

## Convergence properties of Fock's expansion for S-state eigenfunctions of the helium atom

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It is proved by functional analytic methods that for S-state solutions of Schrödinger's equation for the helium atom, Fock's expansion in powers of  $R^{1/2}$  and  $R \ln R$ , where  $R$  is the hyperspherical radius  $r_1^2 + r_2^2$ , converges pointwise for all  $R$ , thereby generalising a result of Macek that the expansion converges in the mean for all  $R < \frac{1}{2}$ . It is shown that for any value (even complex) of the energy  $E$ , Schrödinger's equation, considered as a partial differential equation with no boundary condition at  $R = \infty$ , has infinitely many solutions representable by an expansion of the type proposed by Fock. Some of the open problems are discussed in determining whether for  $E$  in the point spectrum of the atomic Hamiltonian the physical eigenfunction  $\Psi_E$ , which has exponential decay as  $R \rightarrow \infty$ , is representable by Fock's expansion.

**Key words:** Helium atom eigenfunctions — Fock's expansion — Convergence properties — Functional analysis

Finding a series expansion for the eigenfunctions of many-electron atoms in general and the helium atom in particular was the goal of several workers in the twenty years after the discovery of wave mechanics. In 1935, it was observed by Bartlett, Gibbons, and Dunn that no expansion for the wavefunction  $\psi$  of the helium atom in powers of the variables  $r_1$ ,  $r_2$ , and  $r_{12}$  would satisfy Schrödinger's equation [1]. (Here  $r_1$  and  $r_2$  are the distances of each electron from the nucleus and  $r_{12}$  is the interelectronic separation.) Soon thereafter Bartlett pointed out that the physical ground-state wavefunction  $\psi$  can have *no* convergent expansion of the form

$$\psi = \sum_{j=0}^{\infty} (r_1^2 + r_2^2)^{j/2} a^{(j)}(\beta, \phi),$$

where  $\beta$  and  $\phi$  are hyperspherical angles and  $(r_1^2 + r_2^2)^{1/2}$  is the hyperspherical radius [2]. Unfortunately, this conclusion has not always been universally appreciated. Bartlett further observed that *formally* Schrödinger's equation seemed to allow solutions of the form

$$\sum_{j=0}^{\infty} \sum_{k=0}^{\infty} (r_1^2 + r_2^2)^{j/2} (\ln(r_1^2 + r_2^2))^{1/2 k} c^{(j,k)}(\beta, \phi)$$

but the relation of such an expansion to the physical  $\psi$  was not clear.

In 1954, V. A. Fock, who at the time was unaware of Bartlett's work, rediscovered the fact that no expansion in powers of  $(r_1^2 + r_2^2)^{1/2}$  with coefficients which are well-behaved functions of the hyperspherical angles can be a solution of Schrödinger's equation for  $S$ -states of the helium atom. He also proposed that the expansion be generalised to include powers of logarithms of the hyperspherical radius, in which case there do exist formal solutions of Schrödinger's equation (considered as a partial differential equation with no boundary condition at  $r_1^2 + r_2^2 = \infty$ ) with coefficients which are well-behaved functions of the hyperspherical angles [3]. Generalisations of Fock's expansion to many-electron atoms with  $L \neq 0$ , and closed-form expressions for the first few coefficients of Fock's expansion have also been derived [4–6]. However, the convergence properties of Fock's expansion have received comparatively little attention; for 25 years the only study was that of Macek [16]. For most expansions in atomic and molecular physics, such as those for the Stark and the Zeeman effects and the  $1/R$ -expansion for interatomic forces, experiments left no doubt that the expansions represented the physics correctly, even though the precise mathematical nature of the expansions was determined only recently [7]. Thus mathematical results on the convergence of Fock's expansion provide the only method for determining the relationship of Fock's expansion to atomic eigenfunctions.

Finding the analytical structure of the cusp in the wavefunction at  $r_1 = 0$ ,  $r_2 = 0$ ,  $r_{12} = 0$  is of considerable interest to those who do highly accurate variational calculations on few-electron atoms, for it is extremely advantageous to choose basis functions which have the same analytic structure as the wavefunction one is trying to approximate. This intuition, which was discussed by Kato [8], was developed extensively a few years later by Schwartz [9], and recent results have been presented in joint work with Bruno Klahn [10]. A practical example was furnished by the work of Frankowski and Pekeris [11], which has not always received the attention it deserves. In 1959, Pekeris published his famous calculation on the ground state of helium using a basis of 1078 Laguerre functions, which yielded an energy of  $-2.903724375$  a.u. [12]. In 1966, Frankowski and Pekeris included in their basis functions containing up to two powers of logarithms. A variational calculation with 246 basis functions yielded an energy of  $-2.9037243770326$  a.u., which probably is within about  $2 \times 10^{-12}$  a.u. of the 'exact' non-relativistic energy. (Recent work with D. Freund and B. Huxtable [27] has yielded a variational upper bound to the energy of  $-2.9037243770340$  a.u.) In other words, by including functions containing up to two powers of logarithms one is able to use a basis only  $\frac{1}{4}$  as large and simultaneously to reduce the error

from  $2 \times 10^{-9}$  a.u. to about  $2 \times 10^{-12}$  a.u., an improvement in accuracy by about a factor of 1000. This striking example of the accelerated rate of convergence was interpreted by Frankowski and Pekeris as confirming the presence of logarithmic terms in the wavefunction for the helium atom. However, we should remember that the improved convergence when one includes logarithmic terms resembling those proposed by Fock does not *necessarily* imply that Fock's expansion represents an eigenfunction of the helium atom. For example, it was found by Schwartz that the inclusion of terms containing fractional powers such as  $(r_1 + r_2)^{1/2}$  resulted in an improved rate of convergence of the variational calculations for the helium atom [13], but no one would maintain that such terms are present in the expansion of helium eigenfunctions about the point  $r_1 + r_2 = 0$  [14].

In this paper we shall prove that Schrödinger's equation for  $L=0$  states of the helium atom, or any other two-electron ion, considered as a partial differential equation with *no* boundary condition at  $r_1^2 + r_2^2 = \infty$ ,

$$\left( -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \right) \psi_E = E\psi_E$$

has infinitely many solutions  $\psi_E$  for any  $E$  (even complex) which are representable by convergent expansions in powers of  $(r_1^2 + r_2^2)^{1/2}$  and  $\ln(r_1^2 + r_2^2)$  of the type proposed by Fock. The main question which we have not yet been able to answer is whether for  $E$  in the discrete spectrum, one of the solutions  $\psi_E$  of the partial differential equation which have a convergent Fock expansion has exponential fall-off instead of exponential blowup as  $r_1$  or  $r_2$  tends to infinity. We firmly believe that the answer to this question is "yes", but finding a mathematical proof would require the generalisation of the theory of ordinary differential equations with regular singular points to partial differential equations. Recently, in a series of announcements Jean Leray [25] has sketched a proof that the physical eigenfunction is representable by a series of the type proposed by Fock which converges for all  $R$  less than some constant  $R_c$ ; the details have not yet been published.

The proof of the convergence of Fock's expansion is presented in seven sections. In Section 1 we shall review the derivation of the recursive differential equations which determine the coefficients of Fock's expansion. The second-order partial differential operator  $\square^*$ , the Laplace-Beltrami operator on the 3-dimensional hypersphere ( $S^3$ ) imbedded in the 4-dimensional space ( $\mathbb{R}^4$ ), plays a fundamental role in the recursive differential equations.  $\square^*$  is the analogue of the square of the angular momentum operator on the ordinary 2-dimensional sphere ( $S^2$ ) imbedded in the ordinary 3-dimensional space ( $\mathbb{R}^3$ ). The spectral properties of  $-\square^*$  are discussed in Sect. 2, where a closed-form expression for the integral kernel of the square of the resolvent of  $-\square^*$  is also obtained. In Sect. 3, we derive estimates of the norms of certain operators which appear frequently in our proofs. In Sect. 4 an inductive proof of the internal consistency of Fock's differential recurrence relation is given. In Sect. 5 we outline how a proof of convergence would go if the recursive differential equation were rather simpler. In Sect. 6 the full recurrence relation is tackled, and we prove that for each non-negative value of  $R = r_1^2 + r_2^2$ , the series for  $\psi_E(R)$  converges to a function

in  $L^2(S^3)$ . In Sect. 7, we prove that for all non-negative  $R$ , the series for  $\psi_E(R)$  converges to a function in  $L^\infty(S^3)$ , and that the function  $\psi_E(R)$  satisfies the partial differential equation with no boundary condition at  $R = \infty$ . Our conclusions and suggestions for further research are presented in Sect. 8. An integral, the evaluation of which is rather involved, is treated in the Appendix.

After this article was written the author became aware of a short article by Macek [15], which modulo a few technical details provides a proof that the Fock expansion converges in  $L^2(S^3)$  for all  $R < \frac{1}{2}$ . This little-known article deserves far more attention than it has received in the literature. My own Sect. 6 would have been somewhat shorter if I had used Macek's line of attack, but the proof given here of the stronger result that the Fock expansion converges in  $L^\infty(S^3)$  for all  $R$  requires lengthy derivations of upper bounds to the kernels of various integral operators.

### 1. Fundamental equations of Fock's expansion

It is well known that  $S$ -states of two-electron atoms and ions can be described by the three variables  $r_1$ ,  $r_2$ , and  $r_{12}$ , where  $r_1$  and  $r_2$  are the distances of each electron from the nucleus and  $r_{12}$  is the interelectronic separation. In these variables the kinetic energy is a rather complicated operator [16], while the potential energy is quite simple. Since most mathematical treatments of Schrödinger's equation make use of the fact that the kinetic energy operator dominates the potential energy operator, it is very convenient to have a simple representation of the kinetic energy operator regardless of how complicated the potential energy operator may then become. In other words, we shall use simple closed-form expressions for the kinetic energy operator and powers of its resolvent and the specific form of the potential energy operator will matter relatively little since we shall need to know only its qualitative properties. One of the major benefits of Fock's work was the discovery of a coordinate system which made the kinetic energy operator particularly simple. Let us now review Fock's treatment of Schrödinger's equation for a two-electron atom [3].

Fock's idea was to define three new variables  $R$ ,  $\alpha$ , and  $\theta$  by

$$\begin{aligned} R &= r_1^2 + r_2^2 \\ \alpha &= 2 \arccos (r_2 / R^{1/2}) = 2 \arcsin (r_1 / R^{1/2}) \\ \cos \theta &= \mathbf{r}_1 \cdot \mathbf{r}_2 / (r_1 r_2) = \frac{1}{2}(r_1^2 + r_2^2 - r_{12}^2) / r_1 r_2. \end{aligned} \tag{1.1}$$

Notice that  $R$  is *quadratic* in the usual distance variables, so  $R^{1/2}$  is *linear* in them. The variable  $\theta$  is the angle between the vectors  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , where both are considered to be elements of the same 3-dimensional space  $\mathbb{R}^3$ . The variable  $\alpha$  does not seem to have a simple interpretation within the usual space  $\mathbb{R}^3$ . The inverse transformation is given by

$$\begin{aligned} r_1 &= R^{1/2} \sin (\alpha / 2) \\ r_2 &= R^{1/2} \cos (\alpha / 2) \\ r_{12} &= R^{1/2} (1 - \sin \alpha \cos \theta)^{1/2}. \end{aligned} \tag{1.2}$$

In these hyperspherical variables Schrödinger's equation for a two-electron atom with  $L = 0$  is

$$\left( R^2 \frac{\partial^2}{\partial R^2} + 3R \frac{\partial}{\partial R} + \square^* \right) \psi = \left( \frac{1}{2} R^{1/2} U - \frac{1}{2} R E \right) \psi \quad (1.3)$$

where  $\square^*$  is the Laplace-Beltrami operator on  $S^3$

$$\square^* = \frac{1}{\sin^2 \alpha} \left\{ \frac{\partial}{\partial \alpha} \left( \sin^2 \alpha \frac{\partial}{\partial \alpha} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right\} \quad (1.4)$$

and  $U$  is the usual potential energy operator multiplied by  $R^{1/2}$

$$\begin{aligned} U(\alpha, \theta) &= R^{1/2} \left\{ -\frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \right\} \\ &= -Z \left[ \frac{1}{\sin(\alpha/2)} + \frac{1}{\cos(\alpha/2)} \right] + (1 - \sin \alpha \cos \theta)^{-1/2}. \end{aligned} \quad (1.5)$$

(Since both  $U$  and a physical wavefunction  $\Psi$  are constant in the third hyperspherical angle  $\phi$ , the trivial  $\phi$ -dependence of all quantities will be suppressed.) If one tries the *ansatz* for  $\Psi$

$$\psi(R, \alpha, \theta) = \sum_{j=0}^{\infty} R^{j/2} \psi_j(\alpha, \theta) \quad (1.6)$$

one obtains a coupled recursive differential equation for the  $\psi_j$ 's

$$\left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \psi_j = -\frac{1}{2} U \psi_{j-1} + \frac{1}{2} E \psi_{j-2}.$$

This equation can be solved for  $j=0$  and  $j=1$ ; if we take  $\psi_0=1$ , then  $\psi_1 = -Z(\sin(\alpha/2) + \cos(\alpha/2)) + \frac{1}{2}(1 - \sin \alpha \cos \theta)^{1/2}$ . However, if  $j=2$ , then a contradiction is obtained. The right side  $-\frac{1}{2} U \psi_1 + \frac{1}{2} E \psi_0$  is in the Hilbert space  $L^2(S^3)$ , so  $\psi_2$  must be in  $D(-\square^*)$ , the domain of  $-\square^*$ . In order for the equation to have a solution in  $D(-\square^*)$ , it is necessary that the right side be orthogonal to every function in the kernel of  $(-\square^* - 3)$ , in particular, to  $\sin \alpha \cos \theta$ . However, the right side has a non-zero projection on this function. Therefore, Fock suggested that powers of  $\ln R$  be included in the expansion:

$$\psi(R, \alpha, \theta) = \sum_{j=0}^{\infty} \sum_{k=0}^{[j/2]} R^{j/2} (\ln R)^k \psi_{j,k}(\alpha, \theta). \quad (1.7)$$

The expression  $[j/2]$  means "the largest integer which does not exceed  $j/2$ ". (Our summation index  $j$  is slightly different from Fock's. Fock summed up *half-integral* powers of  $R$ , while we sum over *integral* powers of  $R^{1/2}$ .) If the *ansatz* (1.7) is inserted into Schrödinger's equation (1.3), the following differential recurrence relation for the  $\psi_{j,k}$ 's is obtained:

$$\begin{aligned} \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \psi_{j,k} &= (j+2)(k+1) \psi_{j,k+1} + (k+1)(k+2) \psi_{j,k+2} \\ &\quad - \frac{1}{2} U \psi_{j-1,k} + \frac{1}{2} E \psi_{j-2,k}. \end{aligned} \quad (1.8)$$

The first few  $\psi_{j,k}$ 's have been obtained in closed form by Fock [3] and Ermolaev [5]. Within a normalisation constant, it has been found for singlet states that

$$\begin{aligned} \psi_{0,0} &= 1 \\ \psi_{1,0} &= -Z(\sin(\alpha/2) + \cos(\alpha/2)) + \frac{1}{2}(1 - \sin\alpha \cos\theta)^{1/2} \\ \psi_{2,1} &= -Z \frac{\pi - 2}{6\pi} \sin\alpha \cos\theta. \end{aligned} \tag{1.9}$$

$\psi_{2,0}$  and all the other  $\psi_{j,k}$ 's with  $j \geq 3$  have never been obtained in closed form. This lack of knowledge of all but the first few  $\psi_{j,k}$ 's probably is the primary reason that there has been only one previous study, that of Macek, on the convergence properties of Fock's expansion (1.7).

In proving the convergence of (1.7), the first hurdle one faces is that the expansion does not seem to be a power series in a single function of  $R$ , so the usual theory of analytic functions is not applicable immediately. However, if we define the variables  $s$  and  $t$  by

$$s = R^{1/2}, \quad t = R \ln R \tag{1.10}$$

and replace the summation index  $j$  with a new index  $n$ , where  $n = j - 2k$ , we can rewrite the series (1.7) as

$$\psi(s, t; \alpha, \theta) = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} s^n t^k \psi_{n+2k,k}(\alpha, \theta). \tag{1.11}$$

This expansion is a standard power series in the variables  $s$  and  $t$ . If we can prove that (1.11) converges for all values of  $s$  and  $t$ , it certainly will converge for those real values of  $s$  and  $t$  which satisfy

$$t = s^2 \ln(s^2) \tag{1.12}$$

the equation for those  $s$  and  $t$  which are related in the physical manner by Eqs. (1.10). Since the theory of the convergence of power series in two independent variables is very much analogous to the theory of the convergence of power series in a single variable [17], if one wants to prove that the series (1.11) converges for all complex  $s$  and  $t$ , it suffices to prove that the coefficient of  $s^n t^k$  falls off factorially quickly in  $n$  and  $k$ . In particular, an estimate of the form

$$\|\psi_{n+2k,k}\| \leq C \frac{A^n B^k}{(n!)^{3/16} k!} \tag{1.13}$$

will be sufficient to prove that the series (1.11) converges for all complex  $s$  and  $t$ . (In (1.13), the symbol  $\|\psi\|$  will denote first the  $L^2$ -norm and then the  $L^\infty$ -norm, which latter is essentially the maximum absolute value of the function.) Since  $n \leq n + 2k$ , it would also suffice to have an estimate of the form (1.13) with  $n!$  replaced by  $(n + 2k)!$ , and transforming back to the summation index  $j = n + 2k$ , we see that it will be enough to prove an estimate of the form

$$\|\psi_{j,k}\| \leq C \frac{A^j B^k}{(j!)^{3/16} k!} \tag{1.14}$$

for some fixed positive numbers  $A$ ,  $B$ , and  $C$ .

We shall use the differential recurrence relation (1.8) to derive an estimate of the form (1.14). To begin, it will be helpful to simplify (1.8) by eliminating the factors of  $(k+1)$  and  $(k+1)(k+2)$  from the right side of (1.8). To this end let  $\phi_{j,k}$  be defined by

$$\psi_{j,k} = \frac{\phi_{j,k}}{4^k k!}. \quad (1.15)$$

If we substitute  $\phi_{j,k}$  for  $\psi_{j,k}$  in the recurrence relation (1.8), we obtain

$$\left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} = \frac{1}{4}(j+2)\phi_{j,k+1} + \frac{1}{16}\phi_{j,k+2} - \frac{1}{2}U\phi_{j-1,k} + \frac{1}{2}E\phi_{j-2,k}. \quad (1.16)$$

In Eq. (1.15), the factor of  $k!$  results in a simpler equation. The factor of  $4^k$  appears only for technical reasons which later will become clearer. Our goal is to derive an estimate on the  $\phi_{j,k}$ 's of the form

$$\|\phi_{j,k}\| \leq C \frac{A^j}{(j!)^{3/16}} \quad (1.17)$$

which is equivalent to (1.14) because of the definition (1.15). Notice that there is no  $k$ -dependence on the right side of (1.17); this feature will simplify our treatment later in the paper.

Equation (1.16) will play a fundamental role throughout the rest of this article. The basic fact which we shall use is that the operator  $-\square^*$  which appears on the left side of (1.16) dominates the operator  $U$  on the right side. To make these notions precise it is necessary to discuss the spectral properties of the operator  $-\square^*$ , which is done in Sect. 2.

## 2. Spectral properties of $-\square^*$

In order to study the properties of the operator  $-\square^*$ , it is particularly helpful to have a closed-form representation of the resolvent and the square of the resolvent of  $-\square^*$  as integral kernels. To this end we shall use the fact that  $P_n$ , the projection onto the eigenspace of  $-\square^*$  with eigenvalue  $n(n+2)$  [ $n = 0, 1, 2, 3, \dots$ ], has a kernel given by

$$P_n(\Theta) = \frac{(n+1) \sin((n+1)\Theta)}{2\pi^2 \sin(\Theta)} = \frac{n+1}{2\pi^2} C_n^1(\Theta) \quad (2.1)$$

where  $C_n^1(\Theta)$  is a Gegenbauer polynomial (see [24], p. 273). Here capital  $\Theta$  is to be distinguished from lower case  $\theta$ . Capital  $\Theta(\omega, \omega')$  is the geodesic distance between the two points  $\omega$  and  $\omega'$  on the hypersphere  $S^3$ ; more colloquially, it is the angle between  $\omega$  and  $\omega'$ . If we have some function  $\psi(\omega)$  in  $L^2(S^3)$ , we can calculate its projection  $[P_n\psi](\omega)$  onto the eigenspace of  $-\square^*$  with eigenvalue  $n(n+2)$  by the formula

$$[P_n\psi](\omega) = \int_{S^3} d\omega' \frac{(n+1) \sin((n+1)\Theta(\omega, \omega'))}{2\pi^2 \sin(\Theta(\omega, \omega'))} \psi(\omega'). \quad (2.2)$$

The situation in  $S^3$  is quite analogous to that in the more usual sphere  $S^2$ . If we were treating  $S^2$ , in formula (2.1) we would replace  $(n + 1) \sin ((n + 1)\Theta)/\sin (\Theta)$ , which is a polynomial in  $\cos (\Theta)$ , with the  $n$ th Legendre polynomial in  $\cos (\Theta)$ , and we would replace  $2\pi^2$ , the “surface area” of  $S^3$ , with  $4\pi$ , the surface area of  $S^2$ .

We first want to show that the domain of  $-\square^*$ , denoted by  $D(-\square^*)$ , the set of all functions  $\psi(\omega)$  in  $L^2(S^3)$  such that  $-\square^*\psi$  is also in  $L^2(S^3)$ , is contained in  $L^\infty(S^3)$ , the set of all functions on  $S^3$  which are uniformly bounded almost everywhere. To prove that  $D(-\square^*) \subset L^\infty(S^3)$ , it suffices to show that  $(-\square^* + 1)^{-1}$  is a bounded operator from  $L^2(S^3)$  to  $L^\infty(S^3)$ . It will be most helpful to have a simple representation of  $(-\square^* + 1)^{-1}$  as an integral operator. In order to derive such a representation, we first observe that since the eigenvalues of  $-\square^*$  are  $n(n + 2)$  [ $n = 0, 1, 2, \dots$ ], the eigenvalues of  $(-\square^* + 1)$  are  $(n(n + 2) + 1) = (n + 1)^2$ . Hence the eigenvalues of  $(-\square^* + 1)^{-1}$  are  $(n + 1)^{-2}$ . Thus we can write the integral kernel of  $(-\square^* + 1)^{-1}$  as

$$\begin{aligned} [(-\square^* + 1)^{-1}](\Theta) &= \sum_{n=0}^{\infty} (n + 1)^{-2} P_n(\Theta) = \frac{1}{2\pi^2 \sin (\Theta)} \sum_{n=0}^{\infty} \frac{\sin ((n + 1)\Theta)}{(n + 1)} \\ &= \frac{1}{2\pi^2 \sin (\Theta)} \frac{\pi - \Theta}{2} = \frac{\pi - \Theta}{2 \cdot (2\pi^2) \sin (\Theta)} \end{aligned} \tag{2.3}$$

where [19], Eq. 14.2.6 was used to evaluate the sum. To show that  $(-\square^* + 1)^{-1}$  is a bounded operator from  $L^2(S^3)$  to  $L^\infty(S^3)$ , we note that

$$\begin{aligned} \|(-\square^* + 1)^{-1}\psi\|_\infty &= \sup_{\omega \in S^3} | [(-\square^* + 1)^{-1}\psi](\omega) | \\ &= \sup_{\omega \in S^3} \left| \int_{S^3} d\omega' \frac{\pi - \Theta(\omega, \omega')}{2 \cdot (2\pi^2) \sin (\Theta(\omega, \omega'))} \psi(\omega') \right|. \end{aligned} \tag{2.4}$$

We apply the Schwarz inequality to the integral in (2.4):

$$\begin{aligned} &\left| \int_{S^3} d\omega' \frac{\pi - \Theta(\omega, \omega')}{2 \cdot (2\pi^2) \sin (\Theta(\omega, \omega'))} \psi(\omega') \right| \\ &\leq \left[ \int_{S^3} d\omega' \left( \frac{\pi - \Theta(\omega, \omega')}{2 \cdot (2\pi^2) \sin (\Theta(\omega, \omega'))} \right)^2 \int_{S^3} d\omega' |\psi(\omega')|^2 \right]^{1/2}. \end{aligned} \tag{2.5}$$

Because of rotational symmetry the integral on the right side of (2.5) has no dependence on  $\omega$ ; in fact, its numerical value is  $\frac{1}{12}$ . Thus inserting (2.5) into (2.4) yields

$$\|(-\square^* + 1)^{-1}\psi\|_\infty \leq (12)^{-1/2} \|\psi\|_2 \tag{2.6}$$

which is to say that  $(-\square^* + 1)^{-1}$  is a bounded operator from  $L^2(S^3)$  to  $L^\infty(S^3)$ . As was stated above, this means that  $D(-\square^*) \subset L^\infty(S^3)$ .

In fact, any function  $\psi$  in  $D(-\square^*)$  is uniformly Hölder continuous with exponent  $\frac{1}{2}$ . In particular, for any  $\psi$  in  $D(-\square^*)$  and for all pairs of points  $\omega$  and  $\omega'$  in  $S^3$ ,

$$|\psi(\omega) - \psi(\omega')| \leq (4\pi)^{-1/2} \|(-\square^* + 1)\psi\|_2 \Theta^{1/2}(\omega, \omega'). \tag{2.7}$$



This can be proved by observing that since

$$\psi = (-\square^* + 1)^{-1} \varphi, \tag{2.8}$$

where  $\varphi = (-\square^* + 1)\psi$  is in  $L^2(S^3)$  if  $\psi$  is in  $D(-\square^*)$ , it follows that

$$\begin{aligned} |\psi(\omega) - \psi(\omega')| &= \left| \int_{S^3} d\omega'' \{ [(-\square^* + 1)^{-1}](\Theta(\omega, \omega'')) \right. \\ &\quad \left. - [(-\square^* + 1)^{-1}](\Theta(\omega', \omega'')) \} \phi(\omega'') \right| \\ &\leq \left[ \int_{S^3} d\omega'' \{ [(-\square^* + 1)^{-1}](\Theta(\omega, \omega'')) \right. \\ &\quad \left. - [(-\square^* + 1)^{-1}](\Theta(\omega', \omega'')) \}^2 \right]^{1/2} \|\phi\|_2 \end{aligned} \tag{2.9}$$

by the Schwarz inequality. Now

$$\begin{aligned} &\int_{S^3} d\omega'' \{ [(-\square^* + 1)^{-1}](\Theta(\omega, \omega'')) - [(-\square^* + 1)^{-1}](\Theta(\omega', \omega'')) \}^2 \\ &= \int_{S^3} d\omega'' \{ [(-\square^* + 1)^{-1}](\Theta(\omega, \omega'')) \}^2 + \int_{S^3} d\omega'' \{ [(-\square^* + 1)^{-1}](\Theta(\omega', \omega'')) \}^2 \\ &\quad - 2 \int_{S^3} d\omega'' [(-\square^* + 1)^{-1}](\Theta(\omega, \omega'')) [(-\square^* + 1)^{-1}](\Theta(\omega', \omega')). \end{aligned} \tag{2.10}$$

The first two integrals are precisely  $\frac{1}{12}$  each, while by the convolution property the second is just  $-2[(-\square^* + 1)^{-2}](\Theta(\omega, \omega'))$ . The latter quantity can be evaluated in closed form by [19], Eq. (14.2.10)

$$\begin{aligned} [(-\square^* + 1)^{-2}](\Theta) &= \sum_{n=0}^{\infty} (n+1)^{-4} P_n(\Theta) = \frac{1}{2\pi^2 \sin(\Theta)} \sum_{n=0}^{\infty} \frac{\sin((n+1)\Theta)}{(n+1)^3} \\ &= \frac{1}{2\pi^2 \sin(\Theta)} \frac{\Theta}{12} (2\pi^2 - 3\pi\Theta + \Theta^2) = \frac{1}{12} \frac{\Theta}{\sin(\Theta)} \left( 1 - \frac{3\Theta}{2\pi} + \frac{\Theta^2}{2\pi^2} \right). \end{aligned} \tag{2.11}$$

Thus (2.10) equals

$$\begin{aligned} 2 \left\{ \frac{1}{12} - \frac{1}{12} \frac{\Theta}{\sin \Theta} \left( 1 - \frac{3\Theta}{2\pi} + \frac{\Theta^2}{2\pi^2} \right) \right\} &= \frac{1}{6} \left\{ 1 - \frac{\Theta}{\sin \Theta} \left( 1 - \frac{3\Theta}{2\pi} + \frac{\Theta^2}{2\pi^2} \right) \right\} \\ &= \frac{1}{6} \left( 1 - \frac{\Theta(\pi - \Theta)}{\pi \sin \Theta} + \frac{\Theta^2(\pi - \Theta)}{2\pi^2 \sin \Theta} \right) \\ &\leq \frac{1}{6} \left( 1 - \frac{\pi - \Theta}{\pi} + \frac{\Theta}{2\pi} \right) = \frac{1}{6} \frac{3\Theta}{2\pi} = \frac{\Theta}{4\pi} \end{aligned} \tag{2.12}$$

where we have used the estimates  $(-\Theta/\sin \Theta) \leq -1$  and  $\Theta(\pi - \Theta) \leq \pi \sin \Theta$ , the latter of which is easily proved by differentiating to obtain

$$\pi \cos \Theta \geq \pi - 2\Theta \tag{2.13}$$

which is true for  $0 \leq \Theta \leq \pi/2$  since  $\pi \cos \Theta$  is a concave function on this interval. By the symmetry of  $\pi \sin \Theta - \Theta(\pi - \Theta)$  the same inequality holds for  $\pi/2 \leq \Theta \leq \pi$ . Combining (2.12) and (2.9) yields (2.7), as desired.

Let us examine Eq. (1.16) again. The operator on its left side is  $[-\square^* - (j/2) \times (j/2 + 2)]$ . If  $j$  is odd, its inverse exists and is a bounded operator from  $L^2(S^3)$  to  $L^2(S^3)$ . However, if  $j$  is even, then  $[j/2(j/2 + 2)]$  is in the point spectrum of  $-\square^*$  and  $[-\square^* - (j/2)(j/2 + 2)]$  has no inverse. However, if we first project out the eigenspace of  $-\square^*$  with eigenvalue  $j/2(j/2 + 2)$ , then the *generalised inverse*

$$\left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right]^{-1} (1 - P_{j/2}) \tag{2.14}$$

does exist and is a bounded operator from  $L^2(S^3)$  to  $L^2(S^3)$ . We shall need to obtain in closed form a representation of the square of the operator (2.14) as an integral kernel. It is convenient to treat the cases  $j$  odd and  $j$  even separately.

First let us do  $j$  odd. Let  $j = 2J + 1$ , where  $J$  is a natural number. Then  $(j/2)(j/2 + 2) = (J + \frac{1}{2})(J + \frac{5}{2})$ , and the eigenvalues of  $[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-2}$  are  $(n(n + 2) - (J + \frac{1}{2})(J + \frac{5}{2}))^{-2} = ((n + 1)^2 - (J + \frac{3}{2})^2)^{-2}$ , so we can write the kernel of  $[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-2}$  as

$$\begin{aligned} [-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-2}(\Theta) &= \sum_{n=0}^{\infty} ((n + 1)^2 - (J + \frac{3}{2})^2)^{-2} P_n(\Theta) \\ &= \sum_{n=0}^{\infty} ((n + 1)^2 - (J + \frac{3}{2})^2)^{-2} \frac{(n + 1) \sin((n + 1)\Theta)}{2\pi^2 \sin \Theta}. \end{aligned} \tag{2.15}$$

We can use [19], Eq. (14.3.17) to evaluate this summation, which turns out to be

$$\frac{1}{2\pi^2 \sin \Theta} \frac{\pi}{4(J + \frac{3}{2})} \left\{ \pi \frac{\sin((J + \frac{3}{2})\Theta)}{\sin((J + \frac{3}{2})\pi)} - \Theta \cos((\pi - \Theta)(J + \frac{3}{2})) \right\} \frac{1}{\sin((J + \frac{3}{2})\pi)}. \tag{2.16}$$

We now expand the cosine and use the facts that  $\cos((J + \frac{3}{2})\pi) = 0$  and  $\sin((J + \frac{3}{2})\pi) = (-1)^{J+1}$  to obtain the simplified expression

$$\frac{\pi}{2\pi^2} \frac{\pi - \Theta}{2J + 3} \frac{\sin((J + \frac{3}{2})\Theta)}{\sin \Theta} \tag{2.17}$$

which is the kernel of the operator  $[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-2}$ .

Now let us do the case of  $j$  even, which is rather more complicated. Let  $j = 2J$ , where  $J$  is a natural number. Then  $j/2(j/2 + 2) = J(J + 2)$ , and the eigenvalues of  $[-\square^* - J(J + 2)]^{-2}(1 - P_J)$  are  $(n(n + 2) - J(J + 2))^{-2} = ((n + 1)^2 - (J + 1)^2)^{-2}$ , where  $n$  runs through all natural numbers except  $J$ ; for  $n = J$ , the factor of  $(1 - P_J)$  adds the eigenvalue 0. Thus we can write the kernel of  $[-\square^* - J(J + 2)]^{-2}(1 - P_J)$  as

$$[(-\square^* - J(J + 2))^{-2}(1 - P_J)](\Theta)$$

$$\begin{aligned}
&= \sum_{\substack{n=0 \\ n \neq J}}^{\infty} ((n+1)^2 - (J+1)^2)^{-2} P_n(\Theta) \\
&= \lim_{\varepsilon \rightarrow 0} \sum_{\substack{n=0 \\ n \neq J}}^{\infty} ((n+1)^2 - (J+1+\varepsilon)^2)^{-2} P_n(\Theta) \\
&= \lim_{\varepsilon \rightarrow 0} \left\{ \sum_{n=0}^{\infty} ((n+1)^2 - (J+1+\varepsilon)^2)^{-2} P_n(\Theta) - ((J+1)^2 - (J+1+\varepsilon)^2)^{-2} P_J(\Theta) \right\} \\
&= \frac{1}{2\pi^2 \sin(\Theta)} \lim_{\varepsilon \rightarrow 0} \left\{ \sum_{n=0}^{\infty} \frac{(n+1) \sin((n+1)\Theta)}{((n+1)^2 - (J+1+\varepsilon)^2)^2} - \frac{(J+1) \sin((J+1)\Theta)}{((J+1)^2 - (J+1+\varepsilon)^2)^2} \right\} \\
&= \frac{1}{2\pi^2 \sin(\Theta)} \lim_{\varepsilon \rightarrow 0} \left\{ \frac{\pi}{4(J+1+\varepsilon)} \left[ \pi \frac{\sin((J+1+\varepsilon)\Theta)}{\sin((J+1+\varepsilon)\pi)} \right. \right. \\
&\quad \left. \left. - \Theta \cos((\pi - \Theta)(J+1+\varepsilon)) \right] \frac{1}{\sin((J+1+\varepsilon)\pi)} \right. \\
&\quad \left. - \frac{(J+1) \sin((J+1)\Theta)}{(2\varepsilon(J+1) + \varepsilon^2)^2} \right\} \tag{2.18}
\end{aligned}$$

where [19], Eq. 14.3.17 was used to evaluate the summation. We expand the cosine in (2.18) and use the facts that  $\sin((J+1+\varepsilon)\pi) = (-1)^{J+1} \sin(\varepsilon\pi)$  and  $\cos((J+1+\varepsilon)\pi) = (-1)^{J+1} \cos(\varepsilon\pi)$  to simplify (2.18) to

$$\begin{aligned}
&\frac{1}{2\pi^2 \sin(\Theta)} \lim_{\varepsilon \rightarrow 0} \left\{ \frac{\pi}{4(J+1+\varepsilon)} \left[ \pi \frac{\sin((J+1+\varepsilon)\Theta)}{\sin^2(\varepsilon\pi)} \right. \right. \\
&\quad \left. \left. - \Theta \left( \frac{\cos(\varepsilon\pi)}{\sin(\varepsilon\pi)} \cos((J+1+\varepsilon)\Theta) + \sin((J+1+\varepsilon)\Theta) \right) \right] \right. \\
&\quad \left. - \frac{(J+1) \sin((J+1)\Theta)}{(2\varepsilon(J+1) + \varepsilon^2)^2} \right\}. \tag{2.19}
\end{aligned}$$

It will be observed that the terms inside the limit have singularities which are  $O(\varepsilon^{-2})$ ,  $O(\varepsilon^{-1})$ , and  $O(\varepsilon^0)$ . We shall now expand each term in (2.19), up to  $O(\varepsilon^0)$ .

To begin, let us examine the first term,

$$\frac{\pi^2 \sin((J+1+\varepsilon)\Theta)}{4(J+1+\varepsilon) \sin^2(\varepsilon\pi)} \tag{2.20}$$

Since  $\sin^{-2}(\varepsilon\pi) = (\varepsilon\pi)^{-2} + \frac{1}{3} + O(\varepsilon^2)$ ,

$$\begin{aligned}
\frac{\pi^2 \sin((J+1+\varepsilon)\Theta)}{4(J+1+\varepsilon) \sin^2(\varepsilon\pi)} &= \left[ \frac{\pi^2}{4(J+1)} \frac{1}{\varepsilon^2 \pi^2} - \frac{\pi^2 \varepsilon}{4(J+1)^2} \frac{1}{\varepsilon^2 \pi^2} + \frac{\pi^2 \varepsilon^2}{4(J+1)^3} \frac{1}{\varepsilon^2 \pi^2} \right. \\
&\quad \left. + \frac{\pi^2}{4(J+1)} \frac{1}{3} + O(\varepsilon) \right] \sin((J+1+\varepsilon)\Theta) \\
&= \left[ \varepsilon^{-2} \frac{1}{4(J+1)} - \varepsilon^{-1} \frac{1}{4(J+1)^2} + \frac{1}{4(J+1)^3} \right. \\
&\quad \left. + \frac{\pi^2}{12(J+1)} + O(\varepsilon) \right] \sin((J+1+\varepsilon)\Theta). \tag{2.21}
\end{aligned}$$

We now use the fact that  $\sin((J+1+\varepsilon)\Theta) = \sin((J+1)\Theta)\cos(\varepsilon\Theta) + \cos((J+1)\Theta)\sin(\varepsilon\Theta)$  and the expansion  $\cos(\varepsilon\Theta) = 1 - (\varepsilon\Theta)^2/2 + O(\varepsilon^4)$  to see that (2.21) equals

$$\begin{aligned} & \left[ \varepsilon^{-2} \frac{1}{4(J+1)} - \varepsilon^{-1} \frac{1}{4(J+1)^2} + \frac{1}{4(J+1)^3} + \frac{\pi^2}{12(J+1)} + O(\varepsilon) \right] \sin((J+1)\Theta) \\ & - \left[ \frac{\Theta^2}{8(J+1)} + O(\varepsilon) \right] \sin((J+1)\Theta) \\ & + \left[ \varepsilon^{-1} \frac{\Theta}{4(J+1)} - \frac{\Theta}{4(J+1)^2} + O(\varepsilon) \right] \cos((J+1)\Theta). \end{aligned} \quad (2.22)$$

Now let us look at the last term in (2.19),

$$-\frac{(J+1)\sin((J+1)\Theta)}{(2\varepsilon(J+1) + \varepsilon^2)^2}. \quad (2.23)$$

We quickly recognise that

$$\begin{aligned} \frac{(J+1)}{(2\varepsilon(J+1) + \varepsilon^2)^2} &= \frac{1}{4(J+1)\varepsilon^2} \left( 1 + \frac{\varepsilon}{2(J+1)} \right)^{-2} \\ &= \frac{1}{4(J+1)\varepsilon^2} \left[ 1 - \frac{2\varepsilon}{2(J+1)} + \frac{3\varepsilon^2}{4(J+1)^2} + O(\varepsilon^3) \right] \\ &= \varepsilon^{-2} \frac{1}{4(J+1)} - \varepsilon^{-1} \frac{1}{4(J+1)^2} + \frac{3}{16(J+1)^3} + O(\varepsilon) \end{aligned} \quad (2.24)$$

so we see that (2.23) equals

$$-\left[ \varepsilon^{-2} \frac{1}{4(J+1)} + \varepsilon^{-1} \frac{1}{4(J+1)^2} + \frac{3}{16(J+1)^3} + O(\varepsilon) \right] \sin((J+1)\Theta). \quad (2.25)$$

It is immediately obvious that the  $O(\varepsilon^{-2})$  and the  $O(\varepsilon^{-1})$  terms in (2.25) will cancel the corresponding terms in (2.22), so the sum of (2.22) and (2.25) is readily seen to be

$$\begin{aligned} & \left[ \frac{1}{16(J+1)^3} + \frac{\pi^2}{12(J+1)} - \frac{\Theta^2}{8(J+1)} + O(\varepsilon) \right] \sin((J+1)\Theta) \\ & + \left[ \varepsilon^{-1} \frac{\Theta}{4(J+1)} - \frac{\Theta}{4(J+1)^2} + O(\varepsilon) \right] \cos((J+1)\Theta) \end{aligned} \quad (2.26)$$

whose singularity if  $O(\varepsilon^{-1})$ . This singularity is cancelled by the second term in (2.19), which also is  $O(\varepsilon^{-1})$ :

$$\frac{\pi\Theta \cos(\varepsilon\pi)}{4(J+1+\varepsilon)\sin(\varepsilon\pi)} \cos((J+1+\varepsilon)\Theta). \quad (2.27)$$

Since  $\cos((J+1+\varepsilon)\Theta) = \cos((J+1)\Theta)\cos(\varepsilon\Theta) - \sin((J+1)\Theta)\sin(\varepsilon\Theta)$ , one sees that (2.27) equals

$$-\frac{\pi\Theta \cos(\varepsilon\pi)\cos(\varepsilon\Theta)}{4(J+1+\varepsilon)\sin(\varepsilon\pi)} \cos((J+1)\Theta) + \frac{\pi\Theta \cos(\varepsilon\pi)\sin(\varepsilon\Theta)}{4(J+1+\varepsilon)\sin(\varepsilon\pi)} \sin((J+1)\Theta). \quad (2.28)$$

The second term in (2.28) is just

$$\frac{\Theta^2}{4(J+1)} \sin((J+1)\Theta) + O(\varepsilon) \tag{2.29}$$

and the first term in (2.28) is

$$-\left[ \varepsilon^{-1} \frac{\Theta}{4(J+1)} - \frac{\Theta}{4(J+1)^2} + O(\varepsilon) \right] \cos((J+1)\Theta) \tag{2.30}$$

It is evident that (2.30) will cancel the term in (2.26) containing the cosine, so the sum of (2.26), (2.29) and (2.30) is

$$\left[ \frac{1}{16(J+1)^3} + \frac{\pi^2}{12(J+1)} + \frac{\Theta^2}{8(J+1)} + O(\varepsilon) \right] \sin((J+1)\Theta). \tag{2.31}$$

Finally, we need to include the third term in (2.19), which is

$$-\frac{\pi\Theta \sin((J+1+\varepsilon)\Theta)}{4(J+1+\varepsilon)} = -\frac{\pi\Theta \sin((J+1)\Theta)}{4(J+1)} + O(\varepsilon). \tag{2.32}$$

The sum of (2.31) and (2.32) is

$$\left[ \frac{1}{16(J+1)^3} + \frac{\pi^2}{12(J+1)} + \frac{\Theta^2}{8(J+1)} - \frac{\pi\Theta}{4(J+1)} + O(\varepsilon) \right] \sin((J+1)\Theta). \tag{2.33}$$

When we take the limit as  $\varepsilon \rightarrow 0$  and then divide by  $(2\pi^2 \sin(\Theta))$ , the factor in front of the limit in (2.19), we obtain the kernel of the operator

$$\begin{aligned} & [(-\square^* - J(J+2))^{-2}(1 - P_J)](\Theta) \\ &= \frac{1}{4 \cdot 2\pi^2} \frac{\sin((J+1)\Theta)}{(J+1) \sin(\Theta)} \left[ \frac{\pi^2}{3} + \frac{\Theta^2}{2} - \pi\Theta + \frac{1}{4(J+1)^2} \right]. \end{aligned} \tag{2.34}$$

The integrals kernels of  $P_J$ ,  $[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-2}$ , and  $[-\square^* - J(J+2)]^{-2}(1 - P_J)$ , which are given by formulae (2.1), (2.17), and (2.34), respectively, will play an important role throughout this paper.

### 3. Upper bounds to norms of integral operators

In this section we shall obtain upper bounds on the norms of various operators which will occur in our proof that the norms of Fock's  $\psi_{j,k}$ 's fall off factorially fast. We shall need to find estimates on the norms of operators considered as maps from  $L^2(S^3)$  to  $L^2(S^3)$ , in which case the norm of the operator will be denoted by  $\| \cdot \|_{2,2}$ , and also for operators considered as maps from  $L^2(S^3)$  to  $L^\infty(S^3)$ , in which case the norm of the operator will be denoted by  $\| \cdot \|_{2,\infty}$ .

To begin, we want to estimate  $\| P_J \|_{2,\infty}$ . From (2.1),

$$\begin{aligned} \| P_J \psi \|_\infty &= \sup_{\omega \in S^3} |[P_J \psi](\omega)| = \sup_{\omega \in S^3} \left| \int_{S^3} d\omega' P_J(\Theta(\omega, \omega')) \psi(\omega') \right| \\ &= \frac{J+1}{2\pi^2} \sup_{\omega \in S^3} \left| \int_{S^3} d\omega' \frac{\sin((J+1)\Theta(\omega, \omega'))}{\sin(\Theta(\omega, \omega'))} \psi(\omega') \right|. \end{aligned} \tag{3.1}$$

Using the Schwarz inequality on the integral in (3.1) yields

$$\|P_J\psi\|_\omega \leq \frac{J+1}{2\pi^2} \left\{ \sup_{\omega \in S^3} \int_{S^3} d\omega' \left[ \frac{\sin((J+1)\Theta(\omega, \omega'))}{\sin(\Theta(\omega, \omega'))} \right]^2 \right\}^{1/2} \|\psi\|_2. \tag{3.2}$$

The integral in (3.2) does not depend on  $\omega$ ; in fact, its value is also independent of  $J$  and is precisely  $2\pi^2$ , the volume of  $S^3$ . Substituting this value into (3.2) yields the estimate

$$\|P_J\psi\|_\infty \leq (J+1)(2\pi^2)^{-1/2} \|\psi\|_2 \tag{3.3}$$

which is to say that

$$\|P_J\|_{2,\infty} \leq (J+1)(2\pi^2)^{-1/2}. \tag{3.4}$$

The factor of  $(J+1)$  on the right side of (3.4) should not be surprising. It is a reflection of the fact that in  $L^2(S^3)$  the normalised hyperspherical harmonics of order  $J$  have maxima which go like  $(J+1)$ . If we were considering the usual 2-dimensional sphere  $S^2$ , we would have

$$\|P_l\|_{2,\infty} \leq (2l+1)^{1/2}(4\pi)^{-1/2} \tag{3.5}$$

although it is of course true that  $\|P_l\|_{2,2} = 1$ . This example helps to illustrate the importance of remembering that the norm of an operator depends on the image space.

Later in this paper we shall apply the operator  $P_J$  to Eq. (1.16). It will then be necessary to have an estimate of the norm of the operator  $P_J U$ , considered as a map from  $L^2(S^3)$  to  $L^2(S^3)$ , where  $U$  is the ‘‘hyperspherical potential energy’’ operator defined by (1.5). The qualitative property of  $U(\alpha, \theta)$  which will play an important role in the rest of this paper is that  $U$  is in  $L^p(S^3)$  for all  $1 \leq p < 3$ . (This is quite analogous to the fact that in  $\mathbb{R}^3$  the short-range spike of the Coulomb potential  $r^{-1}$  is locally in  $L^p(\mathbb{R}^3)$  for all  $1 \leq p < 3$ .)  $U$  is an *unbounded* operator from its domain  $D(U) \subset L^2(S^3)$  to  $L^2(S^3)$ ; however,  $P_J$  is an operator of finite rank from  $L^2(S^3)$  to  $L^2(S^3)$ , so it is reasonable to expect that the smoothing action of  $P_J$  will control the singular nature of  $U$ . To estimate  $\|P_J U\|_{2,2}$ , we observe that since  $P_J$  is a projection,

$$\begin{aligned} \|P_J U\psi\|_2^2 &= (P_J U\psi, P_J U\psi) = (U\psi, P_J U\psi) \\ &= \int_{S^3} d\omega \int_{S^3} d\omega' \psi^*(\omega) U(\omega) P_J(\Theta(\omega, \omega')) U(\omega') \psi(\omega'). \end{aligned} \tag{3.6}$$

We first apply the Schwarz inequality to the integration over  $\omega$ :

$$\begin{aligned} \|P_J U\psi\|_2^2 &\leq \left\{ \int_{S^3} d\omega |\psi(\omega)|^2 \right. \\ &\quad \left. \times \int_{S^3} d\omega \left[ U(\omega) \int_{S^3} d\omega' P_J(\Theta(\omega, \omega')) U(\omega') \psi(\omega') \right]^2 \right\}^{1/2} \end{aligned} \tag{3.7}$$

and then to the integration over  $\omega'$  in (3.7)

$$\begin{aligned} \|P_J U \psi\|_2^2 &\leq \left\{ \int_{S^3} d\omega |\psi(\omega)|^2 \int_{S^3} d\omega' |\psi(\omega')|^2 \right. \\ &\quad \left. \times \int_{S^3} d\omega \int_{S^3} d\omega' U^2(\omega) P_J^2(\Theta(\omega, \omega')) U^2(\omega') \right\}^{1/2} \\ &= \|\psi\|_2^2 \left\{ \int_{S^3} d\omega \int_{S^3} d\omega' U^2(\omega) P_J^2(\Theta(\omega, \omega')) U^2(\omega') \right\}^{1/2} \end{aligned} \quad (3.8)$$

which is to say that

$$\|P_J U\|_{2,2} \leq \left\{ \int_{S^3} d\omega \int_{S^3} d\omega' U^2(\omega) P_J^2(\Theta(\omega, \omega')) U^2(\omega') \right\}^{1/4}. \quad (3.9)$$

To estimate the right side of (3.9), we apply Hölder's inequality to the  $\omega$  integration with  $p = \frac{4}{3}$  and  $q = 4$ . This is permissible since  $(U^2)^p = (U^2)^{4/3} = |U|^{8/3}$  and  $1 \leq \frac{8}{3} < 3$ . Doing so yields

$$\begin{aligned} &\int_{S^3} d\omega \int_{S^3} d\omega' U^2(\omega) P_J^2(\Theta(\omega, \omega')) U^2(\omega') \\ &\leq \left[ \int_{S^3} d\omega |U(\omega)|^{8/3} \right]^{3/4} \left\{ \int_{S^3} d\omega \left[ \int_{S^3} d\omega' P_J^2(\Theta(\omega, \omega')) U^2(\omega') \right]^4 \right\}^{1/4} \end{aligned} \quad (3.10)$$

and we then apply Hölder's inequality with  $p = 4/3$ ,  $q = 4$  to the  $\omega'$  integration on the right side of (3.10):

$$\begin{aligned} &\int_{S^3} d\omega' P_J^2(\Theta(\omega, \omega')) U^2(\omega') \\ &\leq \left[ \int_{S^3} d\omega' |U(\omega')|^{8/3} \right]^{3/4} \left[ \int_{S^3} d\omega' P_J^8(\Theta(\omega, \omega')) \right]^{1/4}. \end{aligned} \quad (3.11)$$

Taking the fourth power of (3.11) and inserting the result into (3.10) yields

$$\begin{aligned} &\int_{S^3} d\omega \int_{S^3} d\omega' U^2(\omega) P_J^2(\Theta(\omega, \omega')) U^2(\omega') \\ &\leq \left[ \int_{S^3} d\omega |U(\omega)|^{8/3} \right]^{3/4} \left[ \int_{S^3} d\omega' |U(\omega')|^{8/3} \right]^{3/4} \\ &\quad \times \left[ \int_{S^3} d\omega \int_{S^3} d\omega' P_J^8(\Theta(\omega, \omega')) \right]^{1/4} \\ &= \|U\|_{8/3}^4 \left[ \int_{S^3} d\omega \int_{S^3} d\omega' P_J^8(\Theta(\omega, \omega')) \right]^{1/4} \end{aligned} \quad (3.12)$$

Inserting (3.12) into (3.9) gives us

$$\begin{aligned} \|P_J U\|_{2,2} &\leq \|U\|_{8/3} \left[ \int_{S^3} d\omega \int_{S^3} d\omega' P_J^3(\Theta(\omega, \omega')) \right]^{1/16} \\ &= \|U\|_{8/3} ((J+1)/2\pi^2)^{1/2} \left[ \int_{S^3} d\omega \int_{S^3} d\omega' \frac{\sin^8((J+1)\Theta(\omega, \omega'))}{\sin^8(\Theta(\omega, \omega'))} \right]^{1/16} \end{aligned} \tag{3.13}$$

where we have used (2.1) for the explicit form of  $P_J(\Theta)$ . By rotational symmetry, the integral in (3.13) over  $\omega$  does not depend on  $\omega'$ , and a somewhat tedious computation in the Appendix shows that the value of the integral is

$$2\pi^2 \frac{2\pi^2}{3} [(J+1)^5 + (J+1)^3 + (J+1)]. \tag{3.14}$$

(The reader who is so inclined can check this formula in the case  $J=0$  by inspection and in the case  $J=1$  using the relation  $\sin(2\Theta)/\sin(\Theta) = 2\cos(\Theta)$ .) Using (3.14) in (3.13) yields

$$\|P_J U\|_{2,2} \leq \|U\|_{8/3} (2\pi^2)^{-3/8} \left[ \frac{(J+1)^{13} + (J+1)^{10} + (J+1)^7}{3} \right]^{1/16}. \tag{3.15}$$

For large  $J$  this upper bound to  $\|P_J U\|_{2,2}$  goes like  $J^{13/16}$ . Later in this paper we shall divide  $P_J U$  by  $(J+1)$ , so  $\|(J+1)^{-1} P_J U\|_{2,2}$  will behave for large  $J$  like  $J^{13/16-1} = J^{-3/16}$ . This is one of the sources of the exponent  $-\frac{3}{16}$  which appears in (1.14).

We shall also need to estimate  $\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}\|_{2,2}$  and  $\|[-\square^* - J(J+2)]^{-1}(1-P_J)\|_{2,2}$ . It is easy to find these norms since we know the eigenvalues of the operators. Since the eigenvalues of  $[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}$  are  $(n(n+2) - (J+\frac{1}{2})(J+\frac{5}{2}))^{-1} = ((n+1)^2 - (J+\frac{3}{2})^2)^{-1}$ , the eigenvalue with the largest absolute value corresponds to  $n=J$  and is equal to  $((J+1)^2 - (J+\frac{3}{2})^2)^{-1} = -(J+\frac{5}{4})^{-1}$ , so

$$\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}\|_{2,2} = (J+\frac{5}{4})^{-1}. \tag{3.16}$$

Similarly, since the eigenvalues of  $[-\square^* - J(J+2)]^{-1}(1-P_J)$  are  $(n(n+2) - J(J+2))^{-1} = ((n+1)^2 - (J+1)^2)^{-1}$  for  $n \neq J$  together with 0 for  $n=J$ , the eigenvalue with the largest absolute value corresponds to  $n=J-1$  and is equal to  $(J^2 - (J+1)^2)^{-1} = -(2J+1)^{-1}$ , so for  $J \geq 1$

$$\|[-\square^* - J(J+2)]^{-1}(1-P_J)\|_{2,2} = (2J+1)^{-1}. \tag{3.17}$$

We shall never need to know  $\|-\square^{*-1}(1-P_0)\|_{2,2}$ , but for completeness its value is  $\frac{1}{3}$  and it certainly obeys (3.17) if the equality is replaced with an inequality. The two Eqs. (3.16) and (3.17) are essentially due to the fact that since the eigenvalues of  $-\square^*$  increase like  $n^2$ , the gaps between nearest eigenvalues increase like  $n$ .

Additionally, we shall have to find upper bounds to  $\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}\|_{2,\infty}$



and  $\|[-\square^* - J(J+2)]^{-1}(1 - P_J)\|_{2,\infty}$ . To estimate the former, we observe that

$$\begin{aligned} \|[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1}\psi\|_{\infty} &= \sup_{\omega \in S^3} \left\| \int_{S^3} d\omega' h_{J+1/2}(\Theta(\omega, \omega')) \psi(\omega') \right\| \\ &\leq \sup_{\omega \in S^3} \left( \int_{S^3} d\omega' h_{J+1/2}^2(\Theta(\omega, \omega')) \right)^{1/2} \|\psi\|_2 \end{aligned} \quad (3.18)$$

where we have used the Schwarz inequality in the last step and  $h_{J+1/2}(\Theta)$ , the kernel of  $[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1}$ , is given by (2.17)

$$h_{J+1/2}(\Theta) = \frac{\pi}{2\pi^2} \frac{\pi - \Theta}{2J+3} \frac{\sin((J + \frac{3}{2})\Theta)}{\sin(\Theta)}.$$

Since  $\sin((J + \frac{3}{2})\Theta) = \sin((J+1)\Theta) \cos(\Theta/2) + \sin(\Theta/2) \cos((J+1)\Theta)$ ,

$$\begin{aligned} &|(\pi - \Theta) \sin((J + \frac{3}{2})\Theta)| \\ &\leq |\pi - \Theta| |\sin((J+1)\Theta)| + |(\pi - \Theta) \sin(\Theta/2)| |\cos((J+1)\Theta)| \\ &\leq \pi |\sin((J+1)\Theta)| + |(\pi - \Theta) \sin(\Theta/2)| |\cos((J+1)\Theta)| \end{aligned} \quad (3.19)$$

since  $0 \leq \Theta \leq \pi$ . Furthermore, since for  $0 \leq \Theta \leq \pi$

$$\pi - \Theta \leq \pi \cos(\Theta/2) \quad (3.20)$$

which is most easily proved by noting that the two functions coincide at  $\Theta = 0$  and  $\Theta = \pi$  and that  $\pi \cos(\Theta/2)$  is a concave function for  $0 \leq \Theta \leq \pi$ , in (3.19) we can replace  $(\pi - \Theta)$  with  $\pi \cos(\Theta/2)$ , observe that  $\sin(\Theta/2) \cos(\Theta/2) = \frac{1}{2} \sin(\Theta)$ , and obtain

$$|(\pi - \Theta) \sin((J + \frac{3}{2})\Theta)| \leq \pi |\sin((J+1)\Theta)| + \frac{\pi}{2} |\sin(\Theta)| |\cos((J+1)\Theta)|. \quad (3.21)$$

Then since  $(2J+3)^{-1} \leq \frac{1}{2}(J+1)^{-1}$ , using (3.21) in (3.19) yields

$$\begin{aligned} |h_{J+1/2}(\Theta)| &\leq \frac{1}{2\pi^2} \frac{\pi}{2} \frac{1}{J+1} \left( \frac{|\sin((J+1)\Theta)|}{\sin(\Theta)} + \frac{1}{2} |\cos((J+1)\Theta)| \right) \\ &\leq \frac{1}{2\pi^2} \frac{\pi}{2} \frac{1}{J+1} \left( \frac{|\sin((J+1)\Theta)|}{\sin(\Theta)} + \frac{1}{2} \right). \end{aligned} \quad (3.22)$$

Using this estimate in (3.18) together with Minkowski's inequality yields

$$\begin{aligned} &\|[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1}\|_{2,\infty} \\ &\leq \frac{1}{2\pi^2} \frac{\pi}{2} \frac{1}{J+1} \left[ \sup_{\omega \in S^3} \left( \int_{S^3} d\omega' \frac{\sin^2((J+1)\Theta(\omega, \omega'))}{\sin^2(\Theta(\omega, \omega'))} \right)^{1/2} + \frac{1}{2} \left( \int_{S^3} d\omega' \right)^{1/2} \right]. \end{aligned} \quad (3.23)$$

The first integral in (3.23) is independent of  $\omega$  and is just the volume of  $S^3$ ,  $2\pi^2$ , which of course is also the value of the second integral. Thus

$$\|[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1}\|_{2,\infty} \leq (2\pi^2)^{-1/2} \frac{\pi}{2} \frac{3}{2} (J+1)^{-1}. \quad (3.24)$$

To derive an upper bound to  $\|[-\square^* - J(J+2)]^{-1}(1 - P_J)\|_{2,\infty}$ , we note that

$$\begin{aligned} \|[-\square^* - J(J+2)]^{-1}(1 - P_J)\psi\|_\infty &= \sup_{\omega \in S^3} \left| \int_{S^3} d\omega' h_J(\Theta(\omega, \omega')) \psi(\omega') \right| \\ &\leq \sup_{\omega \in S^3} \left( \int_{S^3} d\omega' h_J^2(\Theta(\omega, \omega')) \right)^{1/2} \|\psi\|_2 \end{aligned} \quad (3.25)$$

where the Schwarz inequality was used in the last step and  $h_J(\Theta)$  is the kernel of  $[-\square^* - J(J+2)]^{-1}(1 - P_J)$  given by Eq. (2.37):

$$h_J(\Theta) = \frac{1}{4 \cdot 2\pi^2} \frac{\sin((J+1)\Theta)}{(J+1)\sin(\Theta)} \left[ \frac{\pi^2}{3} + \frac{\Theta^2}{2} - \Theta\pi + \frac{1}{4(J+1)^2} \right]. \quad (3.26)$$

The factor in square brackets in (3.26) attains its maximum absolute value when  $\Theta = 0$ , so

$$\begin{aligned} |h_J(\Theta)| &\leq \frac{1}{4 \cdot 2\pi^2} \frac{|\sin((J+1)\Theta)|}{(J+1)\sin(\Theta)} \left[ \frac{\pi^2}{3} + \frac{1}{4(J+1)^2} \right] \\ &\leq \frac{1}{4 \cdot 2\pi^2} \frac{|\sin((J+1)\Theta)|}{(J+1)\sin(\Theta)} \left( \frac{\pi^2}{3} + \frac{1}{4} \right). \end{aligned} \quad (3.27)$$

Using this upper bound in (3.25) yields

$$\begin{aligned} \|[-\square^* - J(J+2)]^{-1}(1 - P_J)\|_{2,\infty} &\leq \frac{1}{4 \cdot 2\pi^2} \left( \frac{\pi^2}{3} + \frac{1}{4} \right) \frac{1}{J+1} \sup_{\omega \in S^3} \left( \int_{S^3} d\omega' \frac{\sin^2((J+1)\Theta(\omega, \omega'))}{\sin^2(\Theta(\omega, \omega'))} \right)^{1/2}. \end{aligned} \quad (3.28)$$

As with (3.23), the integral in (3.28) is independent of  $\omega$  and its value is just the volume of  $S^3$ , which is  $2\pi^2$ , so

$$\|[-\square^* - J(J+2)]^{-1}(1 - P_J)\|_{2,\infty} \leq \frac{1}{4} (2\pi^2)^{-1/2} \left( \frac{\pi^2}{3} + \frac{1}{4} \right) (J+1)^{-1}. \quad (3.29)$$

We also require estimates of  $\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}U\|_{2,2}$  and  $\|[-\square^* - J(J+2)]^{-1}(1 - P_J)U\|_{2,2}$ . To obtain an upper bound on the former, we observe that

$$\begin{aligned} &\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}U\psi\|_2^2 \\ &= ([-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}U\psi, [-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}U\psi) \\ &= (U\psi, [-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-2}U\psi) \\ &= \int_{S^3} d\omega \int_{S^3} d\omega' \psi^*(\omega) U(\omega) h_{J+1/2}(\Theta(\omega, \omega')) U(\omega') \psi(\omega') \end{aligned} \quad (3.30)$$

where  $h_{J+1/2}(\Theta)$  is the integral kernel of  $[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-2}$  given by (2.17). Applying the Schwarz inequality twice as in steps (3.6) through (3.8) shows that

$$\begin{aligned} &\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}U\psi\|_2^2 \\ &\leq \|\psi\|_2^2 \left[ \int_{S^3} d\omega \int_{S^3} d\omega' U^2(\omega) h_{J+1/2}^2(\Theta(\omega, \omega')) U^2(\omega') \right]^{1/2} \end{aligned} \quad (3.31)$$

which implies that

$$\begin{aligned} & \|[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1} U\|_{2,2} \\ & \leq \left[ \int_{S^3} d\omega \int_{S^3} d\omega' U^2(\omega) h_{J+1/2}^2(\Theta(\omega, \omega')) U^2(\omega') \right]^{1/4}. \end{aligned} \quad (3.32)$$

Using Hölder's inequality as in steps (3.10) through (3.13) finally yields

$$\begin{aligned} & \|[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1} U\|_{2,2} \\ & \leq \|U\|_{8/3} \left[ \int_{S^3} d\omega \int_{S^3} d\omega' h_{J+1/2}^8(\Theta(\omega, \omega')) \right]^{1/16}. \end{aligned} \quad (3.33)$$

We use the estimate (3.22) for  $|h_{J+1/2}(\Theta)|$  and Minkowski's inequality to obtain

$$\begin{aligned} & \left[ \int_{S^3} d\omega \int_{S^3} d\omega' h_{J+1/2}^8(\Theta(\omega, \omega')) \right]^{1/8} \\ & \leq \frac{1}{2\pi^2} \frac{\pi}{2} \frac{1}{J+1} \left[ \int_{S^3} d\omega \int_{S^3} d\omega' \left( \frac{|\sin(J+1)\Theta(\omega, \omega')|}{\sin(\Theta(\omega, \omega'))} + \frac{1}{2} \right)^8 \right]^{1/8} \\ & \leq \frac{1}{2\pi^2} \frac{\pi}{2} \frac{1}{J+1} \left\{ \left[ \int_{S^3} d\omega \int_{S^3} d\omega' \left( \frac{\sin((J+1)\Theta(\omega, \omega'))}{\sin(\Theta(\omega, \omega'))} \right)^8 \right]^{1/8} \right. \\ & \quad \left. + \frac{1}{2} \left[ \int_{S^3} d\omega \int_{S^3} d\omega' \right]^{1/8} \right\}. \end{aligned} \quad (3.34)$$

As we already stated in (3.14), the first integral in (3.34) is

$$2\pi^2 \frac{2\pi^2}{3} [(J+1)^5 + (J+1)^3 + (J+1)] \quad (3.35)$$

so from (3.34) we obtain

$$\begin{aligned} & \left[ \int_{S^3} d\omega \int_{S^3} d\omega' h_{J+1/2}^8(\Theta(\omega, \omega')) \right]^{1/8} \\ & \leq \frac{1}{2\pi^2} \frac{\pi}{2} \frac{1}{J+1} \left[ \left( 2\pi^2 \frac{2\pi^2}{3} [(J+1)^5 + (J+1)^3 + (J+1)] \right)^{1/8} + \frac{1}{2} (2\pi^2)^{2/8} \right] \\ & = (2\pi^2)^{-3/4} \frac{\pi}{2} \left\{ \left( \frac{1}{3} [(J+1)^3 + (J+1)^5 + (J+1)^7] \right)^{1/8} + \frac{1}{2} (J+1)^{-1} \right\} \\ & \leq (2\pi^2)^{-3/4} \frac{\pi}{2} \left\{ (J+1)^{-3/8} + \frac{1}{2} (J+1)^{-1} \right\} \\ & \leq (2\pi^2)^{-3/4} \frac{\pi}{2} \frac{3}{2} (J+1)^{-3/8} = (2\pi^2)^{-3/4} \frac{3\pi}{4} (J+1)^{-3/8}. \end{aligned} \quad (3.36)$$

Taking the square root of (3.36) and inserting the result in (3.33) yields

$$\|[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1} U\|_{2,2} \leq \|U\|_{8/3} (2\pi^2)^{-3/8} \frac{(3\pi)^{1/2}}{2} (J+1)^{-3/16}. \quad (3.37)$$

The factor of  $(J+1)^{-3/16}$  in (3.37) is one of the sources of the exponent  $-\frac{3}{16}$  in (1.14).

Next we shall derive an upper bound to  $\|[-\square^* - J(J+2)]^{-1}(1 - P_J)U\|_{2,2}$ . As in (3.30),

$$\begin{aligned} & \|[-\square^* - J(J+2)]^{-1}(1 - P_J)U\psi\|_2^2 \\ &= \int_{S^3} d\omega \int_{S^3} d\omega' \psi^*(\omega) U(\omega) h_J(\Theta(\omega, \omega')) U(\omega') \psi(\omega') \end{aligned} \tag{3.38}$$

where  $h_J(\Theta)$  is the integral kernel of  $[-\square^* - J(J+2)]^{-2}(1 - P_J)$  given by (2.34). Applying the Schwarz inequality and the definition of the norm of an operator as in (3.31) and (3.32) yields

$$\begin{aligned} & \|[-\square^* - J(J+2)]^{-1}(1 - P_J)U\|_{2,2} \\ & \leq \left[ \int_{S^3} d\omega \int_{S^3} d\omega' U^2(\omega) h_J^2(\Theta(\omega, \omega')) U^2(\omega') \right]^{1/4} \end{aligned} \tag{3.39}$$

and using Hölder's inequality yields in analogy with (3.33)

$$\begin{aligned} & \|[-\square^* - J(J+2)]^{-1}(1 - P_J)U\|_{2,2} \\ & \leq \|U\|_{8/3} \left[ \int_{S^3} d\omega \int_{S^3} d\omega' h_J^8(\Theta(\omega, \omega')) \right]^{1/16}. \end{aligned} \tag{3.40}$$

We use the estimate (3.27) for  $|h_J(\Theta)|$  in (3.40) to obtain

$$\begin{aligned} & \|[-\square^* - J(J+2)]^{-1}(1 - P_J)U\|_{2,2} \\ & \leq \|U\|_{8/3} \left[ \frac{1}{4 \cdot 2\pi^2} \left( \frac{\pi^2}{3} + \frac{1}{4} \right) \frac{1}{J+1} \right]^{1/2} \\ & \quad \times \left[ \int_{S^3} d\omega \int_{S^3} d\omega' \left( \frac{\sin((J+1)\Theta(\omega, \omega'))}{\sin(\Theta(\omega, \omega'))} \right)^8 \right]^{1/16}. \end{aligned} \tag{3.41}$$

As before, the integral over  $\omega$  has no dependence on the value of  $\omega'$  and as in (3.35) the integral is evaluated in closed form in Appendix 2; its value is

$$2\pi^2 \frac{2\pi^2}{3} [(J+1)^5 + (J+1)^3 + (J+1)] \tag{3.42}$$

which when inserted in (3.41) yields

$$\begin{aligned} & \|[-\square^* - J(J+2)]^{-1}(1 - P_J)U\|_{2,2} \\ & \leq \|U\|_{8/3} \left[ \frac{1}{4 \cdot 2\pi^2} \left( \frac{\pi^2}{3} + \frac{1}{4} \right) \frac{1}{J+1} \right]^{1/2} \\ & \quad \times \left( 2\pi^2 \frac{2\pi^2}{3} [(J+1)^5 + (J+1)^3 + (J+1)] \right)^{1/16} \\ & \leq \|U\|_{8/3} \frac{1}{2} (2\pi^2)^{-3/8} \left( \frac{\pi^2}{3} + \frac{1}{4} \right)^{1/2} \end{aligned}$$

$$\begin{aligned} & \times \left\{ \frac{1}{3} [(J+1)^{-3} + (J+1)^{-5} + (J+1)^{-7}] \right\}^{1/16} \\ & \leq \|U\|_{8/3} \frac{1}{2} (2\pi^2)^{-3/8} \left( \frac{\pi^2}{3} + \frac{1}{4} \right)^{1/2} (J+1)^{-3/16}. \end{aligned} \quad (3.43)$$

As before with (3.15) and (3.37), the power  $-\frac{3}{16}$  shows up in (1.14).

Finally, it is proved in [20], pp. 186–687 that if  $T$  is a bounded operator then  $\|T\| = \|T^*\|$ , so if  $A$  and  $B$  are self-adjoint operators and  $AB$  is bounded,  $\|AB\|_{2,2} = \|(AB)^*\|_{2,2} = \|B^*A^*\|_{2,2} = \|BA\|_{2,2}$ , so from (3.37) and (3.43) we see that

$$\begin{aligned} \left\| [-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1} U \right\|_{2,2} &= \|U[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1}\|_{2,2} \\ &\leq \|U\|_{8/3} (2\pi^2)^{-3/8} \frac{(3\pi^2)^{1/2}}{2} (J+1)^{-3/16} \end{aligned} \quad (3.44)$$

and

$$\begin{aligned} & \left\| [-\square^* - J(J+2)]^{-1} (1 - P_J) U \right\|_{2,2} \\ &= \|U[-\square^* - J(J+2)]^{-1} (1 - P_J)\|_{2,2} \\ &\leq \|U\|_{8/3} \frac{1}{2} (2\pi^2)^{-3/8} \left( \frac{\pi^2}{3} + \frac{1}{4} \right)^{1/2} (J+1)^{-3/16}. \end{aligned} \quad (3.45)$$

The estimates (3.4), (3.15), (3.16), (3.17), (3.24), (3.29), (3.44), and (3.45) will be crucial in our proofs on the following pages.

#### 4. Internal consistency of Fock's expansion

We shall now present a proof that the differential recurrence relation (1.16) which defines the coefficients  $\phi_{j,k}$  of Fock's expansion is internally consistent; i.e., that each  $\phi_{j,k}$  is in  $D(-\square^*) \subset L^\infty(S^3) \subset L^2(S^3)$ . Although the ideas behind this proof are not novel, the author is not aware of a previously published rigorous proof. Macek [15] did not address this issue directly, and the discussions of Fock [3] and Ermolaev [4] did not make explicit the integrability condition on  $U$  which ensures that each  $\phi_{j,k}$  is in  $D(-\square^*)$ .

We first observe that the recurrence relation (1.16)

$$\begin{aligned} \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} &= \frac{1}{4}(j+2)\phi_{j,k+1} + \frac{1}{16}\phi_{j,k+2} \\ &\quad - \frac{1}{2}U\phi_{j-1,k} + \frac{1}{2}E\phi_{j-2,k} \end{aligned} \quad (4.1)$$

is equivalent to the pair of recurrence relations

$$\begin{aligned} P_{j/2} \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} &= \frac{1}{4}(j+2)P_{j/2}\phi_{j,k+1} + \frac{1}{16}P_{j/2}\phi_{j,k+2} \\ &\quad + P_{j/2} \left[ -\frac{1}{2}U\phi_{j-1,k} + \frac{1}{2}E\phi_{j-2,k} \right] \end{aligned} \quad (4.2)$$

and

$$(1 - P_{j/2}) \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} = \frac{1}{4}(j+2)(1 - P_{j/2})\phi_{j,k+1} + \frac{1}{16}(1 - P_{j/2})\phi_{j,k+2} + (1 - P_{j/2}) \left[ -\frac{1}{2}U\phi_{j-1,k} + \frac{1}{2}E\phi_{j-2,k} \right] \tag{4.3}$$

where  $P_{j/2}$  is the spectral projection for  $-\square^*$  onto the interval  $[j/2(j/2+2) - \varepsilon, j/2(j/2+2) + \varepsilon]$  for some  $\varepsilon$  satisfying  $0 < \varepsilon < 1$ . If  $j = 2J$ , where  $J$  is a natural number, then  $P_{j/2} = P_J$ . If  $j = 2J + 1$ , where  $J$  is a natural number, then  $P_{j/2} \equiv 0$ . We observe that in any case

$$P_{j/2} \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \equiv 0 \tag{4.4}$$

for all  $j$ , so (4.2) is equivalent to

$$0 = \frac{1}{4}(j+2)P_{j/2}\phi_{j,k+1} + \frac{1}{16}P_{j/2}\phi_{j,k+2} + P_{j/2} \left[ -\frac{1}{2}U\phi_{j-1,k} + \frac{1}{2}E\phi_{j-2,k} \right]. \tag{4.5}$$

It is now convenient to decompose each  $\phi_{j,k}$  as

$$\phi_{j,k} = \omega_{j,k} + \chi_{j,k} \tag{4.6}$$

where

$$\omega_{j,k} = P_{j/2}\phi_{j,k} \text{ and } \chi_{j,k} = (1 - P_{j/2})\phi_{j,k}. \tag{4.7}$$

Notice that for  $j$  odd  $\omega_{j,k} \equiv 0$  and  $\chi_{j,k} \equiv \phi_{j,k}$ . Substituting (4.7) into (4.3) and (4.5) yields

$$\left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] (1 - P_{j/2})\chi_{j,k} = \frac{1}{4}(j+2)\chi_{j,k+1} + \frac{1}{16}\chi_{j,k+2} + (1 - P_{j/2}) \left[ -\frac{1}{2}U\phi_{j-1,k} + \frac{1}{2}E\phi_{j-2,k} \right] \tag{4.8}$$

and

$$0 = \frac{1}{4}(j+2)\omega_{j,k+1} + \frac{1}{16}\omega_{j,k+2} + P_{j/2} \left[ -\frac{1}{2}U\phi_{j-1,k} + \frac{1}{2}E\phi_{j-2,k} \right]. \tag{4.9}$$

These equations are solved in the following order: for *fixed*  $j$ , one starts with the maximum value of  $k$ , which equals  $[j/2]$ , and continues progressively in descending order until  $k = 0$ , and then  $j$  is increased by 1 and one starts over with the maximum value of  $k$ . A schematic chart of the order of progression is presented in Fig. 1.

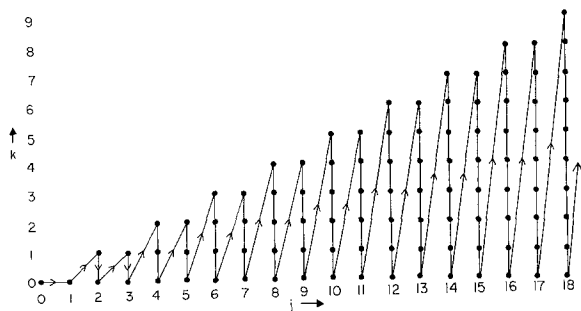


Figure 1

We shall use induction to show that each  $\phi_{j,k}$  is in  $D(-\square^*) \subset L^\infty(S^3)$ . We shall make use of the fact that  $U$  is in  $L^2(S^3)$ . To begin, for  $j=0$  we have  $k=0$ , so  $\chi_{0,0}=0$  and  $\omega_{0,0}$  is an arbitrary constant. Without loss of generality we set  $\omega_{0,0}=1$ , which evidently is in  $D(-\square^*) \subset L^\infty(S^3)$ . We now assume that  $\phi_{j,k}$  is in  $D(-\square^*) \subset L^\infty(S^2) \subset L^2(S^3)$  for all pairs  $(j, k)$  up to but not including some critical  $(\mathcal{J}, K)$ , where the pairs  $(j, k)$  are ordered as in Fig. 1. (Notice that the statement  $\phi_{j,k} \in D(-\square^*)$  is equivalent to the statement that both  $\omega_{j,k}$  and  $\chi_{j,k}$  are in  $D(-\square^*)$  since both  $P_{j/2}(-\square^*) = (-\square^*)P_{j/2}$  and  $(1 - P_{j/2})(-\square^*) = (-\square^*)(1 - P_{j/2})$  are relatively bounded by  $-\square^*$ .) We must demonstrate that  $\phi_{\mathcal{J},K}$  is in  $D(-\square^*)$ .

There are two possibilities: either  $\mathcal{J} = 2J + 1$  or  $\mathcal{J} = 2J$  for some natural number  $J$ . Let us check the former case first. With  $j = \mathcal{J} = 2J + 1$  and  $k = K$ , we have  $\omega_{\mathcal{J},K} = 0$  and Eq. (4.8) becomes

$$\begin{aligned} [-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]\chi_{2J+1,K} &= \frac{1}{4}(2J + 3)\chi_{2J+1,K+1} + \frac{1}{16}\chi_{2J+1,K+2} \\ &\quad - \frac{1}{2}U\phi_{2J,K} + \frac{1}{2}E\phi_{2J-1,K}. \end{aligned} \quad (4.10)$$

By hypothesis the three vectors  $\chi_{2J+1,K+1}$ ,  $\chi_{2J+1,K+2}$ , and  $\phi_{2J-1,K}$  are in  $D(-\square^*) \subset L^\infty(S^3) \subset L^2(S^3)$ , and since  $U \in L^2(S^3)$  and by hypothesis  $\phi_{2J,K} \in D(-\square^*) \subset L^\infty(S^3)$ , we see that  $U\phi_{2J,K}$  is in  $L^2(S^3)$ . Thus each term on the right side of (4.10) is in  $L^2(S^3)$ , and the operator  $[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]$  on the left side has an inverse defined on all of  $L^2(S^3)$  whose norm is bounded by  $(J + \frac{5}{4})^{-1}$ , so we can apply  $[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1}$  to both sides of (4.10) to obtain

$$\begin{aligned} \chi_{2J+1,K} &= [-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1} \{ \frac{1}{4}(2J + 3)\chi_{2J+1,K+1} + \frac{1}{16}\chi_{2J+1,K+2} \\ &\quad - \frac{1}{2}U\phi_{2J,K} + \frac{1}{2}E\phi_{2J-1,K} \} \end{aligned} \quad (4.11)$$

and we see that the right side of (4.11) defines a vector  $\chi_{2J+1,K} = \phi_{2J+1,K}$  in  $D(-\square^*)$  which satisfies equation (4.10)

As usual, the case  $\mathcal{J} = 2J$  is more complicated. Equation (4.8) with  $j = \mathcal{J} = 2J$  and  $k = K$  becomes

$$\begin{aligned} [-\square^* - J(J + 2)](1 - P_J)\chi_{2J,K} &= \frac{1}{2}(J + 1)\chi_{2J,K+1} + \frac{1}{16}\chi_{2J,K+2} \\ &\quad + (1 - P_J)(-\frac{1}{2}U\phi_{2J-1,K} + \frac{1}{2}E\phi_{2J-2,K}) \end{aligned} \quad (4.12)$$

and Eq. (4.9) with  $j = 2J$ ,  $k = K - 1$  (assuming  $K \geq 1$ ) becomes

$$\frac{1}{2}(J + 1)\omega_{2J,K} = -\frac{1}{16}\omega_{2J,K+1} - P_J(-\frac{1}{2}U\phi_{2J-1,K-1} + \frac{1}{2}E\phi_{2J-2,K-1}). \quad (4.13)$$

Let us treat Eq. (4.13) first. By hypothesis,  $\phi_{2J,K+1} \in D(-\square^*)$ ,  $\phi_{2J-2,K-1} \in D(-\square^*) \subset L^2(S^3)$ , and  $\phi_{2J-1,K-1} \in D(-\square^*) \subset L^\infty(S^3)$ . Since  $U$  is in  $L^2(S^3)$  and  $\phi_{2J-1,K-1}$  is in  $L^\infty(S^3)$ ,  $U\phi_{2J-1,K-1}$  is in  $L^2(S^3)$ . Thus  $(-\frac{1}{2}U\phi_{2J-1,K-1} + \frac{1}{2}E\phi_{2J-2,K-1})$  is in  $L^2(S^3)$ . When  $P_J$  is applied to this vector, the result is a *finite* linear combination of hyperspherical harmonics which are eigenfunctions of  $-\square^*$  with eigenvalue  $J(J + 2)$ , so  $P_J(-\frac{1}{2}U\phi_{2J-1,K-1} + \frac{1}{2}E\phi_{2J-2,K-1})$  is in  $D(-\square^*)$ . As we have already stated, by hypothesis  $\omega_{2J,K+1}$  is in  $D(-\square^*)$ , so the right side of (4.13) is in  $D(-\square^*)$ , so  $\omega_{2J,K}$  is in  $D(-\square^*)$ . This conclusion holds for  $K \geq 1$ ; if  $K = 0$ , then  $\omega_{2J,0}$  is a finite linear combination with *undetermined* coefficients

of hyperspherical harmonics of order  $J$ . These coefficients can be determined only by imposing the boundary condition for  $R = \infty$ , that  $\phi_E(R, \alpha, \Theta)$  be in  $L^2(\mathbb{R}^6)$ .

To treat  $\chi_{2J,K}$ , we examine the right side of Eq. (4.12) and note that by hypothesis  $\chi_{2J,K+1} \in D(-\square^*) \subset L^2(S^3)$ ,  $\chi_{2J,K+2} \in D(-\square^*) \subset L^2(S^3)$ ,  $\phi_{2J-2,K} \in D(-\square^*) \subset L^2(S^3)$ , and  $\phi_{2J-1,K} \in D(-\square^*) \subset L^\infty(S^3)$ . Since  $U$  is in  $L^2(S^3)$ ,  $U\phi_{2J-1,K}$  is in  $L^2(S^3)$ , so the right side of (4.12) is in  $L^2(S^3)$ . Since the right side of (4.12) is orthogonal to the kernel of  $[-\square^* - J(J+2)]$  and  $[-\square^* - J(J+2)]^{-1}(1 - P_J)$  is a bounded operator from  $L^2(S^3)$  to  $L^2(S^3)$ , we see that the equation

$$\begin{aligned} \chi_{2J,K} = & [-\square^* - J(J+2)]^{-1}(1 - P_J)\left\{\frac{1}{2}(J+1)\chi_{2J,K+1} + \frac{1}{16}\chi_{2J,K+2} \right. \\ & \left. + \left(-\frac{1}{2}U\phi_{2J-1,K} + \frac{1}{2}E\phi_{2J-2,K}\right)\right\} \end{aligned} \tag{4.14}$$

defines a function  $\chi_{2J,K}$  in  $D(-\square^*)$  which satisfies Eq. (4.12).

Thus since both  $\omega_{2J,K}$  and  $\chi_{2J,K}$  are in  $D(-\square^*)$ , so is  $\phi_{\beta,K} = \phi_{2J,K} = \omega_{2J,K} + \chi_{2J,K}$ . This completes our proof by induction of the internal consistency of Fock's expansion.

Now that we have proved that  $\phi_{i,k}$  and hence  $\psi_{j,k}$  are in the Banach space  $L^\infty(S^3)$ , we can make rigorous the definition of the sum (1.11), which up to now was only a formal expression. In Sects. 6 and 7 we shall prove that the  $\|\psi_{j,k}\|_\infty$  fall off fast enough to ensure that the series (1.11) converges for all  $s$  and  $t$ , so (1.11) can be viewed as a vector-valued analytic function of the two complex variables  $s$  and  $t$ , defined from  $\mathbb{C} \times \mathbb{C}$ , the set of all pairs of complex numbers, to  $L^\infty(S^3)$ .<sup>21</sup>

### 5. The basic idea of the proof of convergence

In this section we shall illustrate the method of our proof of the convergence of Fock's expansion by studying a simpler model problem. We emphasise that this simplified version probably has no physically interesting interpretation; it serves only to illustrate how the estimates in Sect. 3 will be applied later in this article.

In Eq. (1.16) with  $k = 0$

$$\begin{aligned} \left[-\square^* - \frac{j}{2}\left(\frac{j}{2} + 2\right)\right] \phi_{j,0} = & \frac{1}{4}(j+2)\phi_{j,1} + \frac{1}{16}\phi_{j,2} \\ & - \frac{1}{2}U\phi_{j-1,0} + \frac{1}{2}E\phi_{j-2,0} \end{aligned} \tag{5.1}$$

the first two terms on the right side have the primary effect of making the right side orthogonal to all solutions of the inhomogeneous equation. We can mock up this aspect of their effect by dropping them and applying the projection  $(1 - P_{j/2})$  to  $(-\frac{1}{2}U\phi_{j-1,0} + \frac{1}{2}E\phi_{j-2,0})$ , which yields

$$\left[-\square^* - \frac{j}{2}\left(\frac{j}{2} + 2\right)\right] \phi_{j,0} = (1 - P_{j/2})\left(-\frac{1}{2}U\phi_{j-1,0} + \frac{1}{2}E\phi_{j-2,0}\right). \tag{5.2}$$

Since the operator  $U$  is unbounded from its domain  $D(U)$  to  $L^2(S^3)$  while the operator  $E$  times the identity is a well-behaved bounded operator, we can expect



that the dominant term on the right side of Eq. (5.2) will be the one involving  $U\phi_{j-1,0}$ . As an approximation to Eq. (5.2), we study the equation

$$\left[-\square^* - \frac{j}{2}\left(\frac{j}{2}+2\right)\right]\phi_{j,0} = -\frac{1}{2}(1-P_{j/2})U\phi_{j-1,0}. \quad (5.3)$$

Since  $[-\square^* - (j/2)(j/2+2)]^{-1}(1-P_{j/2})$  is a bounded operator from  $L^2(S^3)$  to  $L^2(S^3)$ , we see that one solution of (5.3) is given by

$$\phi_{j,0} = -\frac{1}{2}\left[-\square^* - \frac{j}{2}\left(\frac{j}{2}+2\right)\right]^{-1}(1-P_{j/2})U\phi_{j-1,0} \quad (5.4)$$

and again for simplicity we shall not worry about the indeterminacy of the solution of Eq. (5.3) if  $j$  is even. We can now iterate Eq. (5.4) to obtain

$$\phi_{j,0} = \left(-\frac{1}{2}\right)^j \prod_{i=1}^j \left(\left[-\square^* - \frac{i}{2}\left(\frac{i}{2}+2\right)\right]^{-1}(1-P_{i/2})U\right)\phi_{0,0}, \quad (5.5)$$

We now take the 2-norm of both sides of Eq. (5.4), obtaining

$$\|\phi_{j,0}\|_2 = \left(\frac{1}{2}\right)^j \left\| \prod_{i=1}^j \left(\left[-\square^* - \frac{i}{2}\left(\frac{i}{2}+2\right)\right]^{-1}(1-P_{i/2})U\right)\phi_{0,0} \right\|_2. \quad (5.6)$$

We now make use of two facts [18]: For any bounded operator  $X$  and any vector  $\phi$ ,  $\|X\phi\|_2 \leq \|X\|_{2,2}\|\phi\|_2$ ; and for any two bounded operators  $X$  and  $Y$ ,  $\|XY\|_{2,2} \leq \|X\|_{2,2}\|Y\|_{2,2}$ . Applying these inequalities to (5.6) yields

$$\|\phi_{j,0}\|_2 \leq \left(\frac{1}{2}\right)^j \prod_{i=1}^j \left(\left\| \left[-\square^* - \frac{i}{2}\left(\frac{i}{2}+2\right)\right]^{-1}(1-P_{i/2})U \right\|_{2,2}\right)\|\phi_{0,0}\|_2. \quad (5.7)$$

We can now use (3.44) and (3.45) to estimate the operator norms which appear on the right side of (5.7). The basic conclusion to be drawn from these estimates is that for some constant  $A$ ,

$$\left\| \left[-\square^* - \frac{i}{2}\left(\frac{i}{2}+2\right)\right]^{-1}(1-P_{i/2})U \right\|_{2,2} \leq A(i+1)^{-3/16}. \quad (5.8)$$

Inserting this estimate into (5.7) yields

$$\|\phi_{j,0}\|_2 \leq \left(\frac{1}{2}\right)^j \prod_{i=1}^j (A(i+1)^{-3/16}) = (A/2)^j ((j+1)!)^{-3/16} \|\phi_{0,0}\|_2. \quad (5.9)$$

This inequality is of the desired form (1.17), and it would show that the series

$$\sum_{j=0}^{\infty} s^j \phi_{j,0}(\alpha, \theta) \quad (5.10)$$

converges for all finite  $s$  to a function in  $L^2(S^3)$ .

Of course, the actual recurrence relation (5.1) is much more complicated than the model relation (5.3). However, the intuition one can develop in understanding the argument in this section will prove to be very useful in following our treatment of the full recurrence relation (5.1) in Sects. 6 and 7.

**6. Proof that Fock’s expansion converges in  $L^2(S^3)$**

In this section we shall prove that for every finite value of  $R$ , Fock’s expansion

$$\sum_{j=0}^{\infty} \sum_{k=0}^{[j/2]} R^{j/2} (\ln R)^k \psi_{j,k}(\alpha, \Theta) \tag{6.1}$$

converges to a function  $\psi(R; \alpha, \Theta)$  in  $L^2(S^3)$ . The coefficients  $\psi_{j,k}(\alpha, \Theta)$  are defined by Eq. (1.8). In Sect. I we defined ‘renormalised’ coefficients  $\phi_{j,k}$  by Eq. (1.15)

$$\psi_{j,k} = \frac{\phi_{j,k}}{4^k k!} \tag{6.2}$$

and we saw that the  $\phi_{j,k}$ ’s were determined by the recurrence relation (1.16)

$$\left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} = \frac{1}{4} (j+2) \phi_{j,k+1} + \frac{1}{16} \phi_{j,k+2} - \frac{1}{2} U \phi_{j-1,k} + \frac{1}{2} E \phi_{j-2,k} \tag{6.3}$$

Our goal is to derive an estimate of the form (1.17)

$$\|\phi_{j,k}\|_2 \leq C \frac{A^j}{(j!)^{3/16}} \tag{6.4}$$

We shall prove this by induction. Since  $\phi_{0,0} = 1$ , evidently it obeys an inequality of the form (6.4). We now make the induction hypothesis that an estimate of the form (6.4) holds for all  $j$  smaller than some  $\mathcal{J}$ , and we shall then prove that (6.4) also holds for  $j = \mathcal{J}$ . As before, there are two possibilities: either  $\mathcal{J} = 2J + 1$  or  $\mathcal{J} = 2J$  for some natural number  $J$ . Let us do the former case first.

With  $j = \mathcal{J} = 2J + 1$ , (6.3) becomes

$$\left[ -\square^* - (J + \frac{1}{2})(J + \frac{5}{2}) \right] \phi_{2J+1,k} = \frac{1}{4} (2J+3) \phi_{2J+1,k+1} + \frac{1}{16} \phi_{2J+1,k+2} - \frac{1}{2} U \phi_{2J,k} + \frac{1}{2} E \phi_{2J-1,k} \tag{6.5}$$

Since  $[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1}$  is a bounded operator from  $L^2(S^3)$  to itself with norm  $(J + \frac{5}{4})^{-1}$ , its application to (6.5) yields

$$\begin{aligned} \phi_{2J+1,k} &= \frac{1}{4} (2J+3) [-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1} \phi_{2J+1,k+1} \\ &+ \frac{1}{16} [-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1} \phi_{2J+1,k+2} \\ &+ [-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1} (-\frac{1}{2} U \phi_{2J,k} + \frac{1}{2} E \phi_{2J-1,k}). \end{aligned} \tag{6.6}$$

We recall from Sect. 4 that we solve the equations for the  $\phi_{2J+1,k}$ ’s in order of decreasing  $k$ , so Eq. (6.6) can be viewed as an inhomogeneous three term recurrence relation for the  $\phi_{2J+1,k}$ ’s, where the inhomogeneity is the last term on the right side of (6.6). We need to solve this recurrence relation to obtain each  $\phi_{2J+1,k}$  in terms of  $\phi_{j,k}$ ’s with  $j$  strictly smaller than  $2J + 1$ . Eq. (6.6) was solved by

inspection; the reader can verify that its solution is

$$\begin{aligned}\phi_{2J+1,k} &= \sum_{n=0}^{[(J-k)/2]} \sum_{m=0}^{J-k-2n} \binom{J-k-m-n}{n} \\ &\quad \times \left(\frac{1}{4}(2J+3)[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}\right)^{J-k-2n-m} \\ &\quad \times \left(\frac{1}{16}[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}\right)^n \\ &\quad \times [-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1} \left(-\frac{1}{2}U\phi_{2J,J-m} + \frac{1}{2}E\phi_{2J+1,J-m}\right).\end{aligned}\quad (6.7)$$

We now take the 2-norm of both sides and use the inequality  $\|XY\|_{2,2} \leq \|X\|_{2,2}\|Y\|_{2,2}$  to obtain

$$\begin{aligned}\|\phi_{2J+1,k}\|_2 &\leq \sum_{n=0}^{[(J-k)/2]} \sum_{m=0}^{J-k-2n} \binom{J-k-m-n}{n} \\ &\quad \times \left(\frac{1}{4}(2J+3)\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}\|_{2,2}\right)^{J-k-2n-m} \\ &\quad \times \left(\frac{1}{16}\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}\|_{2,2}\right)^n \\ &\quad \times \left(\frac{1}{2}\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}U\|_{2,2}\|\phi_{2J,J-m}\|_2\right. \\ &\quad \left.+ \frac{1}{2}\|E\|_{2,2}\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}\|_{2,2}\|\phi_{2J-1,J-m}\|_2\right).\end{aligned}\quad (6.8)$$

By Eq. (3.16)

$$\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}\|_{2,2} = (J+\frac{5}{4})^{-1}; \quad (6.9)$$

by inequality (3.44)  $\|[-\square^* - (J+\frac{1}{2})(J+\frac{5}{2})]^{-1}U\|_{2,2} \leq D_{1/2}(J+1)^{-3/16}$ , where

$$D_{1/2} = \|U\|_{8/3}(2\pi^2)^{-3/8}\frac{(3\pi^2)}{2}; \quad (6.10)$$

and by the induction hypothesis

$$\|\phi_{2J,J-m}\|_2 \leq C\frac{A^{2J}}{((2J)!)^{3/16}} \quad \text{and} \quad \|\phi_{2J-1,J-m}\|_2 \leq C\frac{A^{2J}}{((2J-1)!)^{3/16}} \quad (6.11)$$

and inserting these estimates into (6.8) yields

$$\begin{aligned}\|\phi_{2J+1,k}\|_2 &\leq \sum_{n=0}^{[(J-k)/2]} \sum_{m=0}^{J-k-2n} \binom{J-k-m-n}{n} \left(\frac{2J+3}{4J+5}\right)^{J-k-2n-m} \left(\frac{1}{16J+20}\right)^n \\ &\quad \times \left(\frac{1}{2}D_{1/2}(J+1)^{-3/16}CA^{2J}((2J)!)^{-3/16}\right. \\ &\quad \left.+ \frac{1}{2}\|E\|(J+\frac{5}{4})^{-1}CA^{2J-1}((2J-1)!)^{-3/16}\right) \\ &\leq \sum_{n=0}^{[(J-k)/2]} \sum_{m=0}^{J-k-2n} \binom{J-k-m-n}{n} \left(\frac{3}{5}\right)^{J-k-2n-m} \left(\frac{1}{16J+20}\right)^n \\ &\quad \times CA^{2J+1}((2J+1)!)^{-3/16}(D_{1/2}/A + \|E\|/A^2).\end{aligned}\quad (6.12)$$

We observe that the last term in (6.12) is of the desired form (6.4), so our task is to show that the double sum in (6.12) is bounded by a constant independent of  $J$  and  $K$ . To this end, let us reverse the order of the summation on  $m$ . Let

$i = J - k - 2n - m$ ; then  $i$  goes from 0 up to  $J - k - 2n$ , and the double sum in (6.12) becomes

$$\sum_{n=0}^{[(J-k)/2]} \sum_{i=0}^{J-k-2n} \binom{i+n}{n} \left(\frac{3}{5}\right)^i \left(\frac{1}{16J+20}\right)^n \tag{6.13}$$

We can obtain an upper bound to (6.13) by extending both summations up to  $\infty$ , which yields

$$\begin{aligned} &\sum_{n=0}^{\infty} \sum_{i=0}^{\infty} \binom{i+n}{n} \left(\frac{3}{5}\right)^i \left(\frac{1}{16J+20}\right)^n = \sum_{n=0}^{\infty} \left(1 - \frac{3}{5}\right)^{-n-1} \left(\frac{1}{16J+20}\right)^n \\ &= \frac{5}{2} \sum_{n=0}^{\infty} \left(\frac{5}{2} \frac{1}{16J+20}\right)^n = \frac{5}{2} \left(1 - \frac{5}{2} \frac{1}{16J+20}\right)^{-1} \leq \frac{5}{2} \left(1 - \frac{5}{2} \frac{1}{20}\right)^{-1} \\ &= \frac{5}{2} \frac{8}{7} = \frac{20}{7} \end{aligned} \tag{6.14}$$

so inserting this estimate into (6.12) yields

$$\|\phi_{2J+1,k}\|_2 \leq CA^{2J+1} ((2J+1)!)^{-3/16} \frac{20}{7} (D_{1/2}/A + |E|/A^2) \tag{6.15}$$

Obtaining the analogous estimate for  $\mathcal{F} = 2J$  is a little more involved. With  $j = \mathcal{F} = 2J$  Eq. (6.3) becomes

$$\begin{aligned} [-\square^* - J(J+2)]\phi_{2J,k} &= \frac{1}{2}(J+1)\phi_{2J,k+1} + \frac{1}{16}\phi_{2J,k+2} \\ &\quad - \frac{1}{2}U\phi_{2J-1,k} + \frac{1}{2}E\phi_{2J-2,k} \end{aligned} \tag{6.16}$$

As in Sect. 4, Eqs. (4.6) and (4.7), we decompose  $\phi_{2J,k}$  as  $\phi_{2J,k} = \omega_{2J,k} + \chi_{2J,k}$  where

$$\omega_{2J,k} = P_J\phi_{2J,k} \quad \text{and} \quad \chi_{2J,k} = (1 - P_J)\phi_{2J,k} \tag{6.17}$$

and we obtain Eqs. (4.8) and (4.9):

$$\begin{aligned} [-\square^* - J(J+2)](1 - P_J)\chi_{2J,k} \\ = \frac{1}{2}(J+1)\chi_{2J,k-1} + \frac{1}{16}\chi_{2J,k+2} + (1 - P_J)\left(-\frac{1}{2}U\phi_{2J-1,k} + \frac{1}{2}E\phi_{2J-2,k}\right) \end{aligned} \tag{6.18}$$

and

$$\omega_{2J,k+1} = -(J+1)^{-1} \frac{1}{8}\omega_{2J,k+2} - (J+1)^{-1} P_J(-U\phi_{2J-1,k} + E\phi_{2J-2,k}). \tag{6.19}$$

Equation (6.18) can be viewed as an inhomogeneous three-term recurrence relation and Eq. (6.19) as an inhomogeneous two-term recurrence relation. Their solutions were found by inspection. The reader can check that

$$\begin{aligned} \chi_{2J,k} &= \sum_{n=0}^{[(J-k-1)/2]} \sum_{m=0}^{J-k-2n-1} \binom{J-k-m-n-1}{n} \\ &\quad \times \left(\frac{1}{2}(J+1)\right) [-\square^* - J(J+2)]^{-1} (1 - P_J)^{J-k-2n-m-1} \\ &\quad \times \left(\frac{1}{16}\right) [-\square^* - J(J+2)]^{-1} (1 - P_J)^n \\ &\quad \times [-\square^* - J(J+2)]^{-1} (1 - P_J) \left(-\frac{1}{2}U\phi_{2J-1,J-m-1} + \frac{1}{2}E\phi_{2J-2,J-m-1}\right) \end{aligned} \tag{6.20}$$

and

$$\omega_{2J,k} = -(J+1)^{-1} \sum_{n=0}^{J-k} \left(-\frac{1}{8(J+1)}\right)^n P_J(-U\phi_{2J-1,k+n-1} + E\phi_{2J-2,k+n-1}) \tag{6.21}$$

for  $k \geq 1$ ; for the moment we shall assume the convention that  $\omega_{2,J,0} = 0$  for  $J \geq 1$ . Observe that  $\chi_{2,J,J} = 0$  from Eq. (6.20). This is an expression of the fact that  $\phi_{2,J,J} = \omega_{2,J,J}$  is a finite linear combination of the hyperspherical harmonics of order  $J$ .

Let us estimate  $\|\chi_{2,J,k}\|_2$  first. As in (6.8),

$$\begin{aligned} \|\chi_{2,J,k}\|_2 &\leq \sum_{n=0}^{[(J-k-1)/2]} \sum_{m=0}^{J-k-2n-1} \binom{J-k-2n-m-1}{n} \\ &\quad \times \left(\frac{1}{2}(J+1)\right) \|[-\square^* - J(J+2)]^{-1}(1-P_J)\|_{2,2}^{J-k-2n-m-1} \\ &\quad \times \left(\frac{1}{16}\right) \|[-\square^* - J(J+2)]^{-1}(1-P_J)\|_{2,2}^n \\ &\quad \times \left(\frac{1}{2}\right) \|[-\square^* - J(J+2)]^{-1}(1-P_J)U\|_{2,2} \|\phi_{2J-1,J-m-1}\|_2 \\ &\quad + \frac{1}{2}|E| \|[-\square^* - J(J+2)]^{-1}(1-P_J)\|_{2,2} \|\phi_{2J-2,J-m-1}\|_2. \end{aligned} \tag{6.22}$$

By Eq. (3.17) for  $J \geq 1$

$$\|[-\square^* - J(J+2)]^{-1}(1-P_J)\|_{2,2} = (2J+1)^{-1}; \tag{6.23}$$

by inequality (3.45)  $\|[-\square^* - J(J+2)]^{-1}(1-P_J)U\|_{2,2} \leq D_1(J+1)^{-3/16}$ , where

$$D_1 = \|U\|_{8/3} \frac{1}{2} (2\pi^2)^{-3/8} (\pi^2/2 + \frac{1}{4})^{1/2}; \tag{6.24}$$

and by the induction hypothesis

$$\|\phi_{2J-1,J-m-2}\|_2 \leq C \frac{A^{2J-1}}{((2J-1)!)^{3/16}} \quad \text{and} \quad \|\phi_{2J-2,J-m-1}\|_2 \leq \frac{A^{2J-2}}{((2J-2)!)^{3/16}}, \tag{6.25}$$

so inserting these estimates into (6.22) yields

$$\begin{aligned} \|\chi_{2,J,k}\|_2 &\leq \sum_{n=0}^{[(J-k-1)/2]} \sum_{m=0}^{J-k-2n-1} \binom{J-k-m-n-1}{n} \\ &\quad \times \left(\frac{J+1}{4J+2}\right)^{J-k-2n-m-1} \left(\frac{1}{32J+16}\right)^n \\ &\quad \times \left(\frac{1}{2}D_1(J+1)\right)^{-3/16} CA^{2J-1} ((2J-1)!)^{-3/16} \\ &\quad + \frac{1}{2}|E| (2J+1)^{-1} CA^{2J-2} ((2J-2)!)^{-3/16} \\ &\leq \sum_{n=0}^{[(J-k-1)/2]} \sum_{m=0}^{J-k-2n-1} \binom{J-k-m-n-1}{n} \left(\frac{1}{2}\right)^{J-k-2n-m-1} \left(\frac{1}{32J+16}\right)^n \\ &\quad \times (CA^{2J} ((2J!)^{-3/16} (D_1/A + \frac{1}{2}|E|/A^2)). \end{aligned} \tag{6.26}$$

As with (6.12), the last term is of the desired form (6.4), so we need to show that the double sum is bounded independent of  $J$  and  $k$ . Again we reverse the order of the  $m$  summation, letting  $i = J - k - 2n - 1 - m$ . The index  $i$  goes from 0 up to  $J - k - 2n - 1$ , and the double sum in (6.26) becomes

$$\sum_{n=0}^{[(J-k-1)/2]} \sum_{i=0}^{J-k-2n-1} \binom{i+n}{n} \left(\frac{1}{2}\right)^i \left(\frac{1}{32J+16}\right)^n. \tag{6.27}$$

We can obtain an upper bound to (6.27) by extending the  $i$  and  $n$  summations up to  $\infty$ , which yields

$$\begin{aligned} \sum_{n=0}^{\infty} \sum_{i=0}^{\infty} \binom{i+n}{n} \left(\frac{1}{2}\right)^i \left(\frac{1}{32J+16}\right)^n &= \sum_{n=0}^{\infty} \left(1 - \frac{1}{2}\right)^{-n-1} \left(\frac{1}{32J+16}\right)^n \\ &= 2 \sum_{n=0}^{\infty} \left(\frac{1}{16J+8}\right)^n = 2 \left(1 - \frac{1}{16J+8}\right)^{-1} \leq 2 \frac{8}{7} = \frac{16}{7}. \end{aligned} \quad (6.28)$$

Inserting this estimate into (6.26) yields

$$\|\chi_{2J,k}\|_2 \leq CA^{2J} ((2J)!)^{-3/16} \frac{16}{7} (D_1/A + \frac{1}{2}|E|/A^2). \quad (6.29)$$

Finally we need to use Eq. (6.21) to estimate  $\|\omega_{2J,k}\|_2$ . Taking the 2-norm of both sides of (6.21) yields

$$\begin{aligned} \|\omega_{2J,k}\|_2 &\leq \sum_{n=0}^{J-k} \left(\frac{1}{8J+8}\right)^n [\|(J+1)^{-1}P_J U\|_{2,2} \|\phi_{2J-1,k+n-1}\|_2 \\ &\quad + |E|(J+1)^{-1} \|\phi_{2J-2,k+n-1}\|_2]. \end{aligned} \quad (6.30)$$

From (3.15) we conclude that  $\|(J+1)^{-1}P_J U\|_{2,2} \leq D_0(J+1)^{-3/16}$ , where

$$D_0 = \|U\|_{8/3} (2\pi^2)^{-3/8} \quad (6.31)$$

and by the induction hypothesis

$$\|\omega_{2J-1,k+n-1}\|_2 \leq C \frac{A^{2J-1}}{((2J-1)!)^{3/16}} \quad \text{and} \quad \|\omega_{2J-2,k+n-1}\|_2 \leq C \frac{A^{2J-2}}{((2J-1)!)^{3/16}} \quad (6.32)$$

so using these two estimates in (6.30) yields

$$\begin{aligned} \|\omega_{2J,k}\|_2 &\leq \sum_{n=0}^{J-k} \left(\frac{1}{8J+8}\right)^n [D_0(J+1)^{-3/16} CA^{2J-1} ((2J-1)!)^{-3/16} \\ &\quad + |E|(J+1)^{-1} CA^{2J-2} ((2J-2)!)^{-3/16}] \\ &\leq \sum_{n=0}^{J-k} \left(\frac{1}{8J+8}\right)^n CA^{2J} ((2J)!)^{-3/16} (2D_0/A + 2|E|/A^2) \end{aligned} \quad (6.33)$$

where the last term is of the desired form (6.4), and we need only show that the sum is bounded independent of  $J$  and  $k$ . This is easy, since

$$\sum_{n=0}^{J-k} \left(\frac{1}{8J+8}\right)^n \leq \sum_{n=0}^{\infty} \left(\frac{1}{8J+8}\right)^n = \left(1 - \frac{1}{8J+8}\right)^{-1} \leq \frac{8}{7}. \quad (6.34)$$

Thus using (6.34) in (6.33) yields

$$\|\omega_{2J,k}\|_2 \leq CA^{2J} ((2J)!)^{-3/16} \frac{16}{7} (D_0/A + |E|/A^2). \quad (6.35)$$

We accordingly see that the induction hypothesis for  $j = \mathcal{J}$  can be verified provided that  $A$  was originally chosen sufficiently large that all of the quantities

$$\frac{20}{7} (D_{1/2}/A + |E|/A^2), \frac{16}{7} (D_1/A + \frac{1}{2}|E|/A^2), \quad \text{and} \quad \frac{16}{7} (D_0/A + |E|/A^2), \quad (6.36)$$

which appear in (6.15), (6.29), and (6.35), respectively, are smaller than 1.

As was remarked previously in Sect. 4 and immediately after equation (6.21),  $\omega_{2J,0}$ , which is a finite linear combination of the hyperspherical harmonics of order  $J$ , cannot be determined in terms of  $\omega_{0,0}$  if we confine our attention to non-infinite regions of space. In fact, Fock's equation (1.3) has infinitely many formal solutions  $\psi^{(l)}(R; \alpha, \theta)$  whose leading term for small  $R$  is  $R^l \omega_{2l,0}$  and for which  $\omega_{2J,0} = 0$  for  $J \neq l$ .  $R^l \omega_{2l,0}$  is a harmonic polynomial of degree  $2l$ ; i.e.,

$$(-\nabla_1^2 - \nabla_2^2)R^l \omega_{2l,0} = 0. \tag{6.37}$$

The proper coefficients for the functions  $\omega_{2l,0}$  can be determined in terms of  $\omega_{0,0}$  only by imposing the square integrability boundary condition as  $R \rightarrow \infty$  [6]. For obvious reasons this is likely not to be practicable for some time. However, this "large  $R$ " problem decouples to a considerable extent from our "small  $R$ " problem of proving the convergence of the series for all  $R$

$$\sum_{i=0}^{\infty} \psi^{(i)}(R; \alpha, \theta) \tag{6.38}$$

to a function in  $L^2(S^3)$ . We have been able to show that if the series

$$\sum_{l=0}^{\infty} R^l \omega_{2l,0} \tag{6.39}$$

converges for all  $R$  to a function in  $L^2(S^3)$ , then the series (6.38) does as well. In other words, provided that the coefficients for the  $\omega_{2l,0}$ 's are not chosen in so pathological a manner that the series (6.39) is divergent, the series (6.38) will be convergent. The condition that (6.39) be a convergent series is a quite weak hypothesis, and it seems very natural.

In terms of the variables  $s$  and  $t$  defined by Eq. (1.10), Fock's expansion for  $\psi^{(l)}(s, t; \alpha, \theta)$  is

$$\psi^{(l)}(s, t; \alpha, \theta) = \sum_{n=2l}^{\infty} \sum_{k=0}^{\infty} s^n t^k \psi_{n+2k,k}^{(l)}(\alpha, \theta). \tag{6.40}$$

The same methods that were used earlier throughout this section will show that the  $\psi_{j,k}^{(l)}(\alpha, \theta)$ 's obey an estimate of the form

$$\|\psi_{j,k}^{(l)}\|_2 \leq C \frac{A^{j-2l} \left( (2l)! \right)^{3/16}}{4^k k! \left( j! \right)} \|\omega_{2l,0}\|_2. \tag{6.41}$$

If we now use the expansion (6.40) in Eq. (6.38), we obtain

$$\sum_{l=0}^{\infty} \sum_{n=2l}^{\infty} \sum_{k=0}^{\infty} s^n t^k \psi_{n+2k,k}^{(l)}(\alpha, \theta). \tag{6.42}$$

If we eliminate  $n$  in favor of  $m$ , where  $m = n - 2l$ , (6.42) becomes

$$\sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \sum_{k=0}^{\infty} s^{2l+m} t^k \psi_{2l+m+2k,k}^{(l)}(\alpha, \theta). \tag{6.43}$$

Our goal is to show that if (6.39) converges, then (6.43) does as well. We use our estimate (6.41) to obtain an upper bound to the 2-norm (in  $L^2(S^3)$ ) of (6.43):

$$\sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \sum_{k=0}^{\infty} |s|^{2l+m} |t|^k C \frac{A^{m+2k}}{4^k k!} \left( \frac{(2l)!}{(m+2l+2k)!} \right)^{3/16} \|\omega_{2l,0}\|_2. \tag{6.44}$$

Since  $(2l)!/(m+2l+2k)! \leq 1/(m+2k)!$ , (6.44) is bounded above by

$$\sum_{l=0}^{\infty} |s|^{2l} \|\omega_{2l,0}\|_2 \sum_{m=0}^{\infty} \sum_{k=0}^{\infty} |s|^m |t|^k C \frac{A^{m+2k}}{4^k k!} ((m+2k)!)^{-3/16}. \tag{6.45}$$

The convergence of the double sum over  $m$  and  $k$  is immediately obvious, and the convergence of the sum over  $l$  is equivalent to the convergence of (6.37).

In summary, we have proved that if the coefficients for  $\omega_{2l,0}$  are not chosen in a pathological manner, Fock's expansion converges for all  $R$  to a function in  $L^2(S^3)$ . In the next section we shall prove that it also converges in  $L^\infty(S^3)$ .

**7. Proof that Fock's expansion converges in  $L^\infty(S^3)$  and satisfies Schrödinger's equation**

In this section we prove that Fock's expansion (1.7) converges for all finite  $R$  to a function in  $L^\infty(S^3)$  and that this function satisfies Schrödinger's equation (1.3), considered as a partial differential equation with no boundary condition at  $R = \infty$ . We first derive a factorially decaying upper bound to  $\|[-\square^* - j/2(j/2+2)]\phi_{j,k}\|_2$  and then a factorially decaying upper bound to  $\|\phi_{j,k}\|_\infty$ . We then prove that the function defined by Fock's expansion (1.7) obeys Schrödinger's equation (1.7) with no boundary condition as  $R \rightarrow \infty$ .

To begin, we observe that since  $\omega_{2J,k} = P_J \omega_{2J,k}$

$$\|\omega_{2J,k}\|_\infty \leq \|P_J\|_{2,\infty} \|\omega_{2J,k}\|_2. \tag{7.1}$$

By (3.4)  $\|P_J\|_{2,\infty} \leq (J+1)(2\pi^2)^{-1/2}$ , and in the last section we proved that

$$\|\omega_{2J,k}\|_2 \leq CA^{2J} ((2J)!)^{-3/16} \tag{7.2}$$

so using these two estimates in (7.1) demonstrates that

$$\|\omega_{2J,k}\|_\infty \leq C'(A')^{2J} ((2J+2)!)^{-3/16} \tag{7.3}$$

if we choose two new constants  $C' > C$  and  $A' > A$ . Having obtained (7.3), we now go through an induction argument on  $\|[-\square^* + (j/2)(j/2+2)]\phi_{j,k}\|_2$ . For  $j = 0$ ,  $\phi_{0,0} = \omega_{0,0}$  obeys  $[-\square^*]\omega_{0,0} = 0$ . We now make the induction hypothesis that the  $\phi_{j,k}$ 's obey an estimate of the form

$$\left\| \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} \right\|_2 \leq C'(A')^j (j!)^{-3/16} \tag{7.4}$$

for all  $j$  up to but not including some particular  $\mathcal{J}$ , and we set about proving that (7.4) also holds for  $j = \mathcal{J}$ . Let us do the case  $j = \mathcal{J} = 2J + 1$  first.



With  $j = 2J + 1$ , we have from Eq. (6.7) that

$$\begin{aligned} [-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]\phi_{2J+1,k} &= \sum_{n=0}^{[(J-k)/2]} \sum_{m=0}^{J-k-2n} \binom{J-k-m-n}{n} \\ &\times (\frac{1}{4}(2J+3)[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1})^{J-k-2n-m} \\ &\times ((\frac{1}{16})[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1})^n (-\frac{1}{2}U\phi_{2J,J-m} + \frac{1}{2}E\phi_{2J-1,J-m}). \end{aligned} \quad (7.5)$$

We now note that

$$\phi_{2J-1,J-m} = [-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]^{-1}[-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]\phi_{2J-1,J-m} \quad (7.6)$$

and that

$$\begin{aligned} \phi_{2J,J-m} &= \omega_{2J,J-m} + \chi_{2J,J-m} \\ &= \omega_{2J,J-m} + [-\square^* - J(J+2)]^{-1}(1 - P_J)[-\square^* - J(J+2)]\chi_{2J,J-m}. \end{aligned} \quad (7.7)$$

Using (7.6) and (7.7) to re-express the last term in (7.5) yields

$$\begin{aligned} -\frac{1}{2}U\omega_{2J,J-m} - \frac{1}{2}\{U[-\square^* - J(J+2)]^{-1}(1 - P_J)\}[-\square^* - J(J+2)]\chi_{2J,J-m} \\ + \frac{1}{2}E[-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]^{-1}[-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]\phi_{2J-1,J-m} \end{aligned} \quad (7.8)$$

so the 2-norm of (7.8) is bounded above by

$$\begin{aligned} \frac{1}{2}\|U\|_2\|\omega_{2J,J-m}\|_\infty + \frac{1}{2}\|U[-\square^* - J(J+2)]^{-1}(1 - P_J)\|_{2,2} \\ \times \|[-\square^* - J(J+2)]\chi_{2J,J-m}\|_2 \\ + \frac{1}{2}E\|[-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]^{-1}\|_{2,2}\|[-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]\phi_{2J-1,J-m}\|_2 \end{aligned} \quad (7.9)$$

and we can use (3.16), (3.45) and (6.24) to estimate the operator norms, thereby obtaining an upper bound to (7.9) of

$$\begin{aligned} \frac{1}{2}\|U\|_2\|\omega_{2J,J-m}\|_\infty + \frac{1}{2}D_1(J+1)^{-3/16}\|[-\square^* - J(J+2)]\chi_{2J,J-m}\|_2 \\ + \frac{1}{2}E|(J + \frac{1}{4})^{-1}\|[-\square^* - (J + \frac{1}{2})(J + \frac{3}{2})]\phi_{2J-1,J-m}\|_2. \end{aligned} \quad (7.10)$$

By the induction hypothesis and (7.3), we can bound the vector norms in (7.10) to obtain an upper bound to (7.10)

$$C'(A')^{2J+1}((2J+1)!)^{-3/16}(\frac{1}{2}\|U\|_2/A' + D_1/A' + |E|/(A')^2). \quad (7.11)$$

Having estimated the last term in (7.5), we can then take the 2-norm of both sides of (7.5), which gives us

$$\begin{aligned} \|[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]\phi_{2J+1,k}\|_2 \\ \leq \sum_{n=0}^{[(J-k)/2]} \sum_{m=0}^{J-k-2n} \binom{J-k-m-n}{n} \\ \times (\frac{1}{4}(2J+3)\|[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1}\|_{2,2})^{J-k-2n-m} \\ \times ((\frac{1}{16})\|[-\square^* - (J + \frac{1}{2})(J + \frac{5}{2})]^{-1}\|_{2,2})^n \\ \times C'(A')^{2J+1}((2J+1)!)^{-3/16}(\frac{1}{2}\|U\|_2/A' + D_1/A' + |E|/(A')^2)^2. \end{aligned} \quad (7.12)$$

Using Eq. (3.16) to bound  $\|[-\square^* - (J + \frac{1}{2})(J + \frac{3}{2})]^{-1}\|_{2,2}$  yields

$$\begin{aligned} & \|[-\square^* - (J + \frac{1}{2})(J + \frac{3}{2})]\phi_{2J+1,k}\|_2 \\ & \leq \sum_{n=0}^{[(J-k)/2]} \sum_{m=0}^{J-k-2n} \binom{J-k-m-n}{n} \left(\frac{2J+3}{4J+5}\right)^{J-k-2n-m} \left(\frac{1}{16J+20}\right)^n \\ & \quad \times C'(A')^{2J+1} ((2J+1)!)^{-3/16} (\frac{1}{2}\|U\|_2/A' + D_1/A' + |E|/(A')^2). \end{aligned} \tag{7.13}$$

The summation in (7.13) is exactly the same as that in (6.12), so we can use its upper bound of 20/7 derived in (6.14) to conclude that

$$\begin{aligned} & \|[-\square^* - (J + \frac{1}{2})(J + \frac{3}{2})]\phi_{2J+1,k}\|_2 \\ & \leq C'(A')^{2J+1} ((2J+1)!)^{-3/16} \frac{20}{7} (\frac{1}{2}\|U\|_2/A' + D_1/A' + |E|/(A')^2). \end{aligned} \tag{7.14}$$

Now we need to treat the case  $\mathcal{J} = 2J$ . We observe that  $\|[-\square^* - J(J+2)]\phi_{2J,k}\|_2 = \|[-\square^* - J(J+2)]\chi_{2J,k}\|_{2s}$  and we see from (6.20) that

$$\begin{aligned} [-\square^* - J(J+2)]\chi_{2J,k} &= \sum_{n=0}^{[(J-k-1)/2]} \sum_{m=0}^{J-k-2n-1} \binom{J-k-m-n-1}{n} \\ & \quad \times (\frac{1}{2}(J+1))[-\square^* - J(J+2)]^{-1} (1 - P_J)^{J-k-2n-m-1} \\ & \quad \times ((\frac{1}{16})[-\square^* - J(J+2)]^{-1} (1 - P_J))^n \\ & \quad \times (1 - P_J) (-\frac{1}{2}U\phi_{2J-1,J-m-1} + \frac{1}{2}E\phi_{2J-2,J-m-1}). \end{aligned} \tag{7.15}$$

As in (7.6) and (7.7), we note that

$$\phi_{2J-1,J-m-1} = [-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]^{-1} [-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]\phi_{2J-1,J-m-1} \tag{7.16}$$

and

$$\begin{aligned} \phi_{2J-2,J-m-1} &= \omega_{2J-2,J-m-1} + \chi_{2J-2,J-m-1} \\ &= \omega_{2J-2,J-m-1} + [-\square^* - (J-1)(J+1)]^{-1} (1 - P_{J-1}) \\ & \quad \times [-\square^* - (J-1)(J+1)]\chi_{2J-2,J-m-1}. \end{aligned} \tag{7.17}$$

We now use (7.16) and (7.17) to re-express the last term in (7.15) as

$$\begin{aligned} & -\frac{1}{2}(U[-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]^{-1})[-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]\phi_{2J-1,J-m-1} \\ & \quad + \frac{1}{2}E\omega_{2J-2,J-m-1} + \frac{1}{2}E([-\square^* - (J-1)(J+1)]^{-1}(1 - P_{J-1})) \\ & \quad \times [-\square^* - (J-1)(J+1)]\chi_{2J-2,J-m-1} \end{aligned} \tag{7.18}$$

and the 2-norm of (7.18) is bounded above by

$$\begin{aligned} & \frac{1}{2}\|U[-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]^{-1}\|_{2,2} \|[-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})]\phi_{2J-1,J-m-1}\|_2 \\ & \quad + \frac{1}{2}\|E\|(2\pi^2)^{1/2}\|\omega_{2J-2,J-m-1}\|_\infty \\ & \quad + \frac{1}{2}\|E\| \|[-\square^* - (J-1)(J+1)]^{-1}(1 - P_{J-1})\|_{2,2} \\ & \quad \times \|[-\square^* - (J-1)(J+1)]\chi_{2J-2,J-m-1}\|_2. \end{aligned} \tag{7.19}$$

We can now use (3.17), (3.44), and (6.10) to estimate the operator norms in (7.19), thereby obtaining

$$\begin{aligned} & \frac{1}{2} D_{1/2} J^{-3/16} \|[-\square^* - (J - \frac{1}{2})(J + \frac{3}{2})] \phi_{2J-1, J-m-1}\|_2 + \frac{1}{2} |E| (2\pi^2)^{1/2} \|\omega_{2J-2, J-m-1}\|_\infty \\ & + \frac{1}{2} |E| (2J-1)^{-1} \|[-\square^* - (J-1)(J+1)] \chi_{2J-2, J-m-1}\|_2. \end{aligned} \quad (7.20)$$

By the induction hypothesis and (7.3) we can bound the vector norms in (7.20) to obtain the following upper bound to (7.20), assuming  $J \geq 1$ :

$$C'(A')^{2J} ((2J)!)^{-3/16} (D_{1/2}/A' + \frac{1}{2}|E|(2\pi^2)^{1/2}/A' + |E|/(A')^2). \quad (7.21)$$

Now that we have estimated the last term in (7.15), we observe that

$$\begin{aligned} & \|[-\square^* - (J(J+2))] \chi_{2J,k}\|_2 \\ & \leq \sum_{n=0}^{[(J-k-1)/2]} \sum_{m=0}^{J-k-2n-1} \binom{J-k-m-n-1}{n} \\ & \quad \times \left(\frac{1}{2}(J+1)\right) \|[-\square^* - J(J+2)]^{-1} (1-P_J)\|_{2,2}^{J-k-2n-m-1} \\ & \quad \times \left(\frac{1}{16}\right) \|[-\square^* - J(J+2)]^{-1} (1-P_J)\|_{2,2}^n \| (1-P_J)\|_{2,2} \\ & \quad \times C'(A')^{2J} ((2J)!)^{-3/16} (D_{1/2}/A' + \frac{1}{2}|E|(2\pi^2)^{1/2}/A' + |E|/(A')^2). \end{aligned} \quad (7.22)$$

Since  $\|(1-P_J)\|_{2,2} = 1$ , we can use Eq. (3.17) to control  $\|[-\square^* - J(J+2)]^{-1} (1-P_J)\|_{2,2}$  to obtain

$$\begin{aligned} & \|[-\square^* - J(J+2)] \chi_{2J,k}\|_2 \\ & \leq \sum_{n=0}^{[(J-k-1)/2]} \sum_{m=0}^{J-k-2n-1} \binom{J-k-m-n-1}{n} \left(\frac{J+1}{4J+2}\right)^{J-k-2n-m-1} \left(\frac{1}{32J+16}\right)^n \\ & \quad \times C'(A')^{2J} ((2J)!)^{-3/16} (D_{1/2}/A' + \frac{1}{2}|E|(2\pi^2)^{1/2}/A' + |E|/(A')^2). \end{aligned} \quad (7.23)$$

The double sum in this inequality is precisely the same as the double sum in (6.26), for which we found the upper bound of  $\frac{16}{7}$  in (6.28). Thus

$$\begin{aligned} & \|[-\square^* - J(J+2)] \chi_{2J,k}\|_2 \\ & \leq C'(A')^{2J} ((2J)!)^{-3/16} \frac{16}{7} (D_{1/2}/A' + \frac{1}{2}|E|(2\pi^2)^{1/2}/A' + |E|/(A')^2). \end{aligned} \quad (7.24)$$

Provided that  $A'$  is initially chosen sufficiently large so that (7.3) holds and both

$$\frac{20}{7} \left(\frac{1}{2}\right) \|U\|_2/A' + D_1/A' + |E|/(A')^2 \quad (7.25)$$

and

$$\frac{16}{7} \left(\frac{1}{2}\right) |E|(2\pi^2)^{1/2}/A' + D_{1/2}/A' + |E|/(A')^2 \quad (7.26)$$

are smaller than 1, we see from (7.14) and (7.24) that the induction can be verified for  $j = \mathcal{J}$ , so we conclude that for all  $j$  and  $k$

$$\left\| \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} \right\|_2 \leq C'(A')^j (j!)^{-3/16} \quad (7.27)$$

for some suitable positive constants  $C'$  and  $A'$ .

In order to derive a similar estimate for  $\|\phi_{j,k}\|_\infty$ , we observe first that

$$\|\phi_{j,k}\|_\infty \leq \|\omega_{j,k}\|_\infty + \|\chi_{j,k}\|_\infty \tag{7.28}$$

and that  $\|\omega_{j,k}\|_\infty$  obeys the estimate (7.3), and  $\omega_{j,k} \equiv 0$  if  $j$  is odd. Since

$$\chi_{j,k} = \left( \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right]^{-1} (1 - P_{j/2}) \right) \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} \tag{7.29}$$

it follows that

$$\begin{aligned} \|\chi_{j,k}\|_\infty &\leq \left\| \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right]^{-1} (1 - P_{j/2}) \right\|_{2,\infty} \left\| \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} \right\|_2 \\ &\leq (2\pi^2)^{-1/2} \frac{\pi}{2} \frac{3}{2} (2j+1)^{-1} \left\| \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} \right\|_2 \end{aligned} \tag{7.30}$$

from (3.24) and (3.25) and the fact that

$$\frac{1}{4} \left( \frac{\pi^2}{3} + \frac{1}{4} \right) \leq \frac{\pi}{2} \frac{3}{2} \tag{7.31}$$

From (7.30) and (7.27) we conclude that

$$\|\chi_{j,k}\|_\infty \leq C'(A')^j (j!)^{-3/16} \tag{7.32}$$

and using (7.32) in (7.28) implies that for all  $j$  and  $k$ ,

$$\|\phi_{j,k}\|_\infty \leq C'(A')^j (j!)^{-3/16} \tag{7.33}$$

Accordingly we conclude that for all complex values of  $s$  and  $t$ , the expansion

$$\sum_{n=0}^\infty \sum_{k=0}^\infty s^n t^k \psi_{n+2k,k}(\alpha, \theta) \tag{7.34}$$

converges to a function in  $L^\infty(S^3)$ .

The indeterminacy of  $\omega_{2l,0}$  can be treated in a manner similar to our discussion at the end of Sect. 6. If the sum

$$\sum_{l=0}^\infty s^{2l} \|\omega_{2l,0}\|_\infty \tag{7.35}$$

converges for all  $s$ , then the corresponding sum given in (6.43)

$$\sum_{l=0}^\infty \sum_{m=0}^\infty \sum_{k=0}^\infty s^{2l+m} t^k \psi_{2l+m+2k,k}^{(l)}(\alpha, \theta) \tag{7.36}$$

converges for all  $s$  and  $t$  to a function in  $L^\infty(S^3)$ .

Additionally, we note that since  $\|[-\square^* - (j/2)(j/2 + 2)]\phi_{j,k}\|_2$  falls off factorially fast in  $j$  and

$$\|[-\square^* + 1]\phi_{j,k}\|_2 \leq \left\| \left[ -\square^* - \frac{j}{2} \left( \frac{j}{2} + 2 \right) \right] \phi_{j,k} \right\|_2 + \left( \frac{j}{2} + 1 \right)^2 \|\phi_{j,k}\|_2 \tag{7.37}$$

and both terms on the right side of (7.37) have been shown to fall off factorially quickly in  $j$ ,  $\|[-\square^* + 1]\phi_{j,k}\|_2$  falls off factorially fast. Therefore it follows that the series

$$\sum_{n=0}^{\infty} \sum_{k=0}^{\infty} s^n t^k [(-\square^* + 1)\psi_{n+2k,k}](\alpha, \theta) \tag{7.38}$$

converges to a function in  $L^2(S^3)$ . From our discussion of uniform Hölder continuity in Sect. 2, it follows that for *fixed*  $s$  and  $t$  all the truncated sums in (7.34) and the limit function are uniformly Hölder continuous of order  $\frac{1}{2}$  with the *same* constant  $c$  given by

$$c = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} |s|^n |t|^k \|(-\square^* + 1)\psi_{n+2k,k}\|_2. \tag{7.39}$$

If a sequence of functions, all of which are uniformly Hölder continuous with the same constant  $c$ , converges on a dense set, then the sequence of functions converges pointwise. Since we proved in Sect. 6 that the series (7.34) converges in  $L^2(S^3)$  it converges pointwise except on a set of measure 0, and from our remarks on uniform Hölder continuity it follows that (7.34) converges for all points in  $S^3$ .

As before, we also have the convergence in  $L^2(S^3)$  of the summation

$$\sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \sum_{k=0}^{\infty} s^{2l+m} t^k (-\square^* + 1)\psi_{2l+m+2k}^{(l)}(\alpha, \theta) \tag{7.40}$$

provided that the series

$$\sum_{l=0}^{\infty} s^{2l} (-\square^* + 1)\omega_{2l,0} = \sum_{l=0}^{\infty} s^{2l} (l+1)^2 \omega_{2l,0} \tag{7.41}$$

converges in  $L^2(S^3)$ .

We shall now prove that the expansion (1.7) obeys Schrödinger's equation (1.3), considered as a partial differential equation with no boundary condition at  $\infty$ . To begin, we need to express the differential operator in (1.3) in terms of  $s$  and  $t$ . Since

$$\begin{aligned} \frac{\partial}{\partial R} &= \frac{\partial s}{\partial R} \frac{\partial}{\partial s} + \frac{\partial t}{\partial R} \frac{\partial}{\partial t} \\ &= \frac{1}{2} R^{-1/2} \frac{\partial}{\partial s} + (1 + \ln R) \frac{\partial}{\partial t} = \frac{1}{2} \frac{1}{s} \frac{\partial}{\partial s} + \left( 1 + \frac{t}{s^2} \right) \frac{\partial}{\partial t} \end{aligned} \tag{7.42}$$

we see that

$$\begin{aligned}
 R^2 \frac{\partial^2}{\partial R^2} + 3R \frac{\partial}{\partial R} &= R^{-1} \frac{\partial}{\partial R} \left( R^3 \frac{\partial}{\partial R} \right) \\
 &= \left( \frac{1}{2} s^{-3} \frac{\partial}{\partial s} + (s^{-2} + s^{-4} t) \frac{\partial}{\partial t} \right) \left( \frac{1}{2} s^5 \frac{\partial}{\partial s} + (s^6 + s^4 t) \frac{\partial}{\partial t} \right) \\
 &= \frac{1}{4} s^2 \frac{\partial^2}{\partial s^2} + \frac{5}{4} s \frac{\partial}{\partial s} + (s^2 + t)^2 \frac{\partial^2}{\partial t^2} + (4s^2 + 3t) \frac{\partial}{\partial t} + (s^3 + st) \frac{\partial}{\partial s \partial t}.
 \end{aligned} \tag{7.43}$$

(We parenthetically observe that since  $(\frac{1}{2}(s^3 + st))^2 - \frac{1}{4}s^2(s^2 + t)^2 = 0$ , this differential operator is *parabolic* when expressed as a function of  $s$  and  $t$ .) When the differential operator on the right side of (7.43) is applied to the expansion (1.11), one obtains another entire function of  $s$  and  $t$  from  $\mathbb{C} \times \mathbb{C}$  to  $L^2(S^3)$ . We just finished proving that the series (7.38) defines an entire function from  $\mathbb{C} \times \mathbb{C}$  to  $L^2(S^3)$ , so obviously the same conclusion holds if we replace  $(-\square^* + 1)$  in (7.38) with  $(-\square^*)$ . Furthermore, since the series (1.11) defines an entire function from  $\mathbb{C} \times \mathbb{C}$  to  $L^\infty(S^3)$  and  $U$  is in  $L^2(S^3)$ , the series

$$s \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} s^n t^k U(\alpha, \theta) \psi_{n+2k,k}(\alpha, \theta) \tag{7.44}$$

defines an entire function from  $\mathbb{C} \times \mathbb{C}$  to  $L^2(S^3)$ . Thus when  $\psi$  is defined to be the limit of the series (1.11), each term in (1.3) is an entire function from  $\mathbb{C} \times \mathbb{C}$  to  $L^2(S^3)$ . The fact that  $\psi(s, t; \alpha, \theta)$  is a solution of (1.3) follows from the observation that its expansion coefficients  $\psi_{n+2k,k}(\alpha, \theta)$  are determined from the recurrence relation (1.8) derived from the differential equation (1.3).

## 8. Conclusions and suggestions for further research

It has been shown that Fock's expansion for  $S$ -state solutions of Schrödinger's Equation for two-electron atoms and ions has virtually optimal convergence properties. The expansion converges not only in a small neighborhood of  $R = 0$ , but for all finite  $R$ . Better behaviour could not be expected.

Nonetheless, there are important problems which remain to be solved. We have demonstrated that for every complex  $E$ , Schrödinger's equation (1.3), considered as a partial differential equation with no boundary condition at  $R = \infty$ , has infinitely many solutions, each of which has a convergent Fock expansion. If  $E$  is not in the point spectrum of the Hamiltonian, Schrödinger's equation  $(H - E)\psi = 0$ , considered as an operator equation in the Hilbert space  $L^2(\mathbb{R}^6)$ , does not have a square-integrable solution. Thus for  $E$  outside the point spectrum of the Hamiltonian, the functions defined by Fock's expansion cannot represent functions in  $L^2(\mathbb{R}^6)$ . If  $E$  is not even in the continuous spectrum of the Hamiltonian, presumably the functions obtained from Fock's expansion have exponential growth as  $R \rightarrow \infty$ . If  $E$  is in the continuous spectrum of the Hamiltonian, it is conceivable that at least some of the functions defined by Fock's expansion

correspond to improper (continuum) eigenfunctions, which are not in  $L^2(\mathbb{R}^6)$ . It remains to be proved that if  $E$  is in the discrete spectrum of the Hamiltonian and corresponds to an  $S$ -state, at least one of the functions defined by Fock's expansion actually converges to an appropriate  $L^2(\mathbb{R}^6)$  eigenfunction of energy  $E$ . This probably is a very hard problem the resolution of which might well require the development of a theory of partial differential equations with regular singular points, in analogy to the well-known theory of ordinary differential equations with regular singular points. One would like to know whether *any* solution of the partial differential equation (1.3) which is finite at  $R=0$  has a convergent expansion of the form (1.7).

An important step toward an understanding of the cusp behaviour of locally well-behaved solutions of partial differential equations, the coefficients of which are not analytic in Cartesian coordinates, has been accomplished by my colleague Prof. Robert N. Hill [24]. He has proved that if  $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N)$  is a locally well-behaved solution of the Schrödinger equation for an atom or a molecule, then in the vicinity of any two particle collision where one particular  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| = 0$  and all other interparticle distances are bounded away from zero, the wavefunction  $\Psi$  can be decomposed as

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \Psi_a(\mathbf{r}_1, \dots, \mathbf{r}_N) + r_{ij}\Psi_c(\mathbf{r}_1, \dots, \mathbf{r}_N)$$

where both  $\Psi_a$  and  $\Psi_c$  are analytic functions of the Cartesian variables. Hill's result provides a natural extension of the famous Kato cusp conditions [8] to higher order derivatives.

Furthermore, Prof. J. Leray has recently announced some results on the local behavior of solutions of Schrödinger's equation for atomic systems in the vicinity of the point where all electrons are collapsing upon the nucleus [25]; however, the technical details such as estimates of norms of operators have not yet all been published. It is quite possible that his techniques, whose full publication we await with anticipation, will provide the key to determining whether all locally well-behaved solutions of Schrödinger's equation for Coulomb systems have convergent expansions of the type proposed by Fock.

Even when the question of the representability of  $S$ -state eigenfunctions of two electron atoms by Fock's expansion has been solved, we will be left with another unresolved problem, the indeterminacy of the  $\omega_{2l,0}$ 's. As we have already remarked, this indeterminacy is a reflection of the fact that in 2 or more dimensions, there are infinitely many linearly independent harmonic polynomials. The situation in many dimensions is quite different from that in 1 dimension, where there are only two linearly independent harmonic polynomials, which are of the form  $(ax+b)$ . It has been noted by Demkov and Ermolaev [6] that the indeterminacy of the  $\omega_{2l,0}$ 's can be resolved in principle by applying the  $L^2(\mathbb{R}^6)$  condition; in other words, by studying the asymptotic behaviour as  $R \rightarrow \infty$  of the expansion

$$\psi(E; R, \alpha, \theta) = \sum_{l=0}^{\infty} \psi^{(l)}(E; R, \alpha, \theta).$$

In practice, of course, this is likely to be very difficult. Here we shall only observe that if  $E$  corresponds to a *non-degenerate* point eigenvalue, then at most one of the functions  $\psi^{(l)}(E; R, \alpha, \theta)$  can be in  $L^2(\mathbb{R}^6)$ , for if two or more were in  $L^2(\mathbb{R}^6)$ , the eigenvalue  $E$  would be degenerate. For the ground state wavefunction  $\psi$  we know by the recent work of the Hoffmann–Ostenhof's and Barry Simon that  $\psi(R=0) \neq 0$  [1]. Thus we know that the  $l=0$  term is non-vanishing for the ground state. If it also is in  $L^2(\mathbb{R}^6)$ , then all the other terms with  $l \neq 0$  must automatically vanish. Thus a study of the asymptotic behavior of  $\psi^{(0)}(E; R, \alpha, \theta)$  might be sufficient to settle the indeterminacy question, at least for the ground state.

The author hopes that this discussion will encourage others to think about these challenging problems.

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## Appendix

Evaluation of  $\int_0^\pi d\alpha \sin^2 \alpha \left( \frac{\sin(n\alpha)}{\sin \alpha} \right)^8$

In this appendix we shall evaluate the integral

$$\int_{S^3} d\omega' \int_{S^3} d\omega \frac{\sin^8(n\Theta(\omega, \omega'))}{\sin^8(\Theta(\omega, \omega'))} \quad (\text{A.1})$$

which occurs in (3.13), (3.34), and (3.41), where  $n$  is a positive integer. To begin, we observe that by rotational symmetry the result of the integration over  $\omega$  is independent of the value of  $\omega'$ , so we use this fact and the relation

$$d\omega = \sin^2 \alpha \, d\alpha \, \sin \theta \, d\theta \, d\phi \quad (\text{A.2})$$

to see that (A.1) equals

$$\begin{aligned} (2\pi^2) \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \int_0^\pi d\alpha \sin^2 \alpha \frac{\sin^8(n\alpha)}{\sin^8 \alpha} \\ = (2\pi^2) 4\pi \int_0^\pi d\alpha \frac{\sin^8(n\alpha)}{\sin^6 \alpha} = (2\pi^2) 2\pi \int_0^{2\pi} d\alpha \frac{\sin^8(n\alpha)}{\sin^6 \alpha}. \end{aligned} \quad (\text{A.3})$$

Originally this integral was evaluated using [26], Eqs. 1.320.1 and 3.616.7, followed by a Taylor series expansion up to sixth order. I am grateful to William H. Miller for suggesting that I use complex integration instead. If we let



$z = e^{i\alpha}$ , then  $dz = i e^{i\alpha} d\alpha = iz d\alpha$ , so  $d\alpha = i^{-1} z^{-1} dz$ , and

$$\sin \alpha = \frac{1}{2i}(e^{i\alpha} - e^{-i\alpha}) = \frac{1}{2i}(z - z^{-1}) \quad (\text{A.4})$$

and

$$\sin(n\alpha) = \frac{1}{2i}(e^{in\alpha} - e^{-in\alpha}) = \frac{1}{2i}(z^n - z^{-n}) \quad (\text{A.5})$$

so the last integral in (A.3) becomes

$$-\frac{1}{4i} \oint \frac{dz}{z} (z^{-1} - z)^{-6} (z^n - z^{-n})^8 \quad (\text{A.6})$$

where the contour of integration is a circle of radius 1 centered at the origin. Since

$$\frac{z^{-n} - z^n}{z^{-1} - z} = z^{-n+1} \sum_{j=0}^{n-1} z^{2j} \quad (\text{A.7})$$

is analytic in  $z$  away from the origin, we see that the only singularity of the integrand in (A.6) is at the origin. Therefore we can contract the contour of integration down to a circle of radius  $\frac{1}{2}$  centered at the origin. We now use the facts that

$$(z^{-1} - z)^{-6} = z^6 (1 - z^2)^{-6} = z^6 \sum_{j=0}^{\infty} \binom{5+j}{5} z^{2j} \quad (\text{A.8})$$

and

$$(z^{-n} - z^n)^8 = \sum_{k=0}^{\infty} (-1)^k \binom{8}{k} z^{(2kn-8n)} \quad (\text{A.9})$$

to see that the integral (A.6) equals

$$-\frac{\pi}{2} \sum_{k=0}^8 (-1)^k \binom{8}{k} \sum_{j=0}^{\infty} \binom{5+j}{5} \frac{1}{2\pi i} \oint \frac{dz}{z} z^{(6+2kn-8n+2j)} \quad (\text{A.10})$$

For fixed  $k$ , this integral will vanish unless  $(6+2kn-8n+2j)=0$ ; i.e.,  $j = (-3+n(4-k))$ . Since  $j$  is nonnegative, we see immediately that all the terms with  $4 \leq k \leq 8$  automatically vanish. Thus (A.10) equals

$$\begin{aligned} & -\frac{\pi}{2} \sum_{k=0}^3 (-1)^k \binom{8}{k} \binom{2+n(4-k)}{5} \\ & = -\frac{\pi}{2} \frac{1}{5!} \sum_{k=0}^3 (-1)^k \binom{8}{k} ((4-k)n+2)((4-k)n+1)((4-k)n)((4-k)n-1) \\ & \quad ((4-k)n-2). \end{aligned} \quad (\text{A.11})$$

Temporarily ignoring the common factor of  $(-\pi/(2 \cdot 5!))$ , we see that the  $k=0$  term is

$$\begin{aligned} (4n+2)(4n+1)(4n)(4n-1)(4n-2) &= 16n(2n+1)(2n-1)(4n+1)(4n-1) \\ &= 16n(4n^2-1)(16n^2-1) = 16n(64n^4-20n^2+1). \end{aligned} \quad (\text{A.12})$$

The  $k = 1$  term is

$$\begin{aligned} & -8(3n+2)(3n+1)(3n)(3n-1)(3n-2) \\ & = -24n(3n+2)(3n-2)(3n+1)(3n-1) \\ & = -24n(9n^2-4)(9n^2-1) = -24n(81n^4-45n^2+4). \end{aligned} \quad (\text{A.13})$$

The  $k = 2$  term is

$$\begin{aligned} & 28(2n+2)(2n+1)(2n)(2n-1)(2n-2) = 8 \cdot 28n(n+1)(n-1)(2n+1)(2n-1) \\ & = 8 \cdot 28n(n^2-1)(4n^2-1) = 8 \cdot 28n(4n^4-5n^2+1). \end{aligned} \quad (\text{A.14})$$

Finally, the  $k = 3$  term is

$$\begin{aligned} & -56(n+2)(n+1)(n)(n-1)(n-2) = -56n(n+2)(n-2)(n+1)(n-1) \\ & = -56n(n^2-4)(n^2-1) = -56n(n^4-5n^2+4). \end{aligned} \quad (\text{A.15})$$

If we take out a common factor of  $8n$ , the sum of these four terms is

$$\begin{aligned} & 8n\{(128n^4-40n^2+2) - (243n^4-135n^2+12) + (112n^4-140n^2+28) \\ & \quad - (7n^4-35n^2+28)\} \\ & = 8n\{n^4(128-243+112-7) + n^2(-40+135-140+35) + (2-12+28-28)\} \\ & = 8n\{n^4(-10) + n^2(-10) + (-10)\} = -80(n^5+n^3+n). \end{aligned} \quad (\text{A.16})$$

Putting back in the factor of  $(-\pi/(2 \cdot 5!))$  yields

$$\frac{\pi}{2} \frac{80}{120} (n^5+n^3+n) = \pi \frac{n^5+n^3+n}{3}, \quad (\text{A.17})$$

so the final answer for (A.3) is

$$(2\pi^2)^2 \frac{n^5+n^3+n}{3}, \quad (\text{A.18})$$

the desired result.

Finally, we should remark that it is easy to obtain an upper bound to integral in (A.3). Since  $|\sin(n\alpha)/\sin\alpha| \leq n$ ,

$$\int_0^{2\pi} d\alpha \frac{\sin^8(n\alpha)}{\sin^6\alpha} = \int_0^{2\pi} d\alpha \sin^2(n\alpha) \frac{\sin^6(n\alpha)}{\sin^6\alpha} \leq n^6 \int_0^{2\pi} d\alpha \sin^2(n\alpha) = \pi n^6 \quad (\text{A.19})$$

The main effect of using this estimate instead of Eq. (A.3) would be the replacement of the exponent  $-\frac{3}{16}$ , which occurs throughout the text of our article, with  $-\frac{2}{16} = -\frac{1}{8}$ . We certainly could still prove the convergence of Fock's expansion.

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