{\mathbf{P}}_k) = \int_{\alpha\in\mathcal{A}} F(\tilde{W}(\alpha)) d\mu(\alpha). \tag{3.16}$$

Proof: We first address the latter equation. As in the case of the Szegö Theorem for the n-sphere, we approximate the function F by a polynomial on the compact interval $[-\|W\|_\infty, \|W\|_\infty]$. Thus it is enough to prove Eq.(3.16) for the case $F(x) = x^q$ with q any non-negative integer. From Eq.(3.10), and abbreviating D_{k+1} by D we have

$$\begin{aligned}
&\frac{1}{(k+1)^2} tr\hat{\mathbf{P}}_k(\hat{\mathbf{P}}_k D_{k+1} W D_{k+1}^{-1} \hat{\mathbf{P}}_k)^q = \\
&\quad (k+1)^{2(q-1)} \int\int\cdots\int \langle \hat{\Psi}_{\alpha_1,k} \mid D\ W D^{-1} \mid \hat{\Psi}_{\alpha_2,k}\rangle \langle \hat{\Psi}_{\alpha_2,k} \mid D\ W D^{-1} \mid \hat{\Psi}_{\alpha_3,k}\rangle \\
&\qquad\qquad \cdots \times \langle \hat{\Psi}_{\alpha_q,k} \mid D\ W D^{-1} \mid \hat{\Psi}_{\alpha_1,k}\rangle d\mu(\alpha_1) d\mu(\alpha_2)\cdots d\mu(\alpha_q) \\
&\quad = (k+1)^{2(q-1)} \int\int\cdots\int \langle K\Phi_{\alpha_1,k} \mid WJ \mid K\Phi_{\alpha_2,k}\rangle \langle K\Phi_{\alpha_2,k} \mid WJ \mid K\Phi_{\alpha_3,k}\rangle \\
&\qquad\qquad \cdots \times \langle K\Phi_{\alpha_q,k} \mid WJ \mid K\Phi_{\alpha_1,k}\rangle d\mu(\alpha_1) d\mu(\alpha_2)\cdots d\mu(\alpha_q)
\end{aligned} \tag{3.17}$$

where we have used Eqs.(3.5-3.7) and $J = J(p)$ is the multiplicative factor defined in Eq.(3.5). Note that all the scalar products in Eq.(3.17) are taken in $L^2(\mathbf{R}^3)$.

Since for any α and β in $\mathcal{A}$ we have that

$$\langle K\Phi_{\alpha,k} \mid WJ \mid K\Phi_{\beta,k}\rangle_{L^2(\mathbf{R}^3)} = \langle \Phi_{\alpha,k} \mid (WJ)(\mathbf{p}(\boldsymbol{\omega})) \mid \Phi_{\beta,k}\rangle_{L^2(\mathcal{S}^3)}, \tag{3.18}$$

then from the previous equation,

$$\frac{1}{(k+1)^2} tr\hat{\mathbf{P}}_k(\hat{\mathbf{P}}_k D_{k+1} W D_{k+1}^{-1} \hat{\mathbf{P}}_k)^q = \frac{1}{(k+1)^2} tr\mathbf{P}_{\mathbf{S}k}(\mathbf{P}_{\mathbf{S}k} V \mathbf{P}_{\mathbf{S}k})^q \tag{3.19}$$

with V the function defined on $\mathcal{S}^3$ by

$$V(\boldsymbol{\omega}) = J(\mathbf{p}(\boldsymbol{\omega}))W(\mathbf{p}(\boldsymbol{\omega})) \tag{3.20}$$

and $\mathbf{P}_{\mathbf{S}k}$ the projection onto k^{th}-order spherical harmonics defined in Eq.(2.2) of section II.

Note that the function V is initially defined just on the punctured sphere $\mathcal{S}^3$ (without the north pole) but we can extend it continuously to the whole sphere by taking $V = 0$ at the north pole. We denote the extension also by V.

We now take the limit $k \to \infty$ in both sides of Eq.(3.19) and use the Szegö Theorem for the sphere $\mathcal{S}^3$, theorem (2.4), to conclude that the right side of this equation converges to

$$\int_{\alpha\in\mathcal{A}} (\hat{V}(\alpha))^q d\mu(\alpha) = \int_{\alpha\in\mathcal{A}} (\tilde{W}(\alpha))^q d\mu(\alpha), \tag{3.21}$$

since

$$
\begin{aligned}
\hat{V}(\alpha) &= \frac{1}{2\pi}\int_0^{2\pi} V(\boldsymbol{\omega}(s,\alpha))ds \\
&= \frac{1}{2\pi}\int_0^{2\pi} W(\mathbf{p}(s,\alpha))\left(\frac{2}{(\mathbf{p}(s,\alpha))^2+1}\right)ds \\
&= \tilde{W}(\alpha) \qquad (3.22)
\end{aligned}
$$

by the definition of $\hat{V}$, and of $\tilde{W}$, Eq.(3.13). This concludes the proof of the Eq.(3.16) for monomials x^q and hence for arbitrary F.

Finally, the inner product in the left side of Eq.(3.15) in the statement of the theorem is just equal to the inner products in Eq.(3.18) with $\alpha = \beta$ which converge to $\hat{V}(\alpha) = \tilde{W}(\alpha)$ by lemma (2.1) and Eq.(3.22). This concludes the proof of the theorem. □

Section IV. Szegö-Type Theorem for the Hydrogen Bound States in Configuration Space

In this section we prove a Szegö theorem for expectations of multiplication operators in configuration space. In the following, $\Psi_{\alpha,k}$ represents the inverse Fourier transform of $\hat{\Psi}_{\alpha,k}$, i.e., the bound state in the configuration space representation. The dilation operator will act as before, and in particular,

$$D_{(k+1)^2}\Psi(\mathbf{x}) = (k+1)^3\Psi((k+1)^2\mathbf{x}). \qquad (4.1)$$

4.1 *Decaying of the functions* $\{D_{(k+1)^2}\Psi_{\alpha,k}\}$, $\mathbf{x}\to\infty$

As a first step, we need a bound on the mass of the rescaled states $\{D_{(k+1)^2}\Psi_{\alpha,k}\}$ outside a fixed ball.

Lemma 4.1 *There exists a constant $r_0 > 0$ independent of α and k such that for all non-negative integers n and s,*

$$\lim_{k\to\infty} k^s \int_{|\mathbf{x}|\geq r_0} |\ \mathbf{x}\ |^n|\ D_{(k+1)^2}\Psi_{\alpha,k}(\mathbf{x})|^2 d^3x = 0. \qquad (4.2)$$

Remark: The lemma shows, by the Schwarz inequality, that

$$\langle\Psi_{\alpha,k}|D^{-1}_{(k+1)^2}|\mathbf{x}|^n\chi_{|\mathbf{x}|>r_0}D_{(k+1)^2}|\Psi_{\beta,k}\rangle = 0(k^{-\infty}) \qquad (4.3)$$

uniformly in α and β. Here, $\chi_{|\mathbf{x}|>r_0}$ is the characteristic function for the exterior of a ball of radius r_0. Optimizing constants in the proof below, one can show that r_0 can be taken to be any number > 2 which is the maximal apogee distance for a classical orbit of energy $E = -1/2$.
Proof: It suffices to show that for $k \to \infty$,

$$k^s \int_{|\mathbf{x}\cdot\mathbf{b}|\geq r_0/2} |\mathbf{x}\cdot\mathbf{b}|^n |D_{(k+1)^2}\Psi_{\alpha,k}(\mathbf{x})|^2 d^3x \to 0 \tag{4.4}$$

for all unit vectors $\mathbf{b}$, since the integral in the left side of Eq.(4.2) is estimated by a finite sum of terms (with coefficients depending on n) of this form.

To prove Eq.(4.4) we will show below that for $q \geq 0$,

$$\|(\mathbf{x}\cdot\mathbf{b})^q D_{(k+1)^2}\Psi_{\alpha,k}(\mathbf{x})\| \leq c_0\sqrt{k}\frac{q!e^{c_1k/2}}{(k/2)^q}, \tag{4.5}$$

for positive constants c_0, c_1 independent of α and k. Eq.(4.4), and hence the conclusion of the lemma, then follow from Chebyshev's inequality and this inequality (4.5): The integral on the left side of Eq.(4.4) is less than

$$\frac{k^s}{(r_0/2)^m}\|(\mathbf{x}\cdot\mathbf{b})^{(n+m)/2}D_{(k+1)^2}\Psi_{\alpha,k}(\mathbf{x})\|^2 \leq \frac{k^s}{(r_0/2)^m}\left[c_0\sqrt{k}\frac{(\frac{n+m}{2})!e^{c_1k/2}}{(k/2)^{\frac{(n+m)}{2}}}\right]^2, \tag{4.6}$$

with $0 \leq m$ and $\frac{1}{2}(n+m) = q$. We now pick m to be the integer such that $k-1 < (n+m) \leq k$. It then follows from this inequality (4.6) that the integral (4.4) satisfies

$$k^s \int_{|\mathbf{x}\cdot\mathbf{b}|\geq r_0/2} |\mathbf{x}\cdot\mathbf{b}|^n |D_{(k+1)^2}\Psi_{\alpha,k}(\mathbf{x})|^2 d^3x \leq \frac{c_0^2\pi e k^{s+2}}{(r_0/2)^{k-n-1}}e^{(c_1-1)k} \tag{4.7}$$

with $r_0 > 2$. Here, we have used Stirling's formula to estimate the factorial in Ineq.(4.6), c.f. [3]. Provided that r_0 is chosen so that $r_0/2 > e^{c_1-1}$, it is clear that the right side of Ineq.(4.7) goes to zero, $k \to \infty$, so that indeed Ineq.(4.4) and the lemma follow from Ineq.(4.5).

Thus the task at hand is to prove Ineq.(4.5). We have that the left side of this inequality is equal to

$$\begin{aligned} \|(\mathbf{x}\cdot\mathbf{b})^q D_{(k+1)^2}\Psi_{\alpha,k}\| &= \|(\frac{\imath}{(k+1)^2}\mathbf{b}\cdot\nabla_p)^q\hat{\Psi}_{\alpha,k}\| \\ &= \|(\frac{\imath}{(k+1)^2}\mathbf{b}\cdot\nabla_p)^q D_{k+1}J^{1/2}K\Phi_{\alpha,k}\| \\ &= \|(\frac{\imath}{(k+1)}\mathbf{b}\cdot\nabla_p)^q J^{1/2}K\Phi_{\alpha,k}\|. \end{aligned} \tag{4.8}$$

Here, we have gone into the momentum representation where we have explicit expressions for the functions $\hat{\Psi}_{\alpha,k}$, see Eq.(3.7); ∇_p is the gradient with respect to the momentum variables.

To estimate the quantity (4.8), we employ some complex variable techniques. Let z be a complex variable, and consider the function

$$\begin{aligned}\exp\left(\frac{z}{(k+1)}\mathbf{b}\cdot\nabla_p\right)J^{1/2}K\Phi_{\alpha,k}(\mathbf{p}) &= J^{1/2}K\Phi_{\alpha,k}(\mathbf{p}+\frac{z}{(k+1)}\mathbf{b})\\ &= a(k)\left(\frac{2}{(\mathbf{p}+\frac{z}{(k+1)}\mathbf{b})^2+1}\right)^2\left(\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p}+\frac{z}{(k+1)}\mathbf{b})\right)^k. \end{aligned} \tag{4.9}$$

We will need an estimate on the L^2-norm of this function. It is straight-forward to see that, at least for $|z|/(k+1) < 1/2$,

$$\left|\frac{2}{(\mathbf{p}+\frac{z}{(k+1)}\mathbf{b})^2+1}\right|^2 \le \left(\frac{4}{\mathbf{p}^2+1}\right)^2. \tag{4.10}$$

Moreover, recall that $|\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p})| \le 1$ for $\mathbf{p}$ real, and also note that

$$\left|\nabla_p\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p}+\frac{z}{(k+1)}\mathbf{b})\right| \le c_1, \tag{4.11}$$

for some c_1 independent of $\mathbf{p}, \boldsymbol{\alpha}, z/(k+1)$, still with $|z|/(k+1) < 1/2$, as can be seen by considering the derivative of $\boldsymbol{\omega}$ with respect to $\mathbf{p}$ defined in Eq.(3.1). Consequently, we have that

$$\left|\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p}+\frac{z}{(k+1)}\mathbf{b})\right| \le 1+\frac{c_1|z|}{(k+1)} \tag{4.12}$$

and so

$$\left|\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p}+\frac{z}{(k+1)}\mathbf{b})\right|^k \le \left(1+\frac{c_1|z|}{(k+1)}\right)^k \le e^{c_1|z|} \tag{4.13}$$

with the same restriction on $z/(k+1)$. Combining this inequality with Ineq.(4.10) and Eq.(4.9), it follows that

$$\|\exp\left(\frac{z}{(k+1)}\mathbf{b}\cdot\nabla_p\right)J^{1/2}K\Phi_{\alpha,k}\| \le c_0\sqrt{k}e^{c_1|z|} \tag{4.14}$$

for some constant c_0 and $|z| < (k+1)/2$, since $(\mathbf{p}^2+1)^{-2}$ is in L^2 and the normalization constant $a(k)$ is $O(k^{1/2})$.

Finally, we have from Eq.(4.8) and the above Ineq.(4.14) that

$$\begin{aligned}
\|(\mathbf{x}\cdot\mathbf{b})^q D_{(k+1)^2}\Psi_{\alpha,k}(\mathbf{x})\| &= \left\| \frac{q!}{2\pi\imath}\oint_{|z|=k/2}\frac{dz}{z^{q+1}}\exp\left(\frac{z}{(k+1)}\mathbf{b}\cdot\nabla_p\right)J^{1/2}K\Phi_{\alpha,k}\right\| \\
&\leq \frac{q!}{2\pi}\oint_{|z|=k/2}\frac{|dz|}{|z|^{q+1}}\left\|\exp\left(\frac{z}{(k+1)}\mathbf{b}\cdot\nabla_p\right)J^{1/2}K\Phi_{\alpha,k}\right\| \\
&\leq \frac{q!}{(k/2)^q}c_0\sqrt{k}e^{c_1 k/2} \qquad (4.15)
\end{aligned}$$

which establishes Ineq.(4.5). This concludes the proof of the lemma. □

4.2 *Szegö Theorem in Configuration Representation*

We can now state the Szëgo theorem for multiplication operators in configuration space. In the following, the function $(\mathbf{x}(t,\alpha),\ \mathbf{p}(t,\alpha))$ is the classical Kepler motion, defined in Eqs.(3.11-3.12) of the previous section.

Theorem 4.2 Szegö Theorem in Configuration Representation
Let V be a multiplication operator with $V = V(\mathbf{x})$ a polynomially bounded continuous function on configuration space $\mathbf{R}^3$. Let $F:\mathbf{R}\to\mathbf{R}$ be a continuous function. Then

$$\lim_{k\to\infty}\langle\Psi_{\alpha,k}|D^{-1}_{(k+1)^2}VD_{(k+1)^2}|\Psi_{\alpha,k}\rangle = \frac{1}{2\pi}\int_0^{2\pi}V(\mathbf{x}(t,\alpha))dt \qquad (4.16)$$

and

$$\begin{aligned}
&\lim_{k\to\infty}\frac{1}{(k+1)^2}tr\mathbf{P}_k F(\mathbf{P}_k D^{-1}_{(k+1)^2}VD_{(k+1)^2}\mathbf{P}_k) \\
&\quad = \int_{\alpha\in\mathcal{A}}F\left(\frac{1}{2\pi}\int_0^{2\pi}V(\mathbf{x}(t,\alpha))dt\right)d\mu(\alpha). \qquad (4.17)
\end{aligned}$$

Proof: We first note that

$$\langle\Psi_{\alpha,k}|D^{-1}_{(k+1)^2}VD_{(k+1)^2}|\Psi_{\beta,k}\rangle = \langle\Psi_{\alpha,k}|D^{-1}_{(k+1)^2}V\chi_{|\mathbf{x}|\leq r_0}D_{(k+1)^2}|\Psi_{\beta,k}\rangle + O(k^{-\infty}), \qquad (4.18)$$

with $\chi_{|\mathbf{x}|\leq r_0}$ the characteristic function for the ball of radius r_0 and r_0 chosen to be that of the above lemma(4.1). This equation is a consequence of the lemma, the remark below it, and the assumption that V is polynomially bounded . It follows that

$$\mathbf{P}_k D^{-1}_{(k+1)^2} V D_{(k+1)^2} \mathbf{P}_k = \mathbf{P}_k D^{-1}_{(k+1)^2} V \chi_{|\mathbf{x}|\le r_0} D_{(k+1)^2} \mathbf{P}_k + O(k^{-\infty}), \tag{4.19}$$

since $\mathbf{P}_k$ itself is an integral over the $\Psi_{\alpha,k}$'s with a normalization constant $C(k) = (k+1)^2$. This argument shows in particular that the spectrum of $\mathbf{P}_k D^{-1}_{(k+1)^2} V D_{(k+1)^2} \mathbf{P}_k$ is in the interval $[-\|V\chi_{|\mathbf{x}|\le r_0}\|_\infty - O(k^{-\infty}), \|V\chi_{|\mathbf{x}|\le r_0}\|_\infty + O(k^{-\infty})]$.

Since the continuous function F can be approximated by a polynomial on the interval $[-\|V\chi_{|\mathbf{x}|\le r_0}\|_\infty - 1, \|V\chi_{|\mathbf{x}|\le r_0}\|_\infty + 1]$ and, as we have just seen, all of the operators $\mathbf{P}_k D^{-1}_{(k+1)^2} V D_{(k+1)^2} \mathbf{P}_k$ have spectrum in this interval, it suffices to prove the theorem for a monomial, $F(x) = x^q$, (Recall that $\frac{1}{(k+1)^2} tr \mathbf{P}_k(\cdot)$ is a normalized trace).

Let $\epsilon > 0$ and let $V_\epsilon = V_\epsilon(\mathbf{x})$ be a polynomial on $\mathbf{R}^3$ such that $|V(\mathbf{x}) - V_\epsilon(\mathbf{x})| < \epsilon$ for $|\mathbf{x}| \le r_0$. Then

$$\|\mathbf{P}_k D^{-1}_{(k+1)^2} V D_{(k+1)^2} \mathbf{P}_k - \mathbf{P}_k D^{-1}_{(k+1)^2} V_\epsilon D_{(k+1)^2} \mathbf{P}_k\| < \epsilon + O(k^{-\infty}) < 2\epsilon, \tag{4.20}$$

for k sufficiently large, as can be seen by decomposing $V - V_\epsilon$ into a part contained in the ball $\{\mathbf{x} : |\mathbf{x}| \le r_0\}$ and a part in its exterior. For the first part $V - V_\epsilon$ is bounded by ϵ; for the exterior part, one again just employs the lemma(4.1) and the remark, noting that $V - V_\epsilon$ is polynomially bounded. It then follows that

$$\begin{aligned} &\frac{1}{(k+1)^2} tr \mathbf{P}_k (\mathbf{P}_k D^{-1}_{(k+1)^2} V D_{(k+1)^2} \mathbf{P}_k)^q \\ &= \frac{1}{(k+1)^2} tr \mathbf{P}_k (\mathbf{P}_k D^{-1}_{(k+1)^2} V_\epsilon D_{(k+1)^2} \mathbf{P}_k)^q + O(\epsilon). \end{aligned} \tag{4.21}$$

Since $\Psi_{\alpha,k}$ is the Fourier transform of $D_{k+1} J^{1/2} K \Phi_{\alpha,k}$, we have that

$$\langle \Psi_{\alpha,k} | D^{-1}_{(k+1)^2} V_\epsilon D_{(k+1)^2} | \Psi_{\beta,k} \rangle = \langle J^{1/2} K \Phi_{\alpha,k} | V_\epsilon(\frac{\imath}{(k+1)} \nabla) | J^{1/2} K \Phi_{\beta,k} \rangle. \tag{4.22}$$

Thus the trace term on the right side of Eq.(4.21) is equal to

$$\begin{aligned} &\frac{1}{(k+1)^2} tr \mathbf{P}_k (\mathbf{P}_k D^{-1}_{(k+1)^2} V_\epsilon D_{(k+1)^2} \mathbf{P}_k)^q \\ &= (k+1)^{2(q-1)} \int\int \cdots \int \langle J^{1/2} K \Phi_{\alpha_1,k} | V_\epsilon(\frac{\imath}{(k+1)} \nabla) | J^{1/2} K \Phi_{\alpha_2,k} \rangle \cdots \\ &\quad \langle J^{1/2} K \Phi_{\alpha_q,k} | V_\epsilon(\frac{\imath}{(k+1)} \nabla) | J^{1/2} K \Phi_{\alpha_1,k} \rangle d\mu(\alpha_1) \cdots d\mu(\alpha_q), \end{aligned} \tag{4.23}$$

and so we need to investigate the matrix elements in Eq.(4.22).

Lemma 4.3 *For $\delta > 0$,*

$$
\begin{aligned}
&\langle J^{1/2}K\Phi_{\alpha,k}|V_\epsilon(\frac{\imath}{(k+1)}\nabla)|J^{1/2}K\Phi_{\beta,k}\rangle \\
&= \langle J^{1/2}K\Phi_{\alpha,k}|J^{1/2}K\Phi_{\beta,k}\rangle \left(\frac{1}{2\pi}\int_0^{2\pi} V_\epsilon(\mathbf{x}(t,\beta))dt + O(k^{\delta-1/2})\right) \\
&\qquad + O(k^{-\infty})
\end{aligned}
\tag{4.24}
$$

Before proving this lemma, we note that, with $\alpha = \beta$, this lemma, Eq.(4.22), and the fact that V_ϵ approximates V imply the first equation of the theorem, Eq.(4.16).
Proof of lemma: Define $W_\epsilon(\mathbf{p}, \beta, k)$ by the equation

$$
V_\epsilon(\frac{\imath}{(k+1)}\nabla)J^{1/2}K\Phi_{\beta,k}(\mathbf{p}) \equiv W_\epsilon(\mathbf{p}, \beta, k)J^{1/2}K\Phi_{\beta,k}(\mathbf{p}). \tag{4.25}
$$

Then using the definition of $J^{1/2}K\Phi_{\alpha,k}$, (cf. Eq.(4.9) with $z = 0$), one sees that W_ϵ is in fact a polynomial in $\imath\nabla\ln(\boldsymbol{\beta}\cdot\boldsymbol{\omega}(\mathbf{p}))$, $(\imath/(k+1))\nabla\ln(\mathbf{p}^2+1)$, and $1/(k+1)$ times derivatives of these quantities of order no higher than the degree of the polynomial V_ϵ. Away from the set where $\boldsymbol{\beta}\cdot\boldsymbol{\omega}(\mathbf{p}) = 0$, we have that

$$
W_\epsilon(\mathbf{p}, \beta, k) = V_\epsilon(\imath\nabla\ln(\boldsymbol{\beta}\cdot\boldsymbol{\omega}(\mathbf{p})) + O(1/k). \tag{4.26}
$$

Moreover, the expression $V_\epsilon(\frac{\imath}{(k+1)}\nabla)J^{1/2}K\Phi_{\beta,k}$ is equal to a bounded function times $(\boldsymbol{\beta}\cdot\boldsymbol{\omega}(\mathbf{p}))^{k-d}$ where d is the degree of V_ϵ. These remarks can be summarized as follows: That for $0 < \epsilon' < 1/4$, there exists a function $\tilde{W}_\epsilon(\mathbf{p}, \beta, k)$, C^∞ in $\mathbf{p}$, and such that

$$
V_\epsilon(\frac{\imath}{(k+1)}\nabla)J^{1/2}K\Phi_{\beta,k}(\mathbf{p}) = \tilde{W}_\epsilon(\mathbf{p}, \beta, k)J^{1/2}K\Phi_{\beta,k}(\mathbf{p}) + O(k^{-\infty}) \tag{4.27}
$$

with

$$
\begin{aligned}
\tilde{W}_\epsilon(\mathbf{p}, \beta, k) &= W_\epsilon(\mathbf{p}, \beta, k) = V_\epsilon(\imath\nabla\ln(\boldsymbol{\beta}\cdot\boldsymbol{\omega}(\mathbf{p})) + O(1/k) \\
&\qquad\qquad \text{on } |\boldsymbol{\beta}\cdot\boldsymbol{\omega}(\mathbf{p})| \geq 1-\epsilon' \\
&= 0 \qquad\qquad \text{on } |\boldsymbol{\beta}\cdot\boldsymbol{\omega}(\mathbf{p})| < 1-2\epsilon'.
\end{aligned}
\tag{4.28}
$$

Using these remarks, we proceed just as we did in the proof of the Szegö theorem in momentum space Theorem(3.1) to conclude that

$$
\begin{aligned}
&\langle J^{1/2}K\Phi_{\alpha,k}|V_\epsilon(\frac{\imath}{(k+1)}\nabla)|J^{1/2}K\Phi_{\beta,k}\rangle \qquad (4.29)\\
&= \langle J^{1/2}K\Phi_{\alpha,k}|\tilde{W}_\epsilon(\mathbf{p},\beta,k)|J^{1/2}K\Phi_{\beta,k}\rangle + O(k^{-\infty})\\
&= \langle J^{1/2}K\Phi_{\alpha,k}|J^{1/2}K\Phi_{\beta,k}\rangle \left(\frac{1}{2\pi}\int \tilde{W}_\epsilon(\mathbf{p}(t,\beta),\beta,k)dt + O(k^{\delta-1/2})\right)+O(k^{-\infty}).
\end{aligned}
$$

Now the integral of $\tilde{W}_\epsilon(\mathbf{p}(t,\beta),\beta,k)$ in this last expression is equal to

$$\int V_\epsilon(\imath\nabla\ln(\boldsymbol{\beta}\cdot\boldsymbol{\omega}(\mathbf{p}(t,\beta))dt + O(1/k) \qquad (4.30)$$

by Eq.(4.28) since $\mathbf{p}(t,\beta)$ runs over the path where $|\boldsymbol{\beta}\cdot\boldsymbol{\omega}(\mathbf{p})| = 1$. If $\mathbf{x}(t,\beta)$ is defined

$$\mathbf{x}(t,\beta) \equiv \imath\nabla\ln(\boldsymbol{\beta}\cdot\boldsymbol{\omega}(\mathbf{p}(t,\beta)) \qquad (4.31)$$

then, seemingly miraculously, it is equal to the real-valued function $\mathbf{x}(t,\beta)$ defined by Eqs.(3.11)-(3.12) of the previous section (III). Actually, the definition of $\mathbf{x}(t,\beta)$ was motivated by this last equation Eq.(4.31); in so far as there is a miracle, it is that this choice of $\mathbf{x}(t,\beta)$ and $\mathbf{p}(t,\beta)$ satisfy Hamilton's equations for the Kepler orbit β.

Substituting Eq.(4.31) into Eq.(4.30), and in turn substituting this integral into Eq.(4.29), we obtain the statement of the lemma, Eq.(4.24). □

We now complete the proof of the Szegö Theorem, Theorem(4.2). We substitute the asymptotic expressions for the matrix elements of the above lemma, Eq.(4.24) into the multiple integral Eq.(4.23) thereby obtaining an integral which, by the second line of Eq.(4.29), is precisely of the form considered in the proof of the Szegö theorem (3.1) of the last section, (cf. Eq.(3.17)). Hence,

$$
\begin{aligned}
&\frac{1}{(k+1)^2} tr\mathbf{P}_k(\mathbf{P}_k D^{-1}_{(k+1)^2} V_\epsilon D_{(k+1)^2}\mathbf{P}_k)^q\\
&= \int \left(\frac{1}{2\pi}\int V_\epsilon(\mathbf{x}(t,\alpha))dt\right)^q d\mu(\alpha) + O(k^{\delta-1/2})\\
&= \int \left(\frac{1}{2\pi}\int V(\mathbf{x}(t,\alpha))dt\right)^q d\mu(\alpha) + O(k^{\delta-1/2}) + O(\epsilon), \qquad (4.32)
\end{aligned}
$$

the last equality holding since V differs from V_ϵ by at most ϵ in the ball $\{\mathbf{x} : |\mathbf{x}| \le r_0\}$, and the classical orbits $\mathbf{x}(t,\alpha)$ all have apogees of magnitude less than $2 < r_0$. But by Eq.(4.21), we therefore have that

$$\frac{1}{(k+1)^2} tr \mathbf{P}_k (\mathbf{P}_k D^{-1}_{(k+1)^2} V D_{(k+1)^2} \mathbf{P}_k)^q$$
$$= \int \left(\frac{1}{2\pi} \int V(\mathbf{x}(t,\alpha)) dt \right)^q d\mu(\alpha) + O(k^{\delta - 1/2}) + O(\epsilon), \qquad (4.33)$$

implying the theorem for F a monomial x^q, and so the theorem in general. □

4.3 *Probability densities* $|D_{(k+1)^2}\Psi_{\alpha,k}|^2$ *for* k *large*

We conclude this section with some remarks concerning the dilated states $D_{(k+1)^2}\Psi_{\alpha,k}$. These states can be expressed as the Fourier transform,

$$D_{(k+1)^2}\Psi_{\alpha,k}(\mathbf{x}) = \frac{(k+1)^3}{(2\pi)^{3/2}} \int \exp\left(i(k+1)^2 \mathbf{x}\cdot\mathbf{p}\right) \hat{\Psi}_{\alpha,k}(\mathbf{p}) d^3p$$
$$= \frac{(k+1)^{3/2}}{(2\pi)^{3/2}} \int \exp\left(i(k+1)\mathbf{x}\cdot\mathbf{p}\right) D^{-1}_{k+1} \hat{\Psi}_{\alpha,k}(\mathbf{p}) d^3p$$
$$= \frac{a(k)(k+1)^{3/2}}{(2\pi)^{3/2}} \int \left(\frac{2}{\mathbf{p}^2+1} \right)^2 \exp\left[((k+1) i\mathbf{x}\cdot\mathbf{p} + k \ln(\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p})))\right] d^3p \qquad (4.34)$$

by Eq.(3.7) defining the states $\hat{\Psi}_{\alpha,k}$. This latter integral representation for the dilated states suggests an analysis by the saddle point method. The analysis leads immediately to a computation of the critical points of $(i\mathbf{x}\cdot\mathbf{p} + \ln(\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p})))$ where $|\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p})| = 1$. Note that the resulting equation for the critical points is just

$$\mathbf{x} = i\nabla_p \ln(\boldsymbol{\alpha}\cdot\boldsymbol{\omega}(\mathbf{p}))), \qquad (4.35)$$

precisely the same equation Eq.(4.31) encountered in the proof of the Szegö theorem above. A detailed analysis, carried out in [18], shows that in a neighborhood of a point $\mathbf{x}$ on the Kepler orbit α, $D_{(k+1)^2}\Psi_{\alpha,k}$ decays away from $\mathbf{x}$ in a Gaussian-like manner in directions transverse to the orbit and oscillates with frequency $O(k)$ along the orbit. The width of the Gaussian is $O(k^{-1/2})$. Away from the orbit, the function is $O(k^{-\infty})$. Moreover, and somewhat symbolically,

$$|D_{(k+1)^2}\Psi_{\alpha,k}|^2(\mathbf{x}) \overset{k\to\infty}{\longrightarrow} \frac{1}{2\pi} \frac{1}{|\frac{d\mathbf{x}}{dt}|} \delta_{\text{trans}}(\mathbf{x}). \qquad (4.36)$$

Here, δ_{trans} is a delta function in coordinates transverse to the orbit; the reciprocal of the speed $|\frac{d\mathbf{x}}{dt}|$ is the occupation time density of the Kepler orbit at

$\mathbf{x}$, and the normalization factor $1/2\pi$ arises since 2π is the period for all orbits α having energy $-1/2$.

Appendix. Coordinates for integrals over $\mathcal{A}$

In this appendix we provide a parametrization for integrals over $\mathcal{A}$, in particular, a formula for $d\mu(\alpha)$.

We first relate $d\mu(\alpha)$ to Haar measure on the group SO(4). Recall that $\alpha = \boldsymbol{\alpha} \in \mathcal{A}$ is actually a 4-vector. Let $F = F(\alpha)$ be an integrable function, and let $\mathcal{R}(g)$, $g \in SO(4)$, be a 4-dimensional rotation matrix. Then

$$\begin{aligned} \int F(\alpha) d\mu(\alpha) &= \int F(\mathcal{R}(g)\alpha) d\mu(\alpha) \\ &= \int\int F(\mathcal{R}(g)\alpha) d\mu(\alpha) d\mu_H(g) \\ &= \int F(\mathcal{R}(g)\alpha_0) d\mu_H(g), \end{aligned} \tag{A.1}$$

where $d\mu_H(g)$ is normalized Haar measure on $SO(4)$. Here, we have used the group invariance of the (normalized) measure $d\mu(\alpha)$, and interchanged the order of integration in the double integral. Doing the integral over g first, we obtain a function constant in α so that the α-integration is trivial. Finally, α_0 is arbitrary since rotations act transitively on $\mathcal{A}$; a convenient choice for it will be given below.

We proceed to a parametrization of the rotation matrices, $\{\mathcal{R}(g)\}$. We first define three orthonormal 3-vectors,

$$\begin{aligned} \hat{\mathbf{n}} &= (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)), \\ \hat{\mathbf{u}} &= (\sin(\phi), -\cos(\phi), 0), \\ \hat{\mathbf{v}} &= (\cos(\theta)\cos(\phi), \cos(\theta)\sin(\phi), -\sin(\theta)), \end{aligned} \tag{A.2}$$

where θ, ϕ are the usual spherical coordinates on a 2-sphere. Next, in a fairly obvious notation, define the four orthonormal 4-vectors:

$$\begin{aligned} \boldsymbol{\omega} &= (\cos(\psi)(-\sin(\gamma)\hat{\mathbf{u}} + \cos(\gamma)\hat{\mathbf{v}}), \sin(\psi)), \\ \boldsymbol{\xi} &= (-\cos(\gamma)\hat{\mathbf{u}} - \sin(\gamma)\hat{\mathbf{v}}, 0), \\ \boldsymbol{\eta} &= (\sin(\psi)(-\sin(\gamma)\hat{\mathbf{u}} + \cos(\gamma)\hat{\mathbf{v}}, -\cos(\psi)), \\ \boldsymbol{\zeta} &= (\hat{\mathbf{n}}, 0), \end{aligned} \tag{A.3}$$

where $0 \leq \psi \leq \pi/2$ and $0 \leq \gamma \leq 2\pi$. Finally let $\mathcal{R} = \mathcal{R}(\psi, \theta, \phi, \gamma, \beta, \delta)$ be the rotation matrix with column vectors

$$\begin{aligned} \mathcal{R}(\psi, \theta, \phi, \gamma, \beta, \delta) &= (\cos(\beta)\boldsymbol{\omega} + \sin(\beta)\boldsymbol{\xi}, -\sin(\beta)\boldsymbol{\omega} + \cos(\beta)\boldsymbol{\xi}, \\ &\quad \cos(\delta)\boldsymbol{\eta} + \sin(\delta)\boldsymbol{\zeta}, -\sin(\delta)\boldsymbol{\eta} + \cos(\delta)\boldsymbol{\zeta}), \end{aligned} \tag{A.4}$$

where $0 \leq \beta, \delta \leq 2\pi$.

Let $d\mathcal{R} = d\mathcal{R}(\psi, \theta, \phi, \gamma, \beta, \delta)$ be the matrix of differentials of $\mathcal{R}$. Then $\mathcal{R}^{-1}d\mathcal{R}$ has left-invariant 1-forms as entries, and a wedge-product of six independent entries (the upper off-diagonal entries) is proportional to Haar measure, [14]. One finds after considerable computation that

$$d\mu_H(\psi, \theta, \phi, \gamma, \beta, \delta) = \frac{1}{(2\pi)^4} \cos(\psi)\sin(\psi)\sin(\theta) d\psi d\theta d\phi d\gamma d\beta d\delta. \tag{A.5}$$

The rotation matrix $\mathcal{R}$ defined in Eq.(A.4) maps $\alpha_0 \equiv (1, \imath, 0, 0)$ to

$$\alpha(\psi, \theta, \phi, \beta, \gamma) = \exp(-\imath\beta)(\boldsymbol{\omega} + \imath\boldsymbol{\xi}), \tag{A.6}$$

and it maps the great circle $\mathcal{O}_0 = \{(\cos(s), \sin(s), 0, 0)\}$ spanned by the real and imaginary parts of α_0 to the great circle

$$\mathcal{O}(\psi, \theta, \phi, \gamma) = \{\cos(s)\boldsymbol{\omega} + \sin(s)\boldsymbol{\xi}\} \tag{A.7}$$

corresponding to α. Suppose now that $F(\alpha) = f(\mathcal{O})$ is just a function of the orbit only, hence in our parametrization, independent of β, δ. Then by the remarks in the first paragraph and the expression above for Haar measure, we have that

$$\int_{\mathcal{A}} F(\alpha) d\mu(\alpha) = \frac{1}{(2\pi)^2} \int\int\int\int f(\mathcal{O}(\psi, \theta, \phi, \gamma)) \cos(\psi)\sin(\psi)\sin(\theta) d\psi d\theta d\phi d\gamma. \tag{A.8}$$

If instead we are computing an integral over the space of Kepler orbits with energy $E = -1/2$, then such orbits are conveniently specified by the angular momentum $\mathbf{L}$ and the Runge-Lenz vector $\mathbf{A}$, defined by the following equations:

$$\mathbf{L} = \mathbf{x} \times \mathbf{p}, \tag{A.9}$$

$$\mathbf{A} = \mathbf{p} \times \mathbf{L} - \frac{\mathbf{x}}{|\,\mathbf{x}\,|}, \tag{A.10}$$

and where $\mathbf{L}$ and $\mathbf{A}$ must satisfy the restrictions:

$$\begin{aligned} \mathbf{L}^2 + \mathbf{A}^2 &= 1 \qquad \text{(A.11)} \\ \mathbf{L} \cdot \mathbf{A} &= 0, \qquad \text{(A.12)} \end{aligned}$$

the first equation coming from $E = -1/2$, the latter from the definition of $\mathbf{L}$ and $\mathbf{A}$, using that $\mathbf{x}$ and $\mathbf{L}$ must be orthogonal. Taking the cross-product with $\mathbf{L}$ in both sides of Eq.(A.10), we obtain the following equation for the momentum vector:

$$\mathbf{p} - \frac{\mathbf{L} \times \mathbf{A}}{\mid \mathbf{L} \mid^2} = \frac{\mathbf{L} \times \mathbf{x}}{\mid \mathbf{L} \mid^2 \mid \mathbf{x} \mid} \qquad \text{(A.13)}$$

where we are assuming $\mid \mathbf{L} \mid \neq 0$ (i.e. we are just dealing with elliptical orbits but not with collision orbits). Again, since $\mathbf{x}$ and $\mathbf{L}$ are orthogonal, this last equation shows that the vector $\mathbf{p}$ is in the plane perpendicular to $\mathbf{L}$ and that $\mathbf{p}$ winds around a circle with center $\frac{\mathbf{L} \times \mathbf{A}}{|\mathbf{L}|^2}$ and radius $\frac{1}{|\mathbf{L}|}$.

Suppose now that $\mathbf{L}$ and $\mathbf{A}$ are parametrized:

$$\begin{aligned} \mathbf{L} &= \cos(\psi)(\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)) \qquad \text{(A.14)} \\ \mathbf{A} &= \sin(\psi)(\cos(\gamma)\hat{\mathbf{u}} + \sin(\gamma)\hat{\mathbf{v}}) \qquad \text{(A.15)} \end{aligned}$$

with $\psi \in [0, \pi/2]$, θ, ϕ usual spherical coordinates, and $\gamma \in [0, 2\pi]$. (These angles do indeed parametrize the solutions to Eqs.(A.11,A.12).) Then one can check that the momentum circle defined by Eq.(A.13) with $\mathbf{L}, \mathbf{A}$ given by Eqs.(A.14,A.15) is transformed by the standard inverse stereographic map to the great circle $\mathcal{O}(\psi, \theta, \phi, \gamma)$ defined in Eq.(A.7) above. Consequently, if $F(\alpha) = f(\mathbf{L}, \mathbf{A})$ is just a function the great circle orbit, with that orbit equal to the inverse stereographic image of the Kepler orbit specified by $\mathbf{L}, \mathbf{A}$, then

$$\int_{\mathcal{A}} F(\alpha) d\mu(\alpha) = \frac{1}{(2\pi)^2} \int\int\int\int f(\mathbf{L}, \mathbf{A}) \cos(\psi) \sin(\psi) \sin(\theta) d\psi d\theta d\phi d\gamma, \qquad \text{(A.16)}$$

with $\mathbf{L}, \mathbf{A}$ in the integrand on the right side expressed in terms of $\psi, \theta, \phi, \gamma$ by Eqs.(A.14,A.15).

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