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Coordinate space modification of Fock's theory. Harmonic tensors in the quantum Coulomb problem

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Contents

Abstract. We consider Fock's fundamental theory of the hydrogen atom in momentum space, which allows a realization of the previously predicted rotation group of a three-dimensional (3D) sphere in four-dimensional (4D) space. We then modify Fock's theory and abandon the momentum-space description. To transform and simplify the theory, we use invariant tensor methods of electrostatics in 3D and 4D spaces. We find a coordinate 4D space where the Schrödinger equation becomes the 4D Laplace equation. The transition from harmonic 4D polynomials to the original 3D physical space is algebraic and involves derivatives with respect to a coordinate that is interpreted as time. We obtain a differential equation for eigenfunctions in the momentum space and find its solutions. A concise calculation of the quadratic Stark effect is given. The Schwinger resolvent is derived by the method of harmonic polynomials. Ladder operators are also considered.

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1. Introduction

1.1 Essence of the problem

The quantum Coulomb problem, which allows calculating the spectrum of a system of two opposite charges, is still fundamental in quantum theory [1–4]. The names of the founders of twentieth century physics are associated with it: Bohr, Sommerfeld, Pauli, Schrödinger, and Fock. The introduction to the theory of atomic spectra begins with it, and it has been thoroughly studied using methods of the theory of special functions. Due to its simplicity and the underlying symmetry — the group SO(4) of rotations in a four-dimensional (4D) space — it is an extremely useful and fine tool of theoretical physics for constructing various concepts [5–7].

Despite the apparent exhaustive treatment of the quantum Coulomb problem, there are still some questions that have not been fully clarified. In particular, the complexity of calculating the quadratic Stark effect is difficult to understand, even though the perturbation used is unmatched in its simplicity in physics [1, 2]. Fock's result is also surprising: why is the SO(4) symmetry realized in the momentum space wrapped into a three-dimensional (3D) sphere, with an excursion to the 4D space?

Let us recall the background preceding Fock's accomplishment. Two classical vector integrals, the angular momentum and the Runge–Lenz vector, in quantum mechanics correspond to vector operators that commute with the energy operator, i.e., with the Hamiltonian. An analysis of their commutators [1] carried out in [8] shows that they generate a Lie algebra (a linear space with a commutation operation) coinciding with the Lie algebra of operators of small (infinitesimal) rotations in 4D space [1, 3].

For physicists, this correspondence means that some transformation of variables and operators maps the original quantum Coulomb problem into the problem of free motion of a particle over a 3D sphere embedded in a 4D space. The energy operator is then invariant under rotations of the 3D sphere. This is reminiscent of the remarkable effect of Lewis Carroll's soaring grin of the Cheshire Cat.

Fock's approach struck contemporaries [3, 9–11]. The starting point in his theory is the integral Schrödinger equation (SE) in momentum space. This space can be considered a 3D plane in a 4D space. Fock then wraps the 3D plane into a sphere using stereographic projection, known since antiquity [12] as a convenient transformation of a globe into a flat map [13]. (Fock's globe is three-dimensional, as is the map.) At the same time, Fock surmises the factor for psi functions such that the original integral equation turns into an equation for spherical functions on the 3D sphere (to be distinguished from functions on a two-dimensional sphere). This equation, rarely used in physics but known in the theory of special functions, is invariant under rotations in 4D space. Fock does not explain the physical meaning of the transformation he found [9–11]. As a result, the fundamental questions remain: why is the SO(4) symmetry realized in the wrapped momentum space rather than in the coordinate space, and how has the electron "learned about the stereographic projection?"

In this paper, Fock's approach is modified by the inverse 4D Fourier transformation, which is applicable to eigenfunctions continued harmonically to the 4D momentum space. [2] This is a transition to a new 4D coordinate space, because Fock transforms the SE into a 4D momentum space. In the 4D coordinate space, the modified SE is the 4D Laplace equation, and the eigenfunctions are harmonic 4D tensors, i.e., homogeneous polynomials. Their projections (contractions with numerical tensors) are solid spherical 4D functions.

The final transition to solutions of the original SE, unlike the transition to solutions of the original SE in Fock's theory, turns out to be simple algebra with the help of differentiation. The SO(4) symmetry is thus realized in a coordinate space that, in a certain sense, is 'closer here' than the space found by Fock. Although the structure of the functions is preserved, the inverse transformation is remarkably simple, which is of importance for theoretical concepts.

In this paper, spherical functions are replaced by polynomials that have been well known in electrostatics since the time of Maxwell and are associated with multipole moments [14–24]. In particular, instead of solid spherical functions $r^l Y_{l,m}(\theta, \varphi)$, tensor polynomials x_i and $3x_i x_k - r^2\delta_{ik}$ generating the dipole and quadrupole moments are used for $l = 1, 2$, an octupole polynomial is used for $l = 3$, and so on. Spherical functions are convenient in scattering problems. Polynomials are preferable in calculations with differential operators and are therefore introduced from the very beginning. The spherical coordinates θ, φ and θ, φ, ϕ are not involved here.

In physics, dipole and quadrupole moments typically appear because the fundamental concepts of physics are associated precisely with them. But the use of invariant polynomial tensors in Cartesian coordinates, as shown in a number of recent studies, is preferable and simplifies the fundamental scheme of calculations [25–31]. In Section 3, the rules for using harmonic symmetric tensors are demonstrated that directly follow from their properties. These rules are naturally reflected in the theory of special functions, but are not always obvious, even though the group properties are general [32]. At any rate, we recall the main property of harmonic tensors: the trace over any pair of indices vanishes [23, 33].

We here select those properties of tensors that not only make analytic calculations more compact and reduce 'the number of factorials' but also allow correctly formulating some fundamental questions of the theory. The advantage of using such tensors in the perturbation theory is demonstrated in Sections 4 and 9 in calculating the quadratic Stark effect and in deriving the Schwinger resolvent. In Section 7, we present the derivation of the integral equation obtained by Fock with reference to the theory of special functions, using methods of electrostatics in 3D and 4D spaces. In Section 8, we derive the ladder operators in the Coulomb problem and show their relation to inversion with respect to a sphere.

To modify the Fock theory, it is convenient to use harmonic tensors in moving to the 4D coordinate space because, as shown below, their form remains invariant under a rather complex transformation. Of course, the SO(4) symmetry is inherent in invariant 4D tensors. The final algebraic transition to the physical space singles out one coordinate, which can be called complex time. This coordinate is then multiplied by the imaginary unit i and equated to the length of the radius vector $|\mathbf{r}|$, thus being 'absorbed' by the formula. The SO(4) symmetry is thus concealed in the original solution of the SE.

Strictly speaking, the transformation found in this paper is not identical to Fock's theory. There are three fundamental variations here that simplify the transformations used. The first is the extension from the Fock sphere into 4D space, when harmonic tensors are formed. The second is the use of spatial inversion instead of the stereographic projection of the sphere. The third variation amounts to discarding delta functions in the final transformation. The SO(4) symmetry is preserved each time, which leads to the desired result: the SE eigenfunctions are algebraically related to harmonic 4D tensors. We note that the state correspondence found in this paper is generated by the physical symmetry of the problem and is not known in the theory of Laguerre and Gegenbauer polynomials [32].

[1] The Runge–Lenz operator is first multiplied by n [3].

[2] Applying the inverse (3D) Fourier transformation would mean a return to the original SE in the coordinate space.

1.2 Harmonic polynomials instead of spherical functions

The Schrödinger equation for eigenfunctions, using atomic units (the unit of energy being $Z^2me^4/\hbar^2$ and the unit of length being Bohr's radius $a_B = \hbar^2/(Zme^2)$), has the form

$$\left(-\frac{1}{2}\Delta - \frac{1}{r}\right)\Psi_{nl} = -\frac{1}{2n^2}\Psi_{nl}\,. \tag{1}$$

In what follows, it is convenient to reduce the orbits of all radii na_B to a single radius [1], i.e., change the radius vector for each eigenfunction as $\mathbf{r}' = \mathbf{r}/n$. Equation (1) then takes a deceptively simple form,

$$(-\Delta + 1)\Psi_{nl} = \frac{2n}{r}\Psi_{nl}\,, \tag{2}$$

where r is the modulus of the vector $\mathbf{x}$. The eigenfunctions in the momentum representation then have a scaled argument $\mathbf{p}' = n\mathbf{p}$.

In this paper, the angular factor is not taken in the form of spherical functions but as a combination of solid spherical functions, i.e., a harmonic degree-l polynomial $P_l(\mathbf{x})$ homogeneous in coordinates with the properties

$$\Delta P_l(\mathbf{x}) = 0\,, \quad P_l(c\mathbf{x}) = c^l P_l(\mathbf{x})\,, \quad (\mathbf{x}\nabla)P_l(\mathbf{x}) = lP_l(\mathbf{x})\,. \tag{3}$$

The last equality is Euler's theorem, which is valid for all homogeneous functions (not only polynomials but also, for example, the factor $1/r$ and its powers). The operator that arises here has an interpretation that allows calling it the *angular momentum modulus operator*:

$$\hat{l} = \mathbf{x}\nabla\,. \tag{4}$$

Solutions of Eqn (2) and similar equations can be represented as $P_l(\mathbf{x})F(r)$. When substituted into Eqn (2) and other equations containing the Laplace operator, properties (3) give rise to the equation for the radial function, because the factor $P_l(\mathbf{x})$ persists and can be canceled:

$$\Delta\left[P_l(\mathbf{x})F(r)\right] = \left[\Delta P_l(\mathbf{x})\right]F(r) + 2\left[\nabla P_l(\mathbf{x})\right]\left[\nabla F(r)\right]$$
$$+ P_l(\mathbf{x})\Delta F(r) = 2lP_l(\mathbf{x})\frac{1}{r}\frac{\partial F(r)}{\partial r} + P_l(\mathbf{x})\frac{1}{r}\frac{\partial^2}{\partial r^2}\left[rF(r)\right]\,. \tag{5}$$

This transformation, after the substitution in Eqn (2), immediately leads to the Gauss function [3]

$$F(\alpha,\beta,r) = 1 + \frac{\alpha}{\beta}\frac{r}{1!} + \frac{\alpha(\alpha+1)}{\beta(\beta+1)}\frac{r^2}{2!} + \frac{\alpha(\alpha+1)(\alpha+2)}{\beta(\beta+1)(\beta+2)}\frac{r^3}{3!}\ldots\,. \tag{6}$$

For a discrete spectrum, parameter α is a negative integer, which converts the series into a polynomial, and the eigenfunction (taking a rescaling of the argument $\mathbf{x}$ into account) in the Coulomb problem is taken in the form [1]

$$P_l(\mathbf{x})F(-k, 2l+2, 2r)\exp(-r)\,, \quad n = l + k + 1\,. \tag{7}$$

The number k is the degree of the second factor in Eqn (7), and hence the degree of the entire polynomial is $n-1$. The normalization here and below is unimportant, unless especially stipulated.

[3] The degenerate hypergeometric function $_1F_1(r)$.

If there is no preferred direction and the spectrum is independent of the quantum number m, then the entire set of eigenfunctions with different values of m can be considered simultaneously. For the transformations considered below, it is convenient to use rank-l tensors invariant under the rotation group SO(3) that were developed in electrostatics. In particular, for the quadrupole state, the solution has the form

$$(3x_ix_k - r^2\delta_{ik})F(-k, 6, 2r)\exp(-r)\,, \quad n = 3 + k\,. \tag{8a}$$

For the octupole state, the solution is

$$3(5x_ix_kx_l - x_i\delta_{kl} - x_l\delta_{ik} - x_k\delta_{li})F(-k, 8, 2r)\exp(-r)\,,$$
$$n = 4 + k\,. \tag{8b}$$

For the dipole state, the solution is obvious: $x_iF(-k, 4, 2r)\exp(-r)$. The general form of an invariant harmonic tensor and its properties that are useful in the quantum Coulomb problem are considered in Section 3.

2. Fock's theory

When moving to the momentum representation, Schrödinger equation (2) (with $\hbar = 1$),

$$\Psi_{nl}(\mathbf{x}) = \frac{1}{(2\pi)^3}\int a_{nl}(\mathbf{p})\exp(i\mathbf{p}\mathbf{x})\,d^3\mathbf{p}\,, \tag{9}$$

contains a convolution with respect to momenta. Because the potential $1/r$ goes to $4\pi/\mathbf{p}^2$, the SE in the momentum space is nonlocal:

$$(\mathbf{p}^2 + 1)a_{nl}(\mathbf{p}) - \frac{2n}{2\pi^2}\int\frac{a_{nl}(\mathbf{p}')\,d^3\mathbf{p}'}{|\mathbf{p}-\mathbf{p}'|^2} = 0\,. \tag{10}$$

The first step of the theory is to multiply the function $a_{nl}(\mathbf{p})$ (done without an explanation) by $(1+\mathbf{p}^2)^2$. The second step is to wrap the 3D plane into a 3D sphere (with four coordinates (ξ, ξ_0); see Fig. 1).[4]

Figure 1 shows that the tangent of the slope of the projecting (red) straight line is

$$\tan\varphi = \frac{1}{|\mathbf{p}|}\,.$$

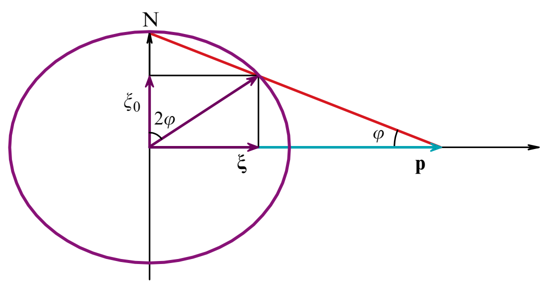

Figure 1. (Color online.) Stereographic projection of a 3d plane $\mathbf{p}$ onto a unit radius 3d sphere.

[4] In [3], the sign of ξ_0 is reversed.

Hence follow the formulas

$$|\xi| = \sin(2\varphi) = \frac{2|\mathbf{p}|}{1+\mathbf{p}^2}\,, \quad \xi = \frac{2\mathbf{p}}{1+\mathbf{p}^2}\,,$$
$$\xi_0 = \cos(2\varphi) = \frac{\mathbf{p}^2-1}{\mathbf{p}^2+1}\,, \quad \xi^2+\xi_0^2 = 1\,. \tag{11}$$

The stereographic projection doubles the tilt angle φ, and this is the effect it produces. The flat drawing correctly reflects the 4D transformation.

In the new variables, with Fock's factor taken into account, the eigenfunction becomes

$$b_{nl}(\xi,\xi_0) = (\mathbf{p}^2+1)^2 a_{nl}(\mathbf{p})\,. \tag{12}$$

It is essential that the projection be given by a conformal transformation. The angles between intersecting curves are preserved. The metric on the sphere in the momentum-space coordinates (of the $\mathbf{p}$ plane) is expressed as

$$\frac{4}{(\mathbf{p}^2+1)^2}\,\mathrm{d}\mathbf{p}^2\,. \tag{13}$$

Hence, the contraction coefficient for elements of the $\mathbf{p}$ space is $(1+\mathbf{p}^2)/2$. The volume element in formula (10) is expressed in terms of the 3D surface element:

$$\mathrm{d}^3\mathbf{p} = \frac{1}{8}(1+\mathbf{p}^2)^3\,\mathrm{d}S_3\,. \tag{14}$$

The kernel of the integral can be (very fortunately but not obviously) transformed as

$$\frac{1}{|\mathbf{p}-\mathbf{p}'|^2} = \frac{2}{\mathbf{p}^2+1}\,\frac{1}{(\xi-\xi')^2+(\xi_0-\xi_0')^2}\,\frac{2}{\mathbf{p}'^2+1}\,, \tag{15}$$

which does not follow from the conformal property. In particular, equality (15) is greatly simplified for two opposite points on the sphere: $|\mathbf{p}|=|\mathbf{p}'|=1,\ \xi_0=\xi_0'=0,\ \mathbf{p}=-\mathbf{p}'$, $\xi=-\xi'$.

Now, substituting relations (12), (14), and (15) into integral equation (10), we obtain

$$b_{nl}(\xi,\xi_0) - \frac{n}{2\pi^2}\int\frac{b_{nl}(\xi',\xi_0')\,\mathrm{d}S_{\xi'}}{(\xi-\xi')^2+(\xi_0-\xi_0')^2} = 0\,, \tag{16}$$

where, as can be seen from the figure, the surface element on the unit 4D sphere with the volume $2\pi^2$ is

$$\mathrm{d}S_{\xi'} = \frac{\mathrm{d}\xi_1'\,\mathrm{d}\xi_2'\,\mathrm{d}\xi_3'}{\xi_0'} = \frac{\mathrm{d}V_{\xi'}}{\xi_0'}\,. \tag{17}$$

(Integration over the flat space $\xi_0'=0$ is convenient for calculations.)

Next, Fock refers to the theory of spherical functions in 4D space. However, any spherical function and a sum of such functions with a fixed index $n-1$ that corresponds to the value of n in the original SE can be substituted into Eqn (16),[5] and hence the equation does not fix the quantum numbers l and m. The property of being conformal is important here. A rotation on the sphere corresponds to a rotation through the same angle in the momentum and coordinate spaces, and therefore a function with the factor $Y_{lm}(\theta,\varphi)$ goes into an eigenfunction with the same factor. If the factor is an invariant tensor, the same tensor is contained in the original function.

Equation (16), as we show below, naturally arises in 3D and 4D electrostatics. This analogy is discussed in Section 7.

3. Harmonic and multipole tensors

3.1 Multipole tensors in 3D electrostatics

We recall that multipole potentials arise when the potential of a point charge is expanded in powers of coordinates x_{0i} of the radius vector $\mathbf{r}_0$ ('Maxwell's poles') [17, 18]. For the $1/|\mathbf{r}-\mathbf{r}_0|$ potential, we have

$$\frac{1}{|\mathbf{r}-\mathbf{r}_0|} = \sum_l(-1)^l\frac{(\mathbf{r}_0\nabla)^l}{l!}\,\frac{1}{r}$$
$$= \sum_l\frac{x_{0i}\ldots x_{0k}}{l!\,r^{2l+1}}\,\mathbf{M}^{(l)}_{i\ldots k}(\mathbf{r}) = \sum_l\frac{\mathbf{r}_0^{\otimes l}\,\mathbf{M}^{(l)}_{[\mathrm{i}]}}{l!\,r^{2l+1}}\,, \tag{18}$$

where the following notation is used. For the lth tensor power of the radius vector, we write

$$x_{0i}\ldots x_{0k} = \mathbf{r}_0^{\otimes l}\,,$$

and for a symmetric harmonic tensor of rank l,

$$\mathbf{M}^{(l)}_{i\ldots k}(\mathbf{r}) = \mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{r})\,. \tag{19}$$

Tensor (19) is a homogeneous harmonic polynomial (with properties (3)). Contraction over any two indices (when the two gradients become the Δ operator) is zero. If tensor (19) is divided by r^{2l+1}, then a multipole harmonic tensor arises,

$$\frac{\mathbf{M}^{(l)}_{i\ldots k}(\mathbf{r})}{r^{2l+1}} = \frac{\mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{r})}{r^{2l+1}}\,, \tag{20}$$

which is also a homogeneous harmonic function with homogeneity degree $-(l+1)$.

The theory typically involves the dipole, quadrupole, and octupole tensors entering relations (8). The higher-rank ones are used less frequently due to their presumed complexity. However, if we recall the obvious property of contraction

$$(2l-1)!!\big(\mathbf{r}_0^{\otimes l},\mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{r})\big) = \big(\mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{r}_0),\mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{r})\big)\,, \tag{21}$$

then, in calculating the potential amplitudes, we do not have to use spherical functions or tensors (19): it suffices to calculate simple power-law moments. This rule is so important in calculations with tensors that it can be formulated as a theorem.

3.2 Theorem on power-law equivalent moments in electrostatics

Let $\rho(\mathbf{x})$ be a distribution of charge. When calculating a multipole potential, power-law moments can be used instead of spherical functions (or instead of harmonic tensors (19)):

$$\int\frac{\rho(\mathbf{r}_0)}{|\mathbf{r}-\mathbf{r}_0|}\,\mathrm{d}V_{\mathbf{r}_0} = \sum_l\int\rho(\mathbf{r}_0)\mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{r}_0)\,\mathrm{d}V_{\mathbf{r}_0}\,\frac{\mathbf{M}^{(l)}_{[\mathrm{i}]}}{(2l-1)!!\,l!\,r^{2l+1}}$$
$$= \sum_l\int\rho(\mathbf{r}_0)\mathbf{r}_0^{\otimes l}\,\mathrm{d}V_{\mathbf{r}_0}\,\frac{\mathbf{M}^{(l)}_{[\mathrm{i}]}}{l!\,r^{2l+1}}\,. \tag{22}$$

[5] In [3], the value of n is given.

Example 1.
For the octupole moment, instead of the integral in the third term in the first sum in (22),

$$\int \rho(\mathbf{r}) 3(5x_i x_k x_l - x_i \delta_{kl} - x_k \delta_{li} - x_l \delta_{ki})\, \mathrm{d}V_{\mathbf{r}}\,,$$

we can take the 'short' integral in the second sum,

$$15 \int \rho(\mathbf{r}_0) x_{0i} x_{0k} x_{0l}\, \mathrm{d}V_{\mathbf{r}_0}\,,$$

and substitute it into the second sum in (22). The moments are different, but the potentials are the same.

3.3 Formula for a harmonic tensor

The formula for the tensor was considered in [26, 27] using a ladder operator. Here, it is derived using the Laplace operator. The first term in the formula, as is easy to see from (18), is equal to

$$\mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{r}) = (2l-1)!!\, x_{i_1} \ldots x_{i_l} + \ldots = (2l-1)!!\, \mathbf{r}^{\otimes l} + \ldots\,. \tag{23}$$

The remaining terms are obtained by repeatedly applying the Laplace operator and multiplying by an even power of the modulus $|\mathbf{r}|^{2k}$. The coefficients are easy to determine by substituting (23) in the Laplace equation (see Appendix A). As a result, we have

$$\mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{r}) = (2l-1)!!\, \mathbf{r}^{\otimes l} - \frac{(2l-3)!!}{1!2^1}\, r^2 \Delta \mathbf{r}^{\otimes l} + \frac{(2l-5)!!}{2!2^2}\, r^4 \Delta^2 \mathbf{r}^{\otimes l} - \frac{(2l-3)!!}{3!2^3}\, r^6 \Delta^3 \mathbf{r}^{\otimes l} + \ldots\,. \tag{24}$$

This form is useful for applying the differential operators of quantum mechanics and electrostatics to it. The differentiation in (24) generates products of the Kronecker symbols.

Example 2.

$$\Delta x_i x_k = 2\delta_{ik}\,, \quad \Delta x_i x_k x_l = 2(\delta_{ik} x_l + \delta_{kl} x_i + \delta_{li} x_k)\,,$$
$$\Delta\Delta x_i x_k x_l x_m = 8(\delta_{ik}\delta_{lm} + \delta_{il}\delta_{km} + \delta_{im}\delta_{kl})\,. \tag{25}$$

The last equality can be verified using the contraction with $i = k$. It is convenient to write the differentiation formula in terms of the symmetrization operation. A symbol for it was proposed in [27], with the sum taken over all independent permutations of indices: [6]

$$\frac{\Delta^k \mathbf{r}^{\otimes l}}{k!2^k} = \langle\langle \delta^{\otimes k}_{[..]} \mathbf{r}^{\otimes(l-2k)} \rangle\rangle\,. \tag{26}$$

As a result, we obtain the formula

$$\mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{r}) = (2l-1)!!\, \mathbf{r}^{\otimes l} - (2l-3)!!\, r^2 \langle\langle \delta^{\otimes 1}_{[..]} \mathbf{r}^{\otimes(l-2)} \rangle\rangle + (2l-5)!!\, r^4 \langle\langle \delta^{\otimes 2}_{[..]} \mathbf{r}^{\otimes(l-4)} \rangle\rangle \ldots\,, \tag{27}$$

where the symbol $\otimes k$ is used for a tensor power of the Kronecker symbol δ_{im}, and the conventional symbol [..] is used for the two subscripts that change under symmetrization.

We follow [26] in finding the relation between the tensor and solid spherical functions. We use two unit vectors: vector $\mathbf{n}_z$ directed along the z-axis and complex vector $\mathbf{n}_x \pm \mathrm{i}\mathbf{n}_y = \mathbf{n}_\pm$. Contraction with their powers gives the required relation

$$\left(\mathbf{M}^{(l)}_{[\mathrm{i}]}, \mathbf{n}^{\otimes(l-m)} \mathbf{n}^{\otimes m}_{\pm}\right) = (l-m)!(x \pm \mathrm{i}y)^m r^{(l-m)} \frac{\mathrm{d}^m}{\mathrm{d}t^m} P_l(t)\Big|_{t=z/r}\,,$$

where $P_l(t)$ is a Legendre polynomial.

3.4 Harmonic 4D tensors

The potential of a point charge [7] in 4D space is equal to $1/r^2$. From the expansion of the point-charge potential of form (18), we obtain the multipole 4D potential

$$\frac{\boldsymbol{\mathcal{M}}^{(n)}_{i\ldots k}(\mathbf{r})}{r^{2n+2}} = (-1)^n \nabla_i \ldots \nabla_k \frac{1}{r^2}\,. \tag{28}$$

The harmonic tensor in the numerator has a structure similar to (27). Its contraction with respect to any two indices must vanish. The dipole and quadrupole 4D tensors, as follows from (28), are expressed as

$$\boldsymbol{\mathcal{M}}^{(1)}_i(\mathbf{r}) = 2x_i\,, \quad \boldsymbol{\mathcal{M}}^{(2)}_{ik}(\mathbf{r}) = 8(x_i x_k - 4\delta_{ik})\,. \tag{29}$$

The leading term of the expansion, as can be seen from (28), is equal to

$$\boldsymbol{\mathcal{M}}^{(n)}_{[\mathrm{i}]}(\mathbf{r}) = (2n)!!\, x_{i_1} \ldots x_{i_n} + \ldots = (2n)!!\, \mathbf{r}^{\otimes n} + \ldots\,. \tag{30}$$

Using the method described in Section 3.3, we obtain two representations (because differentiation rule (26) does not change):

$$\boldsymbol{\mathcal{M}}^{(n)}_{[\mathrm{i}]}(\mathbf{r}) = (2n)!!\, \mathbf{r}^{\otimes n} - \frac{(2n-2)!!}{1!2^1}\, r^2 \Delta \mathbf{r}^{\otimes n} + \frac{(2n-4)!!}{2!2^2}\, r^4 \Delta^2 \mathbf{r}^{\otimes n} + \ldots\,, \tag{31}$$

$$\boldsymbol{\mathcal{M}}^{(n)}_{[\mathrm{i}]}(\mathbf{r}) = (2n)!!\, \mathbf{r}^{\otimes n} - (2n-2)!!\, r^2 \langle\langle \delta^{\otimes 1}_{[..]} \mathbf{r}^{\otimes(n-2)} \rangle\rangle + (2n-4)!!\, r^4 \langle\langle \delta^{\otimes 2}_{[..]} \mathbf{r}^{\otimes(n-4)} \rangle\rangle \ldots\,. \tag{32}$$

We recall the double factorial

$$(2n)!! = 2^n n!\,, \tag{33}$$

which is essential in (32).

Four-dimensional tensors are structurally simpler than 3D tensors. But the SE requires that the eigenfunction be multiplied by a 3D tensor. This forces us to use not the 4D tensor itself but its special projection, which loses 4D invariance as 4D indices are replaced with 3D indices.

3.5 Decomposition of polynomials in terms of harmonic functions

In the perturbation theory, it is necessary to expand the source in terms of spherical functions. If the source is a polynomial, for example, when calculating the Stark effect, then the integrals are standard, but cumbersome. When calculating with the help of invariant tensors, the expansion coefficients are simplified, and there is then no need to use

[6] The factor $k!$ is lost in [26].

[7] We define the unit of charge in terms of the point potential.

integrals. It suffices, as we show here, to calculate contractions that lower the rank of the tensors under consideration.

Instead of integrals, we use the operation of calculating the trace $\hat{\mathrm{T}}\mathrm{r}$ of a tensor over two indices. The following rank reduction formula is useful:[8]

$$\hat{\mathrm{T}}\mathrm{r}\,\langle\langle \delta_{ik}\mathbf{M}^{(l)}_{ik[\mathbf{m}]}\rangle\rangle = (2l+3)\mathbf{M}^{(l-2)}_{[\mathbf{m}]}\,. \tag{34}$$

If the brackets contain several Kronecker symbols, the following relation holds:

$$\hat{\mathrm{T}}\mathrm{r}\,\langle\langle \delta_{i_1p_1}\ldots\delta_{i_kp_k}\mathbf{M}^{(l)}_{i_1p_1[\mathbf{m}]}\rangle\rangle = (2l+2k+1)\langle\langle \delta_{i_2p_2}\ldots\delta_{i_kp_k}\mathbf{M}^{(l-2)}_{[\mathbf{m}]}\rangle\rangle\,. \tag{35}$$

Calculating the trace reduces the number of Kronecker symbols by one, and the rank of the harmonic tensor on the right-hand side of (35) decreases by 2. Repeating the calculation of the trace k times eliminates the Kronecker symbols:

$$\hat{\mathrm{T}}\mathrm{r}_1\ldots\hat{\mathrm{T}}\mathrm{r}_k\,\langle\langle \delta_{i_1p_1}\ldots\delta_{i_kp_k}\mathbf{M}^{(l)}_{[\mathbf{m}]}\rangle\rangle = (2l+2k+1)!!\mathbf{M}^{(l-2k)}_{[\mathbf{m}]}\,. \tag{36}$$

Applying these rules allows decomposing the tensor $x_i\ldots x_p$ with respect to the harmonic ones.

In the perturbation theory, even the third approximation is often considered good. We present the decomposition of the tensor power up to the rank $l=6$:

- $l=2,\quad 3x_ix_k = \mathbf{M}^{(2)}_{ik} + r^2\delta_{ik}\,,$
- $l=3,\quad 5!!x_ix_kx_m = \mathbf{M}^{(3)}_{ikm} + 3r^2\langle\langle\delta_{ik}x_m\rangle\rangle\,,$
- $l=4,\quad 7!!x_ix_kx_lx_m = \mathbf{M}^{(4)}_{iklm} + 5r^2\langle\langle\mathbf{M}^{(2)}_{ik}\delta_{lm}\rangle\rangle + 7r^4\langle\langle\delta_{ik}\delta_{lm}\rangle\rangle\,,$
- $l=5,\quad 9!!x_ix_kx_lx_mx_n = \mathbf{M}^{(5)}_{iklmn} + 7r^2\langle\langle\mathbf{M}^{(3)}_{ikl}\delta_{mn}\rangle\rangle + 3\times 9r^4\langle\langle\delta_{ik}\delta_{lm}x_n\rangle\rangle\,,$
- $l=6,\quad 11!!x_ix_kx_lx_mx_nx_p = \mathbf{M}^{(6)}_{iklmnp} + 9r^2\langle\langle\mathbf{M}^{(4)}_{iklm}\delta_{np}\rangle\rangle + 5\times 11r^4\langle\langle\mathbf{M}^{(2)}_{ik}\delta_{lm}\delta_{np}\rangle\rangle + 9\times 11r^6\langle\langle\delta_{ik}\delta_{lm}\delta_{np}\rangle\rangle\,. \quad (37)$

To derive formulas, it is useful to calculate the trace. The formula for $l=6$ then implies the formula for $l=4$. The trace is calculated using rule (35). For even values of l, the last term in (37) has the form

$$\frac{(2l-1)!!}{(l+1)!!}\,. \tag{38}$$

When averaging over the directions of the vector x_i (i.e., when integrating over the unit sphere), it is convenient to use a simple relation for even values of l [21],

$$\frac{1}{4\pi}\int_{|\mathbf{x}|=1} x_{i_1}\ldots x_{i_l}\,\mathrm{d}S_{\mathbf{x}} = \frac{1}{(2l-1)!!}\langle\langle\delta_{i_1i_2}\ldots\delta_{i_{(l/2-1)}i_{l/2}}\rangle\rangle\,, \tag{39}$$

which is easy to verify by calculating the trace (see (36)). In particular, the most commonly used averaging in physics is obviously the one with $l=2$ [1, 21]:

$$\frac{1}{4\pi}\int_{|\mathbf{x}|=1} x_ix_k\,\mathrm{d}S_{\mathbf{x}} = \frac{1}{3}\,\delta_{ik}\,. \tag{40}$$

Also useful is the frequently occurring contraction over all indices without integration,

$$\left(\mathbf{M}^{(l)}_{[\mathrm{i}]},\mathbf{M}^{(l)}_{[\mathrm{i}]}\right) = \mathbf{M}^{(l)}_{i\ldots k}(\mathbf{x})\mathbf{M}^{(l)}_{i\ldots k}(\mathbf{x}) = \frac{(2l)!}{2^l}\,r^{2l}\,,$$

which arises when normalizing the states.

In *four-dimensional* space, formulas preserve their simplicity. The positions of indices in (31) are unique and can therefore be omitted. Instead of formula (35), we then have

$$\hat{\mathrm{T}}\mathrm{r}\,\langle\langle\delta^{\otimes k}_{[..]}\boldsymbol{\mathcal{M}}^{(n)}_{[..][\mathbf{m}]}\rangle\rangle = (2l+2k+2)\langle\langle\delta^{\otimes(k-1)}_{[..]}\boldsymbol{\mathcal{M}}^{(n-2)}_{[\mathbf{m}]}\rangle\rangle\,. \tag{41}$$

The decomposition of tensor powers of a vector is also compact in four dimensions:

- $n=2,\quad 4!!x_ix_k = \boldsymbol{\mathcal{M}}^{(2)}_{ik} + 2r^2\delta_{ik}\,,$
- $n=3,\quad 6!!x_ix_kx_m = \boldsymbol{\mathcal{M}}^{(3)}_{ikm} + 8r^2\langle\langle\delta_{ik}x_m\rangle\rangle\,,$
- $n=4,\quad 8!!x_ix_kx_lx_m = \boldsymbol{\mathcal{M}}^{(4)}_{iklm} + 6r^2\langle\langle\boldsymbol{\mathcal{M}}^{(2)}_{ik}\delta_{lm}\rangle\rangle + 16r^4\langle\langle\delta_{ik}\delta_{lm}\rangle\rangle\,,$
- $n=5,\quad 10!!x_ix_kx_lx_mx_n = \boldsymbol{\mathcal{M}}^{(5)}_{iklmn} + 8r^2\langle\langle\boldsymbol{\mathcal{M}}^{(3)}_{ikl}\delta_{mn}\rangle\rangle + 10\times 8r^4\langle\langle\delta_{ik}\delta_{lm}x_n\rangle\rangle\,,$
- $n=6,\quad 12!!x_ix_kx_lx_mx_nx_p = \boldsymbol{\mathcal{M}}^{(6)}_{iklmnp} + 10r^2\langle\langle\boldsymbol{\mathcal{M}}^{(4)}_{iklm}\delta_{np}\rangle\rangle + 12\times 6r^4\langle\langle\boldsymbol{\mathcal{M}}^{(2)}_{ik}\delta_{lm}\delta_{np}\rangle\rangle + 24\times 10r^6\langle\langle\delta_{ik}\delta_{lm}\delta_{np}\rangle\rangle\,. \quad (42a)$

When using the tensor notation (with indices suppressed), the last equality becomes

$$12!!\mathbf{x}^{\otimes 6} = \boldsymbol{\mathcal{M}}^{(6)}_{[\mathbf{i}]} + 10r^2\langle\langle\boldsymbol{\mathcal{M}}^{(4)}_{[\mathbf{i}]}\delta_{[..]}\rangle\rangle + 12\times 6r^4\langle\langle\boldsymbol{\mathcal{M}}^{(2)}_{[\mathbf{i}]}\delta^{\otimes 2}_{[..]}\rangle\rangle + 24\times 10r^6\langle\langle\delta^{\otimes 3}_{[..]}\rangle\rangle\,. \tag{42b}$$

We note that the derivation of coordinate-wise relations (37) and (41) by integrating spherical functions is rather cumbersome. Decomposition of higher powers is not more difficult using contractions over two indices.

4. Quadratic Stark effect

4.1 Method of the first correction

To demonstrate the effectiveness of calculations with polynomials (and with harmonic tensors), we consider the quadratic Stark effect in the case where the linear effect is absent. The appropriate formula was obtained in [34–38] by moving to parabolic coordinates. A modern presentation can be found in [1, 39, 40]. The SE then separates and two sets of orthogonal functions arise. The perturbation matrix automatically becomes diagonal, which immediately leads to the well-known formula for the dipole moment proportional to the difference between parabolic quantum numbers n_1-n_2.

If $n_1=n_2=m$ and there is no linear effect, then the quadratic effect must be calculated. In parabolic coordinates, the calculation of the second approximation is not so

[8] The symmetrization operation is *not* associative. Here, it is applied to the tensor as a whole. Formula (27) can be applied to the left-hand side of (34) only after symmetrization. In particular, $\langle\langle\delta_{[..]}\langle\langle\delta_{[..]}x_m\rangle\rangle\rangle\rangle = 2\langle\langle\delta_{[..]}\delta_{[..]}x_m\rangle\rangle$.

obvious and requires some effort [1]. The final formula is as follows. The dipole moment d_z is proportional to the electric field $\mathcal{E}$:

$$d_z = \frac{n^4}{8}(17n^2 - 9m^2 + 19)\mathcal{E}\,, \tag{43}$$

where n and m are the quantum numbers of the hydrogen atom. For the ground state with $n = 1$ and $m = 0$, the electric polarizability is $(9/2)a_{\mathrm{B}}^3$, which is a fundamental law of nature.

Here, we consider the calculation of the quadratic Stark effect using a technique known in physics, when the symmetry properties (for example, the unitarity of the scattering matrix) allow obtaining the next approximations algebraically in terms of the preceding ones [25]. The calculation of matrix elements is not required.

When expanded in powers of $\mathcal{E}$, the original SE for the first correction to the state Ψ_1 has the form

$$\left(\frac{1}{2}\,\Delta + E_0 + \frac{1}{r}\right)\Psi_1 = \mathcal{E}z\Psi_0\,, \tag{44}$$

when the electron charge is negative. We are interested in the second approximation to the energy E_2 in the case where the first correction vanishes:

$$E_1 = (\Psi_0, z\mathcal{E}\Psi_0) = 0\,. \tag{45}$$

Then, the second correction to the energy is calculated linearly in terms of the first correction:

$$E_2 = \frac{1}{2}(\Psi_1, \mathcal{E}z\Psi_0)\,.$$

If the function Ψ_0 is not normalized, the right-hand side must be divided by the norm squared:

$$E_2 = \frac{1}{2}(\Psi_1, \mathcal{E}z\Psi_0)\,\frac{1}{(\Psi_0, \Psi_0)}\,. \tag{46}$$

We note that Eqn (44) gives a non-unique solution for the function Ψ_1. We can always add Ψ_0 to it, because the left-hand side of (44) vanishes for Ψ_0. But this does not change the quadratic correction (46), because the linear correction is equal to zero. Thus, the problem reduces to calculating the first correction Ψ_1. In this case, the polynomial decomposition reduces the number of computations. As an illustration, we consider two problems that are simple in their original formulation.

4.2 Ground state $n = 1$

For $\Psi_0 = \exp(-r)$, Eqn (44) takes the form

$$\left(\frac{1}{2}\,\Delta - \frac{1}{2} + \frac{1}{r}\right)\Psi_1 = \mathcal{E}z\exp(-r)\,. \tag{47}$$

The solution in the form of a polynomial times an exponential is easy to guess:

$$\Psi_1 = -\left(1 + \frac{r}{2}\right)\mathcal{E}z\exp(-r)\,.$$

When substituting this into Eqn (47), it is helpful to use Euler's theorem. Simple integration[9] immediately allows deriving the desired answer from (46):

$$E_2 = -\frac{9}{4}\,\mathcal{E}^2\,.$$

4.3 State $l = n - 1$

Let us consider the calculation for the parameters when l is maximum and equals m: $l = m = n - 1$. The unperturbed state is the product of a homogeneous polynomial and an exponential:

$$\Psi_0 = \exp\left(-\frac{r}{n}\right)(x + \mathrm{i}y)^{n-1}\,.$$

Following the method in Section 4.2, we seek a function in the form

$$\Psi_1 = -(c_1 + c_2 r)\mathcal{E}z\Psi_0\,.$$

Substituting into (44) yields the solution

$$\Psi_1 = -\frac{n^2}{2}\left(n + 1 + \frac{r}{n}\right)\mathcal{E}z\Psi_0 = -\frac{n^2}{2}\left(n + 1 + \frac{r}{n}\right)\mathcal{E}z(x + \mathrm{i}y)^{n-1}\exp\left(-\frac{r}{n}\right). \tag{48}$$

The integrals are easy to calculate, and formula (46) leads to the dipole moment

$$d_z = \frac{n^4(n+1)(4n+5)}{4}\,\mathcal{E}\,, \tag{49}$$

which coincides with (43) for $m = n - 1$. In dimensional units, the moment is expressed as

$$d_z = \frac{n^4(n+1)(4n+5)}{4}\,a_{\mathrm{B}}^3\mathcal{E}\,.$$

An even more direct derivation of this result is possible if we note that correction (48) is equal to the combination of two states with $n + 1$ and $n + 2$ for $l = n$:

$$|n+2, n\rangle = \mathcal{E}z\exp(-r)(x + \mathrm{i}y)^{n-1}\left(1 - \frac{r}{n+1}\right),$$

$$|n+1, n\rangle = \mathcal{E}z\exp(-r)(x + \mathrm{i}y)^{n-1}.$$

The radii of the orbits are reduced to unity, and, hence, these states are not orthogonal. However, they satisfy Eqns (2) with different eigenvalues:

$$\left(-\Delta + 1 - \frac{2n}{r}\right)|n+2, n\rangle = \frac{4}{r}\,|n+2, n\rangle\,,$$

$$\left(-\Delta + 1 - \frac{2n}{r}\right)|n+1, n\rangle = \frac{2}{r}\,|n+1, n\rangle\,.$$

We must now compose such a combination of them such that the factor $1/r$ on the right-hand side cancels, leading to the source $\Psi_{n(n-1)} = (x + \mathrm{i}y)^{n-1}\mathcal{E}z\exp(-r)$, which gives

$$\frac{n^2(n+1)}{2}\left[|n+2, n\rangle - 2|n+1, n\rangle\right].$$

Substitution in the SE turns out to be not very complicated. (When integrating, we must return to the corresponding radii $n + 2$, $n + 1$, and n.)

[9] The integral $\int_0^\infty \exp(-r)r^k\,\mathrm{d}r = k!$ accompanied by averaging (40).

5. Differential form of the Schrödinger equation in momentum space

5.1 Derivation and solution

We apply the method of harmonic tensors to the SE in momentum space. In the traditional approach, only the integral form of the SE is assumed [1–4, 39, 40], which is Eqn (10) or Fock equation (16). The eigenfunctions then contain a factor in the form of Gegenbauer polynomials with a modified argument [39]. The second factor is a harmonic 3D tensor (or a solid spherical function) in momentum space. Direct application of the Fourier transformation reduces to the Hankel transformation [40], which presents no fundamental difficulty, even if specific calculations can be bulky. It is shown below that the differential equation exists, and its derivation is rather simple. Its solution is found using harmonic polynomials similar in form to the 'original' ones (7).

We proceed from Eqn (2) when the radius of the orbit (when multiplied by n) is reduced to unity. We multiply (2) by modulus r and square both sides:

$$r(-\Delta+1)r(-\Delta+1)\Psi_{nl} = 4n^2\Psi_{nl}\,. \tag{50}$$

Hence,

$$\left[r^2(\Delta-1)^2 + 2(\hat{l}_{\mathbf{x}}+1)(\Delta-1)\right]\Psi_{nl} = 4n^2\Psi_{nl}\,, \tag{51}$$

where the 'angular momentum modulus' operator is $\hat{l}_{\mathbf{x}} = \mathbf{x}\nabla$.

We move to the new function

$$\Phi_{nl} = (\Delta-1)^2\Psi_{nl}\,,$$

which corresponds to multiplying the spectrum by $(p^2+1)^2$ (see Fock's method (12)). For this, we apply the operator $(\Delta-1)^2$ to Eqn (51) and swap the operators $\hat{l}_{\mathbf{x}}$ and Δ. We then obtain an equation for the function $\Phi_{nl}(\mathbf{x})$,

$$\left[(\Delta-1)^2 r^2 + 2(\Delta-1)(\hat{l}_{\mathbf{x}}+3)\right]\Phi_{nl} = 4(n^2-1)\Phi_{nl}\,.$$

We can now move to the spectra $a_{nl}(\mathbf{p})$ and $b_{nl}(\mathbf{p})$ by changing $\nabla_{\mathbf{r}} \to \mathrm{i}\mathbf{p}$ and $\mathbf{x} \to \mathrm{i}\nabla_{\mathbf{p}}$,

$$\begin{gathered}\left[\left(-\frac{p^2+1}{2}\right)^2\Delta_{\mathbf{p}} + \frac{p^2+1}{2}\,\hat{l}_{\mathbf{p}}\right]b_{nl} = (n^2-1)b_{nl}\,,\\ b_{nl}(\mathbf{p}) = (p^2+1)^2 a_{nl}(\mathbf{p})\,,\end{gathered} \tag{52}$$

where $\hat{l}_{\mathbf{p}} = \mathbf{p}\nabla_{\mathbf{p}}$. Instead of integral equation (10), we obtain a problem that is no more complicated than the SE in coordinate space, because the equation for it resembles the SE with the sum of two potentials. The operator on the left-hand side of (52) is equal to the operator square of a vector, whence

$$\left[-\left((p^2+1)\nabla_{\mathbf{p}}\right)^2 + 4(p^2+1)\,\hat{l}_{\mathbf{p}}\right]b_{nl}(\mathbf{p}) = 4(n^2-1)b_{nl}(\mathbf{p})\,.$$

We seek a solution of the equation in the product form

$$b_{nl}(\mathbf{p}) = Y_l(\mathbf{p})\,\frac{1}{(p^2+1)^l}\,P_k\left(\frac{1}{p^2+1}\right), \tag{53}$$

where $Y_l(\mathbf{p})$ is a solid spherical function (or a harmonic tensor) and the factor $P_k(u)$ is a polynomial of degree k.

Relation (5) is useful when substituting. For the factor $P_k(u)$, Eqn (52) gives the second Gauss function[10]

$${}_2F(\alpha,\beta,\gamma,u) = 1 + \frac{\alpha\beta}{\gamma}\,\frac{u}{1!} + \frac{\alpha(\alpha+1)\beta(\beta+1)}{\gamma(\gamma+1)}\,\frac{u^2}{2!} + \ldots\,,$$

where the parameters are

$$\begin{gathered}\alpha = -k\,,\quad \beta = 2l+k+2\,,\quad \gamma = l+\frac{3}{2}\,,\\ k = n-l-1\,,\quad u = \frac{1}{p^2+1}\,.\end{gathered} \tag{54}$$

We recall that the transition to the real spectrum requires multiplying the argument $\mathbf{p}$ by n.

Using the properties of Gauss functions [1, 32], we can represent solution (53) in another form:

$$\begin{aligned}a_{nl}(\mathbf{p}) = {}& Y_l(\mathbf{p})\,\frac{1}{(p^2+1)^{n+1}}\,p^{2k}\\ &\times {}_2F\left[-k, \left(-n+\frac{1}{2}\right), \left(l+\frac{3}{2}\right), -\frac{1}{p^2}\right].\end{aligned}$$

Example 3.

(a) $n=2,\ l=0,\ k=1$ (isotropic state). We double the momentum, returning to radius 2:

$$a_{20}(\mathbf{p}) = \mathrm{const}\,\frac{1}{(1+4p^2)^2}\left(1-\frac{2}{1+4p^2}\right).$$

The derivation of this formula using the Hankel transform is rather cumbersome [41].

(b) $n = l+1$, $k=0$ (l is maximum):

$$\Psi_{n(n-1)}(\mathbf{x}) = Y_{n-1}(\mathbf{x})\exp\left(-\frac{r}{n}\right),$$

where the first factor is a solid spherical function (or a harmonic tensor). We move to the argument $\mathbf{x}/n$ and apply the Fourier transform. The polynomial turns into a differential operator applied to $1/(1+p^2)^2$:

$$a_{nl}(\mathbf{p}) = \hat{Y}_l(\mathrm{i}\nabla_{\mathbf{p}})\,\frac{1}{(1+p^2)^2} = \mathrm{const}\,\frac{Y_l(\mathbf{p})}{(1+p^2)^{2+l}}\,.$$

The action of the differential operator generates the same solid spherical function (or tensor), and the next function must be differentiated l times with respect to the argument p^2 (see formula (B.1) in Appendix B).

Returning to the physical argument $n\mathbf{p}$ and using the homogeneity of the polynomial $Y_l(\mathbf{p})$, we obtain

$$a_{nl}(\mathbf{p}) = \mathrm{const}\,\frac{Y_{n-1}(\mathbf{p})}{(1+n^2p^2)^{n+1}}\,,$$

which coincides with the general formula (53).

5.2 Group meaning of the solution

Harmonic 4D polynomials satisfy the 4D SO(4)-invariant Laplace equation, which in the momentum Fock space on a

[10] The hypergeometric function ${}_2F_1$.

sphere $|\xi|^2 + \xi_0^2 = \rho_\xi^2 = 1$ has the form

$$\Delta_\xi Y_{n-1} = \Delta_{\perp\xi} Y_{n-1} + \frac{1}{\rho^3}\frac{\partial}{\partial\rho}\rho^3\frac{\partial}{\partial\rho} Y_{n-1} = \left[\Delta_{\perp\xi} + (n^2-1)\right] Y_{n-1} = 0\,. \quad (55)$$

We recall that the degree of a homogeneous polynomial is $n-1$; hence, its radial dependence is ρ^{n-1} (see footnote 5 in Section 2). On a sphere $\rho = 1$, the transverse operator $\Delta_{\perp\xi}$ becomes a differential operator (with three angles) with an eigenvalue equal to n^2-1. Comparing (52) and (55), we can see that the derived equation (52) after Fock transformation (11) with the scaling factor $(1+\mathbf{p}^2)/2$ switches to the problem for eigenvalues of the angular part of the 4D Laplace equation on the surface of a sphere shown in the figure.

6. Modifying Fock's theory

6.1 Extension to 4D momentum space

Knowing the method of harmonic tensors (or spherical functions), we consider the inverse transition from 4D spherical functions in momentum space to the SE in physical space (where the radius of the orbits is reduced to unity), without repeating it literally. The main point in each transformation is to preserve the SO(4) symmetry. The first modification of the Fock theory is the transition from spherical functions to 4D solid spherical functions inside the sphere. They coincide on the surface $|\xi|^2 + \xi^2 = \rho_\xi^2 = 1$.

The starting point of the theory is therefore given by the solid spherical 4D functions

$$Y_l(\xi)\rho_\xi^k C_k^{l+1}\left(\frac{\xi_0}{\rho_\xi}\right), \quad (56)$$

where the first factor is a 3D solid spherical function (or a harmonic tensor in 3D space), and the second is a Gegenbauer polynomial with the argument ξ_0/ρ_ξ multiplied by ρ_ξ^k. The properties of Gegenbauer polynomials useful in physical problems are discussed in Section 6.3. Now, we only use the homogeneity property in the coordinates of the first and second factors. This polynomial is some projection of the harmonic tensor $\mathcal{M}_{[i]}^{n-1}(\xi, \xi_0)$ from formula (32), i.e., a contraction over indices with a numerical tensor.

Instead of a stereographic projection of a sphere, we consider a closely related 4D spatial transformation consisting of three steps:

- shift of the sphere upward by one: $\xi_0' = \xi_0 + 1$;
- the '$2/\rho$' inversion of space: $(\xi', \xi_0') = 2/(\mathbf{p}^2 + p_0'^2)\times(\mathbf{p}, p_0')$ with multiplication by $2/(\mathbf{p}^2 + p_0^2)$;
- shift of the plane $p_0' = 1$ downward by one: $p_0 = p_0' - 1$.

The point $(\xi, 0)$ on the sphere with the modulus $|\xi| = 1$ then goes to the point $\mathbf{p} = \xi$, which is exactly what happens under the stereographic projection. The sphere maps onto the plane. In physics, the inversion of the radius vector relative to the sphere is more common than 'cartography,' although the latter has a universal geometric description.

For the 4D harmonicity property to be preserved, it is necessary not only to replace the argument but also to divide the solid spherical function by $(\mathbf{p}^2 + p_0^2)$ after inversion. We temporarily postpone the second shift of the plane along axis p_0', and apply the Taylor expansion to the polynomial of degree $n-1$ shifted along the ξ_0 axis by 1,

$$Y_l(\xi) C_k^{l+1}\left(\frac{\xi_0 - 1}{\tilde\rho}\right)\tilde\rho^k = Y_l(\xi)\sum_{m=1}^{n-1}\frac{(-1)^m}{m!} \times \left(\frac{\partial}{\partial\xi_0}\right)^m\left[C_k^{l+1}\left(\frac{\xi_0}{\rho}\right)\rho^k\right], \quad (57)$$

where $\tilde\rho^2 = \xi^2 + (\xi_0 - 1)^2$ (the shifted radius). The 3D function $Y_l(\xi)$ is not affected by the shift.

We use the important property of homogeneity, which persists under differentiation. An individual term in the sum has the homogeneity degree $n-1-m$, and the factor $Y_l(\xi)$ in front of the sum is homogeneous of degree l. Under inversion, the form of the functions is preserved, but inverse powers of the 4D radius vector appear. The additional factor $1/(\mathbf{p}^2 + p_0^2) = 1/\rho_\mathbf{p}^2$ turns the terms into multipole potentials:

$$\sum_{m=1}^{n-1}\frac{\mathcal{M}^{n-1-m}}{(\mathbf{p}^2 + p_0^2)^{n-m}} = \sum_{m=1}^{n-1}\frac{\mathcal{M}^{n-1-m}}{\rho_\mathbf{p}^{2(n-m)}}\,. \quad (58)$$

The numerator in (58) contains solid spherical 4D functions (or 4D tensors):

$$\mathcal{M}^{n-1-m} = Y_l(\mathbf{p})\frac{(-1)^m 2^{n-m}}{m!}\left(\frac{\partial}{\partial p_0}\right)^m\left[C_k^{l+1}\left(\frac{p_0}{\rho_\mathbf{p}}\right)\rho_\mathbf{p}^k\right], \quad (59)$$

where $\rho_\mathbf{p}^2 = \mathbf{p}^2 + p_0^2$.

Recall that a shift of the plane down by one remains to be implemented.

6.2 Introduction of the factor $1/r$ in the physical space

It can be seen from SE (2) that applying the operator $(-\Delta + 1)$ to the function $\Psi_{nl}(\mathbf{x})$ is equivalent (up to a constant) to dividing it by r. The spectrum $a(\mathbf{p})$ is then multiplied by $(\mathbf{p}^2 + 1)$. We discard one factor in (12), modifying Fock's theory once again in order to work with harmonic functions. The final result, as is to be shown, is the function $\Psi_{nl}(\mathbf{x})/r$.

6.3 Transition to the 4D coordinate space

The Fourier transformation

$$\int \exp\left[\mathrm{i}(\mathbf{px} + p_0\tau)\right] a_{nl}(\mathbf{p}, p_0)\,\mathrm{d}^3\mathbf{p}\,\mathrm{d}p_0$$

maps the eigenfunctions $a_{nl}(\mathbf{p}, p_0)$ into the 4D coordinate space, i.e., into functions of four coordinates ($\hbar = 1$). We then apply the inverse transformation with respect to the 'extra' variable τ. The reason for such a 'knight's move' is that multipole tensors become harmonic ones with a factor $1/(\mathbf{x}^2 + \tau^2)$ (see Appendix C). The transformations are performed up to a 'floating' constant; we specify the normalization later.

The original function is given in (58) and (59). The 4D Fourier transformation of the sum replaces the argument $(\mathbf{p}, p_0)$ with $(\mathbf{x}, \tau)$, changes the factorial coefficients, and adds the factor $1/(\mathbf{x}^2 + \tau^2)$. From (C.5), we then have

$$\frac{4\pi^2}{x^2 + \tau^2}\sum_{m=1}^{n-1}\frac{\mathrm{i}^{n-1-m}\mathcal{M}^{n-1-m}(\mathbf{x}, \tau)}{2^{n-1-m}(n-1-m)!}\,. \quad (60)$$

Substituting (59) into (60), we use Newton's binomial formula,

$$\text{const}\,\frac{Y_l(\mathbf{x})}{x^2+\tau^2}\sum_{m=1}^{n-1}\frac{\mathrm{i}^m}{(n-1-m)!}\,\frac{(n-1)!}{m!}\times\left(\frac{\partial}{\partial\tau}\right)^m\left[C_k^{l+1}\left(\frac{\tau}{R}\right)R^k\right]=\text{const}\,\frac{Y_l(\mathbf{x})}{x^2+\tau^2}\left(1+\mathrm{i}\,\frac{\partial}{\partial\tau}\right)^{n-1}\left[C_k^{l+1}\left(\frac{\tau}{R}\right)R^k\right],\quad(61)$$

where $R=\sqrt{\mathbf{x}^2+\tau^2}$. Here, it is necessary to take the plane shift $p_0'=p_0+1$ into account. An extra essential factor $\exp(-\mathrm{i}\tau)$ arises.

We have thus obtained the coordinate space $(\mathbf{x},\tau)$, where the transformed eigenfunctions are proportional to the $(n-1)$th derivative of solid spherical functions,

$$\tilde{\Psi}_{nl}(\mathbf{x},\tau)=\frac{\exp(-\mathrm{i}\tau)\,Y_l(x)}{\mathbf{x}^2+\tau^2}\left(1+\mathrm{i}\,\frac{\partial}{\partial\tau}\right)^{n-1}\left[C_k^{l+1}\left(\frac{\tau}{R}\right)R^k\right],\quad(62)$$

where $R^2=\mathbf{x}^2+\tau^2$.

It remains to calculate the Fourier transforms with respect to the variable τ:

$$\frac{1}{2\pi}\int\tilde{\Psi}_{nl}(\mathbf{x},\tau)\exp(-\mathrm{i}\omega\tau)\,\mathrm{d}\tau\,.\quad(63)$$

6.4 From harmonic 4D polynomials to states of the hydrogen atom

Fourier transforms (63) must be understood in a generalized sense, because the numerator contains a polynomial. The result is a combination of delta functions, which must be discarded. This is achieved by closing the integration contour in the lower half-plane, where the exponential decays and the pole $\tau=-\mathrm{i}r$ is present:[11]

$$Y_l(\mathbf{x})\oint_{\mathrm{Im}\,\tau\leqslant 0}\exp(-\mathrm{i}\tau)\frac{1}{\mathbf{x}^2+\tau^2}\times\left(1+\mathrm{i}\,\frac{\partial}{\partial\tau}\right)^{n-1}\left[C_k^{l+1}\left(\frac{\tau}{R}\right)R^k\right]\mathrm{d}\tau\,.\quad(64)$$

At $\omega=0$, the integral is therefore equal to

$$\frac{\Psi_{nl}(\mathbf{x})}{r}=\text{const}\,Y_l(\mathbf{x})\frac{\exp(-r)}{r}\left(1-\frac{\partial}{\partial t}\right)^{n-1}\times\left[C_k^{l+1}\left(\frac{\mathrm{i}t}{R}\right)R^k\right]\bigg|_{t=r},\quad(65)$$

where we recall that the polynomial $C_k^{l+1}(\mathrm{i}t)$ is either an even or an odd function.

The squared 4D radius $R^2=r^2+\tau^2=r^2-t^2$ is equated to zero only after differentiating. Each derivative with a minus sign can be pulled out of the exponential:

$$\Psi_{nl}(\mathbf{x})=\text{const}\,Y_l(\mathbf{x})\frac{1}{r}\,\frac{\partial^{n-1}}{\partial t^{n-1}}\left[\exp(-t)C_k^{l+1}\left(\frac{\mathrm{i}t}{R}\right)R^k\right].\quad(66)$$

[11] Adding an arbitrary polynomial times an exponential does not change integral (64). The polynomial can be chosen such that the delta function does not appear in (63).

In deriving relations (65) and (66), we deviated from Fock's theory in three points. The validity of the final result must now be verified. We take a specific state for the verification.

Example 4.
State: n, $l=n-4$:

$$\Psi_{n(n-4)}=Y_{n-3}(\mathbf{x})\left(1-\frac{2r}{n-2}+\frac{2r^2}{(n-2)(2n-3)}\right),$$

$$R^2C_2^{n-2}\left(\frac{\mathrm{i}t}{R}\right)=\text{const}\left[(\mathrm{i}t)^2-\frac{(\mathrm{i}t)^2+r^2}{2(n-1)}\right],$$

$$\left(1-\frac{\partial}{\partial t}\right)^{n-1}=1-(n-1)\frac{\partial}{\partial t}+\frac{(n-1)(n-2)}{2}\left(\frac{\partial}{\partial t}\right)^2\ldots\,.$$

Substitution into (65) gives an equality (with a 'floating' constant).

The general formula is verified in Appendix D, where the constant is found. For the Laguerre polynomials, we have

$$L_k^{2l+1}(r)=\frac{\mathrm{i}^k l!}{(l+k)!}\left[\left(1-\frac{\partial}{\partial t}\right)^k R^k C_k^{l+1}\left(\frac{\mathrm{i}t}{R}\right)\right]\bigg|_{t=r},\quad(67)$$

where $R^2=r^2-t^2$.

Thus, there is no need to apply Fock's transformations. It suffices to choose a harmonic polynomial (or tensor), differentiate it, and make the change $\tau=-\mathrm{i}r$. We note here that the substitution $\tau=-\mathrm{i}t$ signifies a transition from the 4D Laplace equation to the wave equation with the wave propagation speed $Ze^2/(\hbar n)$ in dimensional coordinates.

7. Derivation of the Fock equation by electrostatic methods

7.1 In 3D electrostatics

We consider the potential of charges $\sigma(\mathbf{x})$ on the surface of a unit sphere in the case where the charge density is a spherical function with index l (or a homogeneous harmonic polynomial of degree l):

$$\sigma(\mathbf{x})=Y_l(\mathbf{x})\,,\quad|\mathbf{x}|=1\,.\quad(68)$$

This is the simplest problem in electrostatics. The potential $\varphi(\mathbf{x})$ is then outside and inside the sphere:

$$\varphi(\mathbf{x})=c_l\,\frac{Y_l(\mathbf{x})}{r^{2l+1}}\,,\quad|r|\geqslant 1\,,\qquad \varphi(\mathbf{x})=c_l\,Y_l(\mathbf{x})\,,\quad|r|\leqslant 1\,,\quad(69)$$

where $Y_l(\mathbf{x})$ is a polynomial of degree l.

At the boundary, the potential is continuous, and the electric field has a discontinuity $4\pi\sigma$:

$$-\frac{\partial}{\partial r}\,c_l\,\frac{Y_l(\theta,\varphi)}{r^{l+1}}\bigg|_{r=1}+\frac{\partial}{\partial r}\,c_l Y_l(\theta,\varphi)r^l\bigg|_{r=1}=c_l(2l+1)\,Y_l(\theta,\varphi)\bigg|_{r=1}=4\pi\sigma\,,\quad r=1\,.\quad(70)$$

Hence,

$$c_l=\frac{4\pi}{2l+1}\,.\quad(71)$$

On the other hand, the potential is determined by Newton's integral formula

$$\int_{r'=1} \frac{\sigma(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\,\mathrm{d}S' = \varphi(\mathbf{x})\,. \tag{72}$$

We substitute here the potential from (69) and let $\mathbf{x}$ tend to the surface. We then obtain an integral equation for 3D spherical functions,

$$Y_l(\mathbf{x}) - \frac{2l+1}{4\pi}\int_{r'=1} \frac{Y_l(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\,\mathrm{d}S' = 0\,, \quad |\mathbf{x}| = 1\,. \tag{73}$$

We use this analogy to derive the Fock equation (16), i.e., for 4D spherical functions.

7.2 In 4D space

On the surface of a 3D sphere, we choose the charge density

$$\sigma(\mathbf{x}) = \boldsymbol{\mathcal{M}}_{n-1}(\mathbf{x})\,, \quad |\mathbf{x}| = 1\,,$$

where $\boldsymbol{\mathcal{M}}_{n-1}(\mathbf{x})$ is a harmonic homogeneous polynomial of degree $n-1$ (that is, it is any combination of 4D spherical functions with the principal number $n-1$ on the surface). Then, the potential $\varphi(\mathbf{x})$ is as follows outside and inside the sphere:

$$\begin{aligned} \varphi(\mathbf{x}) &= c_{n-1}\frac{\boldsymbol{\mathcal{M}}_{n-1}(\mathbf{x})}{r^{2n}}\,, \quad |r| \geqslant 1\,, \\ \varphi(\mathbf{x}) &= c_{n-1}\boldsymbol{\mathcal{M}}_{n-1}(\mathbf{x})\,, \quad |r| \leqslant 1\,. \end{aligned} \tag{74}$$

The electric field discontinuity in this case is $4\pi^2\sigma$:

$$-\frac{\partial}{\partial r}\,c_{n-1}\frac{Y_n(\theta,\varphi,\psi)}{r^{n+1}}\bigg|_{r=1} + \frac{\partial}{\partial r}\,c_{n-1}\,Y_n(\theta,\varphi,\psi)r^{n-1}\bigg|_{r=1}$$

$$= c_{n-1}2nY_{n-1}(\theta,\varphi,\psi)\big|_{r=1} = 4\pi^2\sigma\,, \quad r = 1\,.$$

Hence,

$$c_{n-1} = \frac{4\pi^2}{2n}\,.$$

Now, instead of Eqn (73), we obtain the Fock equation (16) for homogeneous harmonic polynomials of degree $n-1$ (see footnote 5 in Section 2):

$$\boldsymbol{\mathcal{M}}_{n-1}(\mathbf{x}) - \frac{n}{2\pi^2}\int_{r'=1} \frac{\boldsymbol{\mathcal{M}}_{n-1}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\,\mathrm{d}S' = 0\,, \quad |\mathbf{x}| = 1\,. \tag{75}$$

Thus, the equation is easier to understand in coordinate than in momentum space.

8. Ladder operators in the Coulomb problem

8.1 Raising operator $\hat{\mathbf{D}}$

Ladder operators are useful for representing eigenfunctions in a compact form. They are a basis for constructing coherent states [44–49]. In the Coulomb problem, they are in many respects close to the 'creation' and 'annihilation' operators of an oscillator.

The squared momentum operator

$$\hat{\mathbf{L}}^2 = -r^2\Delta + \hat{l}(\hat{l}+1)\,,$$

where the momentum modulus operator $\hat{l}$ is equal to $\mathbf{x}\boldsymbol{\nabla}$, becomes $\hat{l}(\hat{l}+1)$ when acting on the space of harmonic (or solid spherical) functions. In invariant form, the eigenfunctions $\hat{\mathbf{L}}^2$ are harmonic tensors (19).

The operator $\hat{\mathbf{D}}$ that increases the value of l by one was introduced in [26]. It can be obtained from relation (18):

$$\nabla_i \frac{\mathbf{M}^{(l)}_{k\ldots m}(\mathbf{r})}{r^{2l+1}} = -\frac{\mathbf{M}^{(l+1)}_{ik\ldots m}(\mathbf{r})}{r^{2l+3}}\,. \tag{76}$$

Straightforward differentiation on the left-hand side of (76) yields a vector operator acting on a harmonic tensor:

$$\hat{D}_i M^{(l)}_{k\ldots m}(\mathbf{r}) = M^{(l+1)}_{ik\ldots m}(\mathbf{r})\,, \quad \hat{\mathbf{D}} = (2\hat{l}-1)\mathbf{x} - r^2\boldsymbol{\nabla}\,. \tag{77}$$

In particular,

$$\hat{D}_i x_k = 3x_i x_k - r^2\delta_{ik}\,,$$

$$\hat{D}_i\hat{D}_k\hat{D}_m 1 = 3\big[5x_i x_k x_m - r^2(\delta_{ik}x_m + \delta_{km}x_i + \delta_{mi}x_k)\big]\,.$$

Applying the operator to representation (27) with the help of the differentiation formula

$$\nabla_i x^{\otimes l} + x_i\langle\langle\delta_{[..]}x^{\otimes(l-2)}\rangle\rangle = \langle\langle\delta_{[i.]}x^{\otimes(l-1)}\rangle\rangle$$

increases the rank of the harmonic tensor.

As a result of an l-fold application to 1, we obtain the harmonic tensor

$$\hat{D}_i\hat{D}_k\ldots\hat{D}_m 1 = M^{(l)}_{ik\ldots m} = \hat{\mathbf{D}}^{\otimes l}_{[i]}1 = \mathbf{M}^{(l)}_{[i]}\,, \tag{78}$$

written here in different forms.

The relation of this tensor to the momentum operator $\hat{\mathbf{L}}$ is as follows:

$$\hat{\mathbf{D}} = \hat{l}\mathbf{x} + \mathrm{i}[\mathbf{x}\times\hat{\mathbf{L}}]\,. \tag{79}$$

As indicated in [26], when functions are inverted with respect to a sphere, $r \to 1/r$ (with an additional factor $1/r$), a harmonic tensor passes into multipole (20), and the operator $\hat{\mathbf{D}}$ into the operator $(-\nabla)$. If we multiply the operators by $\mathrm{i}\hbar$, then the raising operator acquires the physical meaning of a *momentum operator in the space inverted with respect to the sphere*. The lowering operator is obvious: it is the gradient. Under inversion, it becomes $-\hat{\mathbf{D}}$.

We give some useful properties of operators in vector form:

$$\hat{D}_i\hat{D}_i = r^2\Delta\,, \tag{80}$$

which for tensors yields a vanishing trace over any two indices. The scalar product of vectors $\hat{\mathbf{D}}$ and $\mathbf{x}$ is

$$\mathbf{x}\hat{\mathbf{D}} = r^2(\hat{l}+1)\,, \quad \hat{\mathbf{D}}\mathbf{x} = r^2\hat{l}\,, \tag{81}$$

and, hence, the contraction of the tensor with the vector $\mathbf{x}$ can be expressed as

$$x_i M^{(l)}_{ik\ldots m} = 2lr^2 M^{(l-1)}_{k\ldots m}\,, \tag{82}$$

where l is a number.

The commutator in the scalar product on the sphere is equal to unity:

$$\mathbf{x}\hat{\mathbf{D}} - \hat{\mathbf{D}}\mathbf{x} = r^2\,.$$

To calculate the divergence of a tensor, a useful formula is

$$\nabla \mathbf{D} = (\hat{l}+1)(2\hat{l}+1)\,,$$

whence

$$\nabla_i M^{(l)}_{ik\ldots m} = (l+1)(2l+1) M^{(l-1)}_{k\ldots m} \tag{83}$$

(l on the right-hand side is a number).

The raising operator is useful for constructing the factor $Y_l(\mathbf{x})$ in front of the radial function in the solution structure of SE (7).

8.2 Four-dimensional operator $\hat{\boldsymbol{\mathcal{D}}}$

The raising operator in 4D space

$$\hat{\boldsymbol{\mathcal{D}}}_i \boldsymbol{\mathcal{M}}^{(n)}_{k\ldots m}(\mathbf{r},\tau) = \boldsymbol{\mathcal{M}}^{(n+1)}_{ik\ldots m}(\mathbf{r},\tau) = \boldsymbol{\mathcal{M}}^{(n+1)}_{ik\ldots m}(\mathbf{y}) \tag{84}$$

has largely similar properties. There is a raising operator

$$\hat{\boldsymbol{\mathcal{D}}} = 2\hat{n}\mathbf{y} - |\mathbf{y}|^2 \nabla_{\mathbf{y}}\,,$$

where y_i is a 4D vector, $i = 1, \ldots, 4$,

$$\mathbf{y} = (\mathbf{x}, \tau)\,, \quad \rho_{\mathbf{y}}^2 = |\mathbf{y}|^2 = \mathbf{x}^2 + \tau^2\,,$$

and the $\hat{n}$ operator multiplies a homogeneous polynomial by its degree, [12]

$$\hat{n} = \left(\mathbf{x}\nabla_{\mathbf{x}} + \tau\,\frac{\partial}{\partial\tau}\right) = \mathbf{y}\nabla_{\mathbf{y}}\,. \tag{85}$$

In particular,

$$\hat{\boldsymbol{\mathcal{D}}}_i 1 = 2y_i\,, \quad \hat{\boldsymbol{\mathcal{D}}}_i y_k = 2(4y_i y_k - \rho_{\mathbf{y}}^2 \delta_{ik})\,,$$
$$\hat{\boldsymbol{\mathcal{D}}}_i \hat{\boldsymbol{\mathcal{D}}}_k \hat{\boldsymbol{\mathcal{D}}}_m 1 = 4!!\left[6x_i x_k x_m - \rho_{\mathbf{y}}^2(\delta_{ik}x_m + \delta_{km}x_i + \delta_{mi}x_k)\right].$$

The scalar product of $\hat{\boldsymbol{\mathcal{D}}}$ and $\mathbf{y}$ is as simple as (81)

$$\mathbf{y}\hat{\boldsymbol{\mathcal{D}}} = \hat{l}_{\mathbf{y}}\rho_{\mathbf{y}}^2\,, \quad \hat{\boldsymbol{\mathcal{D}}}\mathbf{y} = (\hat{l}_{\mathbf{y}}+2)\rho_{\mathbf{y}}^2\,.$$

The scalar product of ladder operators $\hat{\boldsymbol{\mathcal{D}}}$ and $\boldsymbol{\nabla}$ is

$$\hat{\boldsymbol{\mathcal{D}}}\boldsymbol{\nabla} = 2(\hat{l}_{\mathbf{y}}+2)(\hat{l}_{\mathbf{y}}+1)\,.$$

The transformed solution of the SE can be regarded as an invariant tensor in the 4D coordinate space $\mathbf{y}$. It is then convenient to use the $\hat{\boldsymbol{\mathcal{D}}}$ raising operator.

As in (79), operator $\hat{\boldsymbol{\mathcal{D}}}$ is now associated with the momentum operator and the Runge–Lenz operator, which in the 4D coordinate space takes the simple form

$$\hat{\mathbf{A}} = \mathrm{i}\left(\tau\,\frac{\partial}{\partial\mathbf{x}} - \mathbf{x}\,\frac{\partial}{\partial\tau}\right).$$

Separately for the 3D $\mathbf{x}$-component and the fourth coordinate τ of the raising operator, we have

$$\hat{\boldsymbol{\mathcal{D}}}_{\mathbf{x}} = (\hat{n}+1)\mathbf{x} + \mathrm{i}[\mathbf{x}\times\hat{\mathbf{L}}] + \mathrm{i}\tau\mathbf{A}_{\mathbf{x}}\,,$$
$$\hat{\boldsymbol{\mathcal{D}}}_{\tau} = (\hat{n}+1)\tau + \mathrm{i}(\mathbf{x}\mathbf{A}_{\mathbf{x}})\,.$$

[12] Separating the τ variable is necessary in order to pass to the physical space.

9. Schwinger resolvent

We consider perturbed the Fock equation (16) in the 4D coordinate space on a sphere, using the unit 4D vectors $\mathbf{x}, \mathbf{y}$. When the perturbation is a delta function on the sphere, the solution is called resolvent $G(\mathbf{x},\mathbf{y})$. The Fock equation thus turns into an equation for the resolvent,

$$G(\mathbf{x},\mathbf{y}) - \frac{\lambda}{2\pi^2}\int_{|\mathbf{y}'|=1}\frac{G(\mathbf{x},\mathbf{y}')}{|\mathbf{y}-\mathbf{y}'|^2}\,\mathrm{d}S_{\mathbf{y}'} = \delta(\mathbf{x}-\mathbf{y})\,, \tag{86}$$

where instead of n we have a continuous parameter λ.

Schwinger applied the entire series of the integral perturbation theory to the solution of Eqn (86) in order to show that some series in quantum electrodynamics (QED) are summable [50]. This assumption is confirmed in some cases [56]. For the Coulomb problem, the answer is expressed in terms of elementary functions.

The solution to this problem can be obtained by a simple calculation [3] of the Gegenbauer polynomials with the properties listed in Appendix E [51–53]. We seek a solution of problem (86) in the form of a sum of polynomials. We use the obvious expansions

$$\frac{1}{|\mathbf{x}-\mathbf{y}|^2} = \sum_{k=0}^{\infty} C_k^1(\mathbf{x}\mathbf{y})\,, \tag{87}$$

$$\frac{1}{2\pi^2}\sum_{k=0}^{\infty}(k+1)C_k^1(\mathbf{x}\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y})\,, \tag{88}$$

which immediately gives a simple series

$$G(\mathbf{x},\mathbf{y}) = \frac{1}{2\pi^2}\sum_{k=0}^{\infty} C_k^1(\mathbf{x}\mathbf{y})\,\frac{(k+1)^2}{k+1-\lambda}\,. \tag{89}$$

To improve convergence, we subtract series (87) times the coefficient $\lambda/(2\pi^2)$ from it, and then series (88). We thus obtain [13]

$$G(\mathbf{x},\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y}) + \frac{\lambda}{2\pi^2|\mathbf{x}-\mathbf{y}|^2} + \frac{\lambda^2}{2\pi^2}\sum_{k=0}^{\infty} C_k^1(\mathbf{x}\mathbf{y})\,\frac{1}{k+1-\lambda}\,. \tag{90}$$

This is already a useful result for calculations, given the vector properties of the Gegenbauer polynomials. [14]

The resolvent has poles at $\lambda = 1, 2\ldots$, which corresponds to polynomials with the numbers $k = 0, 1, 2\ldots$. The values of the main quantum number n in the SE are $1, 2, \ldots$, respectively.

10. Conclusion

We illustrate the result of this study with the ground state of the SE ($n = 1$): $\exp(-r)$. Moving to the momentum description gives the function $1/(p^2+1)^2$. Fock's transformation gives the state with the number $n - 1 = 0$ *on the surface of a sphere*, i.e., the function 1. In the coordinate 4D space, we must take the harmonic polynomial with the number 0 *in the ball*, i.e., the polynomial 1, and then multiply the unit by

[13] The sign of λ was changed in [3].

[14] Schwinger sums the series by introducing a parameter ζ in the integral: $\int_0^1 \zeta^{k+1-\lambda}\,\mathrm{d}\zeta$.

$\exp(-r)$. This brings us back to the physical space without integrals.

The general formula for the transformation from the 4D space is just as simple. In any solution of the Laplace equation given by a homogeneous polynomial of degree $(n-1)$, including in the form of invariant tensor (32), we replace the coordinate $\tau \to -\mathrm{i}t$. Then, we multiply the polynomial by $\exp(-r)$ and calculate the $(n-1)$th derivative. The last step is to equate $t = r$ and obtain the n state.

To obtain states with a fixed value of l, we must take a harmonic 3D polynomial of degree l (or 3D tensor (27)) in the 4D space and then compose a polynomial of the form (66), which includes the Gegenbauer polynomial, and carry out a simple recalculation as in (65).

We note that, although it is no longer necessary to apply the Fock transformations, some results obtained using the 4D spherical functions carry over to the coordinate 4D space, including the Schwinger resolvent and the Fock integral equation. It is only necessary to replace the 'momentum' argument $(\boldsymbol{\xi}, \xi_0)$ with the coordinate argument $(\mathbf{x}, \tau)$.

As regards the method, we can see that solutions of the 3D and 4D Laplace equations play an important role, and tensor invariant methods of electrostatics are applicable. Importantly, the replacement $\tau \to -\mathrm{i}t$ means the transition to the wave equation with the wave propagation speed $Ze^2/(\hbar n)$. Then, the time parameter is set equal to the radius and disappears. The space in which the SO(4) symmetry is realized turns out to be 'closer' to the physical one than does the wrapped momentum space.

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11. Appendices

A. Structure of a harmonic tensor

We apply the operator Δ to the sum of tensors (24). Using the properties of homogeneous polynomials (5), we obtain two terms for the kth term of the sum:

$$\Delta\left[(-1)^k \frac{(2l-2k-1)!!}{k!2^k}\, r^{2k}\Delta^k \mathbf{r}^{\otimes l}\right]$$
$$= \left[(-1)^k \frac{(2l-2k-1)!!}{k!2^k}\, r^{2k}\Delta^{(k+1)} \mathbf{r}^{\otimes l}\right]$$
$$+ 2k(2l-2k+1)\left[(-1)^k \frac{(2l-2k-1)!!}{k!2^k}\, r^{2k-2}\Delta^k \mathbf{r}^{\otimes l}\right]. \tag{A.1}$$

We next take the second term from the next term of the sum, increasing k by one:

$$2(k+1)\left[(-1)^{k+1} \frac{(2l-2(k+1)+1)!!}{(k+1)!2^{k+1}}\, r^{2k}\Delta^{(k+1)} \mathbf{r}^{\otimes l}\right]$$
$$= -\left[(-1)^k \frac{(2l-2k-1)!!}{k!2^k}\, r^{2k}\Delta^{(k+1)} \mathbf{r}^{\otimes l}\right]. \tag{A.2}$$

This term 'absorbs' the first one from the previous term of the sum. As a result, the total sum is equal to zero and tensor (24) is a harmonic function.

B. Harmonic tensor as an operator

The Fourier transformation maps a polynomial into a differential operator. An invariant harmonic tensor is mapped into a tensor operator in the momentum space:

$$\mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{x}) \to \mathrm{i}^l \hat{\mathbf{M}}^{(l)}_{[\mathrm{i}]}(\nabla_{\mathbf{p}}).$$

We consider how it acts on a scalar function of the argument $\mathbf{p}^2 = p^2$. The result is quite obvious and has been 'rediscovered' several times [54]. Presumably, it was already known to Hobson [19]. We propose the following derivation.

From the uniqueness of the invariant tensor that is homogeneous in coordinates, it follows that the result is proportional to the harmonic tensor:

$$\hat{\mathbf{M}}^{(l)}_{[\mathrm{i}]}(\nabla_{\mathbf{p}}) f(p^2) = \mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{p})\varphi(p).$$

The unknown function $\varphi(p)$ can be found by taking a power of a complex variable instead of a tensor: $(x+\mathrm{i}y)^l = u^l$. The operator arises raised to the power

$$\left(\frac{\partial}{\partial x} + \mathrm{i}\frac{\partial}{\partial y}\right)^l = 2^l \frac{\partial^l}{\partial \bar{u}^l}.$$

This operator is applied to the function $\varphi(u\bar{u})$, with no differentiation with respect to u. The result is obvious:

$$2^l \frac{\partial^l}{\partial \bar{u}^l} f(u\bar{u}) = 2^l u^l f^{(l)}(u\bar{u}) = 2^l (x+\mathrm{i}y)^l f^{(l)},$$

where $f^{(l)}$ is the lth derivative. Thus, a simple and convenient formula is valid:

$$\hat{\mathbf{M}}^{(l)}_{[\mathrm{i}]}(\nabla_{\mathbf{p}}) f(p^2) = \mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{p}) 2^l f^{(l)}(p^2). \tag{B.1}$$

For the function $f(r^2) = 1/|\mathbf{x}|$, this formula yields the relation

$$\hat{\mathbf{M}}^{(l)}_{[\mathrm{i}]}(\nabla_{\mathbf{x}}) \frac{1}{\sqrt{|\mathbf{x}^2|}} = (-1)^l (2l+1)!!\, \frac{\mathbf{M}^{(l)}_{[\mathrm{i}]}(\mathbf{x})}{r^{(2l+1)}}, \tag{B.2}$$

which can be usefully compared with the definition of tensor (18).

C. The 4D Fourier transform of multipole potentials

The Fourier transform of multipole potentials

$$\int \exp\left[\mathrm{i}(\mathbf{p}\mathbf{x} + p_0\tau)\right] \frac{\boldsymbol{\mathcal{M}}^{(n)}_{[\mathrm{i}]}(\mathbf{p}, p_0)}{(\mathbf{p}^2 + p_0^2)^{(n+1)}}\, \mathrm{d}^3\mathbf{p}\, \mathrm{d}p_0 \tag{C.1}$$

preserves their form up to a scalar factor $1/(\mathbf{x}^2 + \tau^2)$, which, as shown below, follows from the Poisson equation.

We use the definition of multipole potentials in terms of 4D gradients (28):

$$\frac{\boldsymbol{\mathcal{M}}^{(n)}_{i\ldots k}(\mathbf{x}, \tau)}{(\mathbf{x}^2 + \tau^2)^{(n+1)}} = (-1)^n \nabla_i \ldots \nabla_k \frac{1}{\mathbf{x}^2 + \tau^2}$$
$$= \frac{(-1)^n}{2^n n!}\, \hat{\boldsymbol{\mathcal{M}}}^{(n)}_{i\ldots k}(\nabla) \frac{1}{\mathbf{x}^2 + \tau^2}, \tag{C.2}$$

where the argument on the right-hand side involves the 4D gradient. The indices $i, \ldots, k$ are four-dimensional. This replacement is valid because all terms in (28) except the first one contain the 4D Laplace operator (excluding the point 0).

We proceed from the equation for a point charge in 4D space:

$$\left(\Delta_{\mathbf{p}} + \frac{\partial^2}{\partial p_0^2}\right)\frac{1}{\mathbf{p}^2 + p_0^2} = -4\pi^2\delta(\mathbf{p})\delta(p_0)\,. \tag{C.3}$$

We apply the operator $\hat{\boldsymbol{\mathcal{M}}}^{(n)}_{i\ldots k}(\nabla)$to (C.3):

$$\left(\Delta_{\mathbf{p}} + \frac{\partial^2}{\partial p_0^2}\right)\frac{\boldsymbol{\mathcal{M}}^{(n)}_{i\ldots k}}{(\mathbf{p}^2 + p_0^2)^{(n+1)}} = -\frac{4\pi^2(-1)^n}{2^n n!}\,\hat{\boldsymbol{\mathcal{M}}}^{(n)}_{i\ldots k}(\nabla_{\mathbf{p}})\delta(\mathbf{p})\delta(p_0)\,. \tag{C.4}$$

The trace over any two indices on the right- and left-hand sides is equal to zero.

Fourier transform (C.1) can now be applied to Eqn (C.4) by substituting $\nabla_{\mathbf{p}} \to -\mathrm{i}(\mathbf{x}, \tau)$. The delta function goes to unity, and we have

$$\int \exp\left[\mathrm{i}(\mathbf{px} + p_0\tau)\right]\frac{\boldsymbol{\mathcal{M}}^{(n)}_{i\ldots k}(\mathbf{p}, p_0)}{(\mathbf{p}^2 + p_0^2)^{(n+1)}}\,\mathrm{d}^3p\,\mathrm{d}p_0 = \frac{4\pi^2\mathrm{i}^n}{2^n n!}\,\frac{\boldsymbol{\mathcal{M}}^{(n)}_{i\ldots k}(\mathbf{x}, \tau)}{\mathbf{x}^2 + \tau^2}\,. \tag{C.5}$$

The last relation holds for any tensor projection, i.e., contraction over indices with a numerical tensor and, hence, *for any solid spherical* function.

D. Polynomial correspondence

To verify formula (65), we cancel $\exp(-r)/r$ and the spherical function (or the harmonic tensor)

$$F\big(-k, (2l+2), 2r\big) = \mathrm{const}\left(1 - \frac{\partial}{\partial t}\right)^{l+k}\left[C_k^{l+1}\left(\frac{\mathrm{i}t}{R}\right)R^k\right]\Bigg|_{t=r} \tag{D.1}$$

on both sides, where $R^2 = r^2 - t^2$.

The general form of the Gegenbauer polynomial $C_k^{l+1}(t)$ is not needed. It suffices to know two of its characteristics:

$$C_k^{l+1}(1) = \frac{(2l+1+k)!}{k!(2l+1)!}\,, \tag{D.2}$$

$$C_k^{l+1}(t) = \frac{2^k(k+l)!}{k!l!}\,t^k + \ldots\,. \tag{D.3}$$

We note that the derivative with respect to t translates the 4D harmonic function into a function whose k value has decreased by one while maintaining l:

$$Y_l(\mathbf{x})\frac{\partial}{\partial t}\,C_k^{l+1}\left(\frac{t}{R}\right)R^k = c_{lk}\,Y_l(\mathbf{x})C_{k-1}^{l+1}\left(\frac{t}{R}\right)R^{k-1}\,. \tag{D.4}$$

Equating $r = 0$, pulling out t^k and differentiating with the use of (D.2), we find the constant c_{lk}:

$$c_{lk} = 2l + k + 1\,.$$

Hence, the mth derivative is

$$\frac{\partial^m}{\partial t^m}\,C_k^{l+1}\left(\frac{t}{R}\right)R^k = \frac{(2l+k+1)!}{(2l+k+1-m)!}\,C_{k-1}^{l+1}\left(\frac{t}{R}\right)R^{k-1}\,. \tag{D.5}$$

The function $[C_k^{l+1}(\mathrm{i}t/R)R^k]_{t=r}$ does not contain a power of R only in the leading term; for $R = 0$, therefore, the leading coefficients from (D.3) arise in (D.1) with different k:

$$\left[C_k^{l+1}\left(\frac{\mathrm{i}t}{R}\right)R^k\right]\Bigg|_{t=r} = \frac{2^k(k+l)!}{k!l!}\,(\mathrm{i}r)^k\,. \tag{D.6}$$

On the right-hand side of (D.1), we have

$$\sum_m \frac{(l+k)!(-\mathrm{i})^m}{m!(l+k-m)!}\,\frac{(2l+k+1)!}{(2l+k+1-m)!} \times \frac{2^{k-m}(k-m+l)!}{(k-m)!\,l!}\,(\mathrm{i}r)^{k-m}\,. \tag{D.7}$$

We change k to $(k-m)$ and, pulling out the factor, obtain

$$\frac{(-\mathrm{i})^k(l+k)!(2l+k+1)!}{l!}\sum_m \frac{(-1)^m(2r)^m}{m!(k-m)!}\,\frac{1}{(2l+m+1)!}\,. \tag{D.8}$$

This sum is to be compared with the Gauss function (6):

$$F(-k, 2l+2, 2r) = k!(2l+1)!\sum_m \frac{(-1)^m(2r)^m}{m!(k-m)!}\,\frac{1}{(2l+m+1)!}\,(\mathrm{i}r)^{k-m}\,. \tag{D.9}$$

We arrive at a correspondence and derive the constant. For the Laguerre polynomials, this correspondence becomes

$$L_k^{2l+1}(r) = \frac{\mathrm{i}^k l!}{(l+k)!}\left(\left(1 - \frac{\partial}{\partial t}\right)^k R^k C_k^{l+1}\left(\frac{\mathrm{i}t}{R}\right)\right)\Bigg|_{t=r}, \tag{D.10}$$

where $R^2 = r^2 - t^2$.

We note that relation (D.10) is not known in the theory of special functions [32]. For the perturbation theory, it is useful to recalculate the normalized functions. The norm in the physical space is

$$\int |Y_l|^2\,\mathrm{d}S_2 \int_0^\infty \left[L_k^{2l+1}(r)\right]^2 r^{2l+2}\exp(-2r)\,\mathrm{d}r = N_L^2\,, \tag{D.11}$$

where S_2 is a sphere of unit radius; the harmonic functions are normalized on the 3D sphere:

$$\int |Y_l|^2\,\mathrm{d}S_2\,\frac{2}{\pi}\int_{-1}^1 \left[C_k^{l+1}(r)\right]^2(1-t^2)^{l+1/2}\,\mathrm{d}t = N_C^2\,. \tag{D.12}$$

The relation between the norms is given by

$$N_L = \frac{(n+l)!(n-1)!}{2}\,N_C\,. \tag{D.13}$$

We recall that the radius of the orbit is assumed to be unity. When passing to the radius n, norm (D.11) must be multiplied by $n^{l+3/2}$.

E. Vector properties of the Gegenbauer polynomials

The 4D Laplace equation is simpler than the 3D one. This can already be seen from the structure of harmonic tensor (31). To construct harmonic polynomials, a simple but important property is used. Any scalar function of the form

$$\frac{1}{r}\,f(\tau \pm \mathrm{i}r)\,, \tag{E.1}$$

where $r = \sqrt{x_1^2 + x_2^2 + x_3^2}$ is the 3D radius and τ is the fourth coordinate, is a harmonic function. The verification is obvious:

$$\left(\frac{\partial^2}{\partial\tau^2} + \frac{1}{r}\frac{\partial^2}{\partial r^2}\, r\right)\frac{1}{r}\, f(r \pm \mathrm{i}\tau) = 0\,.$$

This gives rise to a harmonic homogeneous polynomial of degree k in four variables:

$$\frac{1}{2\mathrm{i}r}\left[(\tau + \mathrm{i}r)^{k+1} - (\tau - \mathrm{i}r)^{k+1}\right], \tag{E.2}$$

which Gegenbauer writes in the form

$$\frac{1}{2\mathrm{i}r}\left[(\tau + \mathrm{i}r)^{k+1} - (\tau - \mathrm{i}r)^{k+1}\right] = (r^2 + \tau^2)^k C_k^1\left(\frac{\tau}{r^2 + \tau^2}\right), \tag{E.3}$$

where $C_k^1(z)$ is a nonhomogeneous (but definite-parity) polynomial named after him.

On the surface of a sphere, where $r^2 + \tau^2 = 1$, equality (E.3) leads to a simple form of the harmonic polynomial:

$$C_k^1(\cos\varphi) = \frac{1}{2\mathrm{i}\sin\varphi}\left\{\exp\left[\mathrm{i}\varphi(k+1)\right] - \exp\left[-\mathrm{i}\varphi(k+1)\right]\right\} = \frac{\sin\left[(k+1)\varphi\right]}{\sin\varphi}\,, \tag{E.4}$$

where $\cos\varphi = \tau$, $\sin\varphi = r$, $r^2 + \tau^2 = 1$.

Under rotations of the coordinate system, when the vector $(0, 0, 0, 1)$ goes into a 4-vector $\mathbf{x}'$ and the vector (x_1, x_2, x_3, τ) goes into $\mathbf{y}$, a polynomial arises from the scalar product of unit vectors [55],

$$C_k^1(\mathbf{xy}) = \frac{\sin\left[(k+1)\varphi\right]}{\sin\varphi}\,, \quad \cos\varphi = \mathbf{xy}\,, \quad \mathbf{x}^2 = 1\,, \quad \mathbf{y}^2 = 1\,, \tag{E.5}$$

where the prime at $\mathbf{x}$ is omitted. This is the value of the harmonic function in both variables $\mathbf{x}$ and $\mathbf{y}$ in space transferred to the surface of the 3D sphere. The polynomials $C_k^1(\mathbf{xy})$ play an important role in solving the 4D Laplace equation (and 4D electrostatics): they are similar to the Legendre polynomials in 3D space. We list the properties that are invariant in the SO(4) symmetry.

• Decomposition of the kernel on a sphere:

$$\frac{1}{|\mathbf{x} - \mathbf{y}|^2} = \sum_{k=0}^{\infty} C_k^1(\mathbf{xy})\,. \tag{E.6}$$

• Completeness of the system, i.e., the delta function decomposition:

$$\frac{1}{2\pi^2}\sum_{k=0}^{\infty}(k+1)C_k^1(\mathbf{xy}) = \delta(\mathbf{x} - \mathbf{y})\,. \tag{E.7}$$

• Eigenvalue problem (see the Fock equation (16), now with C_{n-1}^1):

$$\int_{|\mathbf{y}'|=1} \frac{C_k^1(\mathbf{xy}')}{|\mathbf{y} - \mathbf{y}'|^2}\, \mathrm{d}S_{\mathbf{y}'} = \frac{2\pi^2}{k+1}\, C_k^1(\mathbf{xy})\,. \tag{E.8}$$

• An important evaluation:

$$C_k^1(1) = k + 1\,. \tag{E.9}$$

• Orthogonality and normalization:

$$\int_{|\mathbf{y}'|=1} C_k^1(\mathbf{xy}')C_l^1(\mathbf{y}'\mathbf{y})\, \mathrm{d}S_{\mathbf{y}'} = \frac{2\pi^2}{k+1}\, C_k^1(\mathbf{xy})\delta_{kl}\,. \tag{E.10}$$

• Almost obvious addition theorem on the surface of a sphere [56]:

$$\frac{2\pi^2}{k+1}\sum_{l,m} Y_{klm}(\mathbf{x})\, Y_{klm}(\mathbf{y}) = C_k^1(\mathbf{xy})\,. \tag{E.11}$$

• Leading term of the expansion of the polynomial in powers:

$$C_k^1(\mathbf{xy}) = (2\mathbf{xy})^k + \ldots\,. \tag{E.12}$$

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