

Quantum Mechanics of H-Atom from Path Integrals

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Abstract

The quantum mechanical Coulomb problem in two and three dimensions is solved completely in terms of path integrals. We derive the integral representations for the Green's functions in configuration space and recover the wave functions from factorized residues.

I. Introduction

In recent years, the path integral formulation of quantum theory has found increasing applications in field theories of both elementary particles as well as of many-body systems [1]. Its main advantage is that different non-perturbative summations of Feynman diagrams can be systematized without the danger of double counting by merely performing changes of integration variables. Also, constraints can be enforced in a much more straightforward fashion than in Dirac's original Hamiltonian approach [2]. In these applications, the path integral formula is used to manipulate the action to different forms. The new forms are then used to derive alternative sets of Feynman diagrams for the same theory with particle lines and vertices differing from the original ones. Another range of applications lies in the study of quasiclassical tunneling phenomena [3] and the related question of analyticity of field theories in the complex coupling constant plane [4].

The basic difficulty in dealing with path integrals lies in the fact that only a few rather trivial examples can be handled analytically [5]. Most of the standard problems solved in every textbook of quantum mechanics via Schrödinger's differential equation have now up to remained inaccessible to an explicit summation of all fluctuating paths. This is one of the main reasons why the path formulation has not succeeded in entering basic courses quantum mechanics in spite of the great conceptual attractiveness as compared with the operator formulation.

A program of solving the well-known quantum mechanical problems via path integrals has therefore two purposes: One is to gain exercise in handling this somewhat involved mathematical technique with the possibility of using it in field theoretic applications. The

other is to lay the groundwork for an alternative complete treatment of quantum mechanics from the point of view of fluctuating paths.

It is the purpose of this paper to present a complete quantum mechanical treatment of one of the most important quantum mechanical systems, the hydrogen atom. Our final result, the full Green's function in configuration space, has been communicated before in a letter [6]. Here we shall extend the discussion and derive also the wave functions of the system. Moreover, since the basic technical procedure can most easily be explained in two dimensions, we start out with a discussion in this reduced space which, we hope, will lead to an improved appreciation of the simplicity and elegance of the approach.

II. A More Flexible Path Integral Formula

The problem to be solved consists in finding the Green's function (or propagator) which is the probability amplitude of a particle to travel from a position x_a at time t_a to x_b at time t_b directly from Feynman's formula [5]

$$K(x_b, t_b; x_a, t_a) = \int_{x_a}^{x_b} \mathcal{D}\mathbf{x} \exp \left\{ i \int_{t_a}^{t_b} dt \left(\frac{m}{2} \dot{\mathbf{x}}^2 - V(\mathbf{x}) \right) \right\} \quad (1)$$

in a Coulomb potential $V(\mathbf{x}) = e^2/|\mathbf{x}|$. Here, $\int \mathcal{D}\mathbf{x}$ denotes the sum over all fluctuating paths connecting the end points. An alternative definition involves phase space and reads

$$K(x_b, t_b; x_a, t_a) = \int_{x_a}^{x_b} \mathcal{D}\mathbf{x} \int \frac{\mathcal{D}\mathbf{p}}{(2\pi)^3} \exp \left\{ i \int_{t_a}^{t_b} dt \left(\mathbf{p}\dot{\mathbf{x}} - \frac{\mathbf{p}^2}{2m} - V(\mathbf{x}) \right) \right\} \quad (2)$$

which generally reduces to (1) upon integrating out the momentum variables.

Actually, there are cases where (1) and (2) are not the same, for example, if the mass parameter m were not a constant but a function $m(\mathbf{x})$. Then (2) is the correct formula rather than (1) apart from ambiguities in defining the path integration, a fact which is related to the ordering problem in the operator formulation. In our case there is no such difficulty. For our purpose it will be useful to generalize formula (2) by parametrizing the paths $\mathbf{x}(t)$ not in terms of the physical time but use a new parameter s . In general, this may be connected with t via some s dependent functional of the path

$$t = t^s[\mathbf{x}]. \quad (3)$$

We shall focus on a special class of such functionals in which all s dependence comes from a simple differential relation involving a local function of position

$$\frac{dt}{ds} \equiv t'(s) = f(\mathbf{x}(s)) \quad (4)$$

$$t(s_b) = t_b, \quad t(s_a) = t_a.$$

In this case, $f(\mathbf{x}(s))$ modifies the Hamiltonian $H(\mathbf{p}, \mathbf{x}) = \mathbf{p}^2/2m + V(\mathbf{x})$ in a multiplication fashion and formula (2) becomes

$$K(x_b, t_b; x_a, t_a) = \int \mathcal{D}\mathbf{x}(s) \frac{\mathcal{D}\mathbf{p}(s)}{(2\pi)^3} \exp \left\{ i \int_{s_a}^{s_b} ds \left\{ \mathbf{p}(s) \mathbf{x}'(s) - f(\mathbf{x}(s)) H(\mathbf{p}(s), \mathbf{x}(s)) \right\} \right\}. \quad (5)$$

Notice that it is the initial and final times of the path t_a and t_b which are fixed. Therefore, the parameters s_b , s_a are path dependent quantities. We can display explicitly this dependence by incorporating the constraint

$$t_b - t_a = \int_{s_a}^{s_b} ds f(\mathbf{x}(s)) \quad (6)$$

into the integral as follows

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = f(\mathbf{x}_b) \int_{s_a}^{\infty} ds_b \delta \left(t_b - t_a - \int_{s_a}^{s_b} ds f(\mathbf{x}(s)) \right) \\ \times \int_{\mathbf{x}_a}^{\mathbf{x}_b} \mathcal{D}\mathbf{x} \int \frac{\mathcal{D}\mathbf{p}}{(2\pi)^3} \exp \left\{ i \int_{s_a}^{s_b} ds (\mathbf{p}\mathbf{x}' - f(\mathbf{x}) H(\mathbf{p}, \mathbf{x})) \right\}. \quad (7)$$

Upon a Fourier representation of the δ -function this becomes

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = f(\mathbf{x}_b) \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{-iE(t_b-t_a)} \int_{s_a}^{\infty} ds_b \mathcal{H}^E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) \quad (8)$$

where

$$\mathcal{H}^E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \int_{\mathbf{x}_a}^{\mathbf{x}_b} \mathcal{D}\mathbf{x} \frac{\mathcal{D}\mathbf{p}}{(2\pi)^3} \exp \left\{ i \int_{s_a}^{s_b} ds (\mathbf{p}\mathbf{x}' - \mathcal{H}^E(\mathbf{p}, \mathbf{x})) \right\}. \quad (9)$$

is the propagator of an auxiliary quantum problem which is governed by an E dependent pseudo Hamiltonian

$$\mathcal{H}^E(\mathbf{p}, \mathbf{x}) = f(\mathbf{x}) (H(\mathbf{p}, \mathbf{x}) - E) \quad (10)$$

with motion taking place along a pseudo times s . In other words, \mathcal{H}^E is the operator conjugate to the parameter s and generates infinitesimal translations of the system along the s axis.

The energy intergration in equ. (8) suggests continuing the discussion in terms of the Fourier transformed Green's function.

$$K(\mathbf{x}_b, \mathbf{x}_a | E) = \int_{t_a}^{\infty} dt_b e^{iE(t_b-t_a)} K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = f(\mathbf{x}_b) \mathcal{K}^E(\mathbf{x}_b, \mathbf{x}_a | 0). \quad (11)$$

Up to the trivial factor $f(\mathbf{x}_b)$, this coincides with the Fourier transformed propagator of the pseudo Hamiltonian \mathcal{H}^E :

$$\mathcal{K}^E(\mathbf{x}_b, \mathbf{x}_a | \varepsilon) \equiv \int_{s_a}^{\infty} ds_b e^{i\varepsilon(s_b-s_a)} \mathcal{H}^E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) \quad (12)$$

evaluated at zero pseudo energy $\varepsilon = 0$. Notice that in this way we have transmuted the original problem at any energy E to a novel form in which the pseudo energy ε vanishes. All dependence of $K(\mathbf{x}_b, \mathbf{x}_a | E)$ on the physical energy E is due to the explicit E dependence of the auxiliary Hamiltonian (10).

Seen from the Schrödinger point of view this correspondence reflects the simple fact that instead of solving the time independence equation

$$H\psi_E(\mathbf{x}) = E\psi_E(\mathbf{x})$$

we may determine the wave functions from the zero-eigenstates of \mathcal{H}^E :

$$\mathcal{H}^E \psi_E(\mathbf{x}) = f(\mathbf{x}) (H - E) \psi_E(\mathbf{x}) = 0.$$

Actually, equ. (5) may be considered as a special case of an even more general path integral formula

$$\begin{aligned} \mathcal{K}(\mathbf{x}_b, t_b, s_b; \mathbf{x}_a, t_a, s_a) &= \int_{\mathbf{x}_a}^{\mathbf{x}_b} \mathcal{D}\mathbf{x}(s) \frac{\mathcal{D}\mathbf{p}(s)}{(2\pi)^3} \int_{t_a}^{t_b} \mathcal{D}t(s) \frac{\mathcal{D}p_0(s)}{(2\pi)^3} \\ &\times \exp \left\{ i \int_{s_b}^{s_b} ds [\mathbf{p}(s) \mathbf{x}'(s) - p_0(s) t'(s) - f(\mathbf{x}(s)) (H(\mathbf{p}(s), \mathbf{x}(s)) - p_0(s))] \right\} \end{aligned} \quad (13)$$

in which also time and energy are conjugate fluctuating variables which depend on the parameter s . Equ. (5) results after integrating out $\mathcal{D}t$ which enforces energy conservation $p_0(s) \equiv \text{const} = E$ along the path such that all $\mathcal{D}p_0$ integrals can be performed and one obtains

$$\mathcal{K}(\mathbf{x}_b, t_b, s_b; \mathbf{x}_a, t_a, s_a) = \delta \left(t_b - t_a - \int_{s_a}^{s_b} f(\mathbf{x}(s)) ds \right) K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a).$$

Therefore, we see that

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = f(\mathbf{x}_b) \int_{s_a}^{\infty} ds_b \mathcal{K}(\mathbf{x}_b, t_b, s_b; \mathbf{x}_a, t_a, s_a) \quad (14)$$

a connection which generalizes (11).

Notice that the Hamiltonian equations of the auxiliary dynamical problem described by (13) are, with

$$\mathcal{H}(p, x, p_0, t) \equiv f(\mathbf{x}) [H(\mathbf{p}, \mathbf{x}) - p_0],$$

$$\frac{d\mathbf{p}}{ds} = -\frac{\partial \mathcal{H}}{\partial \mathbf{x}} = -\frac{\partial H}{\partial \mathbf{x}} f(\mathbf{x})$$

$$\frac{d\mathbf{x}}{ds} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}} = \frac{\partial H}{\partial \mathbf{p}} f(\mathbf{x})$$

$$\frac{dp_0}{ds} = \frac{\partial \mathcal{H}}{\partial t} = 0$$

$$\frac{dt}{ds} = -\frac{\partial \mathcal{H}}{\partial p_0} = f(\mathbf{x})$$

(15)

and give the correct equations of motion for $\mathbf{x}(t)$, $\mathbf{p}(t)$. Similarly, the Schrödinger equation associated with the auxiliary Hamiltonian $\mathcal{H}(p, x, p_0, t)$

$$f(\mathbf{x}) (H - i \partial_t) \psi(\mathbf{x}, t; s) = i \partial_s \psi(\mathbf{x}, t; s) \quad (16)$$

leads to the correct wave functions $\psi(\mathbf{x}, t; s)$ if the zero pseudo-energy projection (12) is incorporated by requiring

$$i \partial_s \psi(\mathbf{x}, t; s) = 0.$$

III. The Two-Dimensional H-Atom

Consider now the Hamiltonian of the H-Atom in two dimensions

$$H = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r}, \quad r \equiv \sqrt{\mathbf{x}^2}.$$

The canonical transformation

$$\begin{aligned} x_1 &= u_1^2 - u_2^2 & p_1 &= \frac{1}{2\mathbf{u}^2} (u_1 p_{u_1} + u_2 p_{u_2}) \\ x_2 &= 2u_1 u_2 & p_2 &= \frac{1}{2\mathbf{u}^2} (-u_2 p_{u_1} + u_1 p_{u_2}) \end{aligned} \tag{17}$$

of $x_{1,2}, p_{1,2}$ to $u_{1,2}, p_{u_{1,2}}$ [7] brings the Hamiltonian to the form

$$H = \frac{1}{\mathbf{u}^2} \left(\frac{1}{8m} \mathbf{p}_u^2 - e^2 \right). \tag{18}$$

This form suggests going over to the Hamiltonian $\mathcal{H}^E(p_u, u)$ by choosing in (10) the function

$$f(\mathbf{x}) = |\mathbf{x}| = \mathbf{u}^2 \tag{19}$$

In fact,

$$\mathcal{H}^E(p_u, u) = \mathbf{u}^2(H - E) = \frac{1}{8m} \mathbf{p}_u^2 - E\mathbf{u}^2 - e^2. \tag{20}$$

Due to this, the propagator $\mathcal{K}^E(x_b, s_b; x_a, s_a)$ becomes simply that of a harmonic oscillator with a trivial phase factor

$$e^{ie^2(s_b - s_a)}$$

which is the only place where the charge of the H-Atom occurs.

Consider now the transformation of the path integral from \mathbf{x}, \mathbf{p} to \mathbf{u}, \mathbf{p}_u variables. With

$$d\mathbf{x} = 2 \begin{pmatrix} u_1 & u_2 \\ -u_2 & u_1 \end{pmatrix} d\mathbf{u} \tag{21}$$

$$d\mathbf{p}|_{u=\text{fixed}} = \frac{1}{2\mathbf{u}^2} \begin{pmatrix} u_1 & u_2 \\ -u_2 & u_1 \end{pmatrix} d\mathbf{p}_u$$

one has

$$d^2p = \frac{1}{4\mathbf{u}^2} d^2p_u = \frac{1}{4|\mathbf{x}|} d^2p_u \tag{22}$$

$$d^2x = 4\mathbf{u}^2 d^2u = 4|\mathbf{x}| d^2u$$

such that

$$d^2x \frac{d^2p}{(2\pi)^2} = d^2u \frac{d^2p_u}{(2\pi)^2} \tag{23}$$

reflecting the canonical property of the transformation (17). The path integrals in (5) is defined on a grated s axis $s_n = s_a + (s_b - s_a) n/(N + 1)$ as the product of individual integrals over $d^2x_n d^2p_n$, one for every $s = s_n$, except for a single integral over

dp_{N+1} which is not accompanied by a d^2x_{N+1} , since $x_{N+1} = x_b$ is the fixed coordinate of the end point. Therefore, the functional measure does not simply transform like (23) but satisfies.

$$\mathcal{D}x \frac{\mathcal{D}p}{(2\pi)^2} = \frac{1}{4|x_{N+1}|} \mathcal{D}u \frac{\mathcal{D}p_u}{(2\pi)^2}. \tag{24}$$

It is gratifying to note that the factor $1/|x_{N+1}|$ is exactly cancelled by $f(x_b) = |x_{N+1}|$ in the expression (11) such that we may write directly:

$$K(x_b, x_a | E) = \int_{s_a}^{\infty} ds_b \mathcal{K}^E(\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) \tag{25}$$

where

$$\mathcal{K}^E(\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) = \frac{1}{4} e^{ie^2(s_b-s_a)} \int_{\mathbf{u}_a}^{\mathbf{u}_b} \mathcal{D}u \int \frac{\mathcal{D}p_u}{(2\pi)^2} \exp \left\{ i \int_{s_a}^{s_b} ds \left(pu' - \left(\frac{p_u^2}{2\mu} - Eu^2 \right) \right) \right\}. \tag{26}$$

As far as counting the paths is concerned, there is a subtlety due to the fact that the mapping (17) is of the square root type:

$$(x_1 + ix_2) = (u_1 + iu_2)^2. \tag{27}$$

Thus, if one considers all paths in the complex $x = x_1 + ix_2$ plane from x_a to x_b , they will be mapped into two different classes of paths in the u -plane: Those which go from

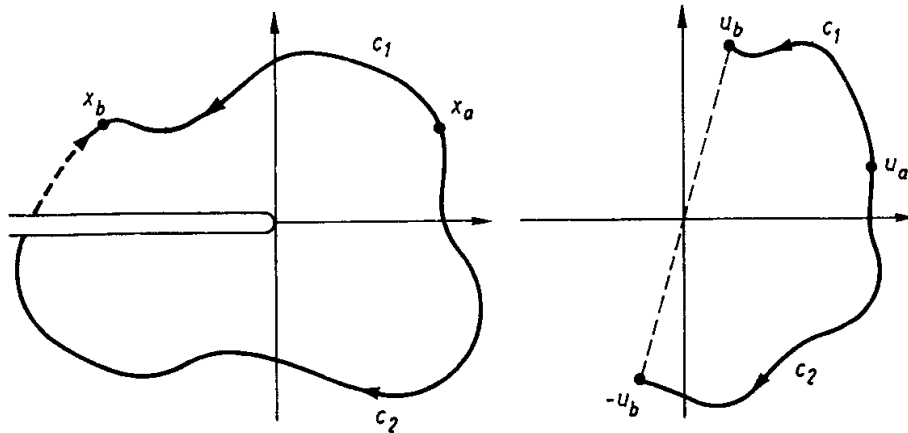


Fig. 1. The correspondence between paths in the x plane from x_a to x_b and those in the u plane. Depending on whether the x path passes an even or odd number of times through the branch cut to the left, the final value u_b is $+\sqrt{x_b}$ or $-\sqrt{x_b}$

u_a to u_b and those going from u_a to $-u_b$. In the cut complex x -plane for the function $u = \sqrt{x^2}$ these are the paths passing an even or odd number of times through the square root cut from $x = 0$ to $x = -\infty$ (see Fig. 1). We may choose the u_a corresponding to the initial x_a to lie on the first sheet (i.e. in the right half u -plane). The final u_b can be in the right as well as the left half plane and all paths on the x -plane go over into all paths from u_a to u_b and those from u_a to $-u_b$. Thus for given the integrand (26) becomes

$$\frac{1}{4} e^{ie^2(s_b-s_a)} (K^E(\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) + K^E(-\mathbf{u}_b, s_b; \mathbf{u}_a, s_a)) \tag{28}$$

where K^E is the usual oscillator Green's function in $\mathbf{u}(s)$ space with mass $\mu = 4m$ and frequency $\omega^2 = -2E/\mu = -E/2m$

$$K^E(\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) = \int \mathcal{D}\mathbf{u} \frac{\mathcal{D}\mathbf{p}_u}{(2\pi)^2} \exp \left\{ i \int_{s_a}^{s_b} ds \left(\mathbf{p}_u \mathbf{u}' - \frac{\mathbf{p}_u^2}{2\mu} + \frac{\mu\omega^2}{2} \mathbf{u}^2 \right) \right\}. \quad (29)$$

This is a Gaussian functional integral which can be performed in the usual fashion with the result [5] ($S \equiv s_b - s_a$)

$$K^E(\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) = \frac{\mu\omega}{2\pi i \sin \omega S} \exp \left\{ i \frac{\mu\omega}{2 \sin \omega S} [(\mathbf{u}_b^2 + \mathbf{u}_a^2) \cos \omega S - 2\mathbf{u}_b \mathbf{u}_a] \right\}.$$

Inserting this into (28) and (25) we find

$$K(\mathbf{x}_b, \mathbf{x}_a | E) = \frac{1}{2} \int_0^\infty dS e^{ie^2 S} F^2(S) \exp \{ -\pi F^2(S) (r_b + r_a) \cos \omega S \} \cos 2\pi F^2(S) u_b u_a \quad (30)$$

where we have used the abbreviation

$$F(S) = \sqrt{\frac{\mu\omega}{2\pi i \sin \omega S}} \quad (31)$$

for the fluctuation factor of the one-dimensional oscillator. We now observe the identity

$$u_b u_a = \sqrt{\frac{1}{2} (x_b x_a + r_b r_a)}$$

and introduce

$$\varrho = e^{-2i\omega S}$$

such that

$$\pi F^2(S) = p_0 \frac{2\sqrt{\varrho}}{1-\varrho} \quad (32)$$

$$e^{ie^2 S} F^2(S) = \frac{2p_0}{\pi} \frac{\varrho^{-(v+(1/2))}}{1-\varrho}$$

where p_0 stands for

$$p_0 = \sqrt{-2mE} = 2m\omega = \frac{\mu\omega}{2} \quad (33)$$

$$v = \frac{e^2}{2\omega}. \quad (34)$$

Then the propagator becomes, after a rotation of the contour of integration in the S plane, such that it runs along the positive imaginary axis and $\varrho = e^{-2i\omega S}$ covers the unit interval:

$$K(\mathbf{x}_b, \mathbf{x}_a | E) = -i \frac{m}{\pi} \int_0^1 d\varrho \frac{\varrho^{-(v+(1/2))}}{1-\varrho} \cos \left(2p_0 \frac{\sqrt{2\varrho}}{1-\varrho} \sqrt{x_b x_a + r_b r_a} \right) e^{-p_0(r_a+r_b)(1+\varrho)/(1-\varrho)}. \quad (35)$$

This integral representation of the Coulomb Green's function in configuration space can be used to determine all wave functions of the system. Rather than doing this, however,

we find it more convenient to begin with a special decomposition of the oscillator Green's function (30) and use the resulting expansion in formulas (25), (26). For this we recall the well-known summation formula [8] for Hermite polynomials.

$$e^{-x^2-y^2} \sum_{n=0}^{\infty} \frac{z^n}{2^n n!} H_n(x) H_n(y) = \frac{1}{\sqrt{1-z^2}} e^{-(1/(1-z^2))(x^2+y^2-2xyz)} \quad (36)$$

with the identification

$$x = \sqrt{\mu\omega} u_{a1,2} \quad y = \sqrt{\mu\omega} u_{b1,2} \quad z = e^{-i\omega S} \quad (37)$$

(1 and 2 refers to the two components of \mathbf{u} vector) we can write (29) in the form, valid for $E < 0$:

$$K^E(\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) = \sum_{n_1, n_2=0}^{\infty} \psi_{n_1, n_2}(\mathbf{u}_b) \psi_{n_1, n_2}^*(\mathbf{u}_a) e^{-i\omega(n_1+n_2+1)(s_b-s_a)} \quad (38)$$

where

$$\psi_{n_1 n_2}(\mathbf{u}) = \sqrt{\frac{\mu\omega}{\pi}} \frac{1}{2^{(n_1+n_2)/2} \sqrt{n_1! n_2!}} e^{-\mu\omega \mathbf{u}^2/2} H_{n_1}(\sqrt{\mu\omega} u_1) H_{n_2}(\sqrt{\mu\omega} u_2) \quad (39)$$

are the oscillator wave functions. The symmetrization has the effect of eliminating odd values of $n_1 + n_2$, such that we can introduce the principal quantum number $n = 0, 1, 2, \dots$ with $n_1 + n_2 = 2n$. Performing now the integral in (25) for $E < 0$, the propagator becomes

$$K(\mathbf{x}_b, \mathbf{x}_a | E) = \frac{1}{2} \sum_{n_1, n_2}^{\infty} \frac{i}{e^2 - (2n+1)\omega} \psi_{n_1, n_2}(\mathbf{u}_b) \psi_{n_1, n_2}^*(\mathbf{u}_a) \quad (40)$$

$$= -\frac{m}{p_0^2} \sum_{n=0}^{\infty} \frac{i}{1 - \frac{\nu}{n + \frac{1}{2}}} \frac{p_0}{2\left(n + \frac{1}{2}\right)} \sum_{n_1+n_2=2n} \psi_{n_1, n_2}(\mathbf{u}_b) \psi_{n_1, n_2}^*(\mathbf{u}_a). \quad (41)$$

Here we used again

$$p_0 \equiv \sqrt{-2mE} = 2m\omega = \frac{\mu\omega}{2}$$

and introduced, in addition,

$$\nu \equiv \frac{e^2}{2\omega} = \sqrt{-\frac{me^4}{2E}}.$$

The mapping of energy into the complex ν plane is displayed in Fig. 2. Notice that the oscillator wave functions multiplied by the factor $\sqrt{p_0/(2n+1)}$

$$\psi_{n_1, n_2}^H(\mathbf{x}) = \sqrt{\frac{p_0}{2n+1}} \psi_{n_1, n_2}(\mathbf{u}) \quad (42)$$

are orthonormal under the scalar product $\int d^2x = \int dr r d\varphi$. This follows from the virial theorem according to which $\mu\omega^2 \mathbf{u}^2/2 = p_0 \mathbf{u}^2 \omega$ has expectation values $\omega(n+1/2)$ and therefore

$$\int dr r d\varphi \frac{p_0}{2n+1} |\psi_{n_1, n_2}(\mathbf{u})|^2 = \int d^2u \frac{p_0 \mathbf{u}^2}{n + \frac{1}{2}} |\psi_{n_1, n_2}(\mathbf{u})|^2 = 1 \quad (43)$$

where it should be remembered that the full x space integral transforms by (17) only into half of the u space integral.

It is now curious to observe in which way the linearly rising oscillator spectrum is converted into the spectrum of the H atom. Looking at (41) we see that the Green's function has poles at the energies

$$E = E_n = -\frac{me^4}{2\left(n + \frac{1}{2}\right)^2}. \tag{44}$$

In the neighborhood of these poles, the factor $-i \frac{m}{p_0^2} \left(1 - \frac{\nu}{n + \frac{1}{2}}\right)^{-1}$ behaves as

$i/E - E_n$ such that the factorized residues $\psi_{n_1 n_2}^H = \sqrt{p_0/2n + 1} \psi_{n_1 n_2}$ represent the properly normalized wave functions of the H atom.

These correspond to the solution of the Schrödinger equation for the bound two-dimensional H-atom. They can be brought to a more familiar form by using a wellknown

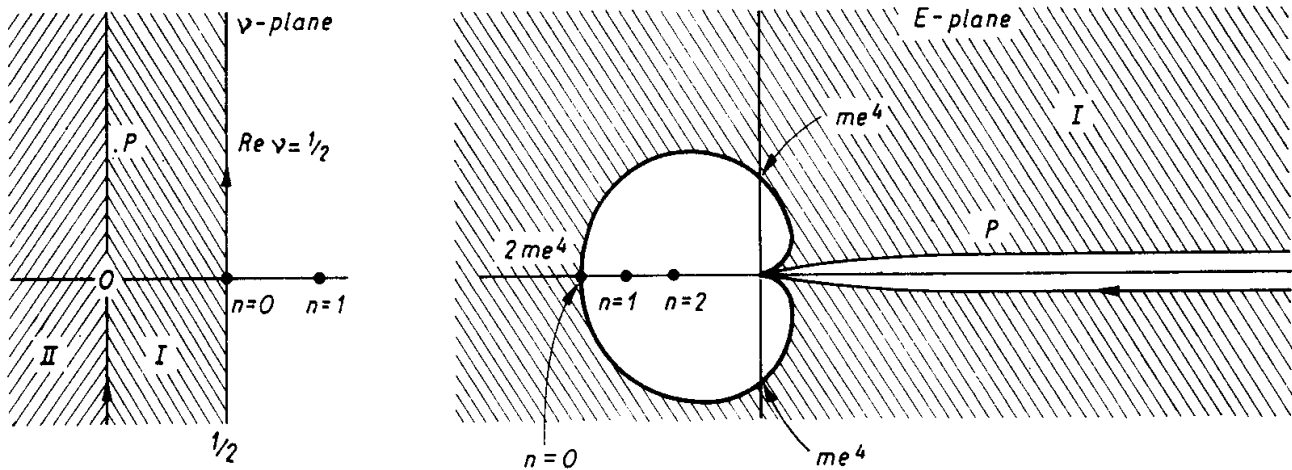


Fig. 2. The correspondence between ν and E planes ($\nu = \sqrt{-me^4/2E}$). The imaginary axis in the ν plane is mapped into the branch cut of the E plane. The left half plane II goes over into the full second sheet of the E plane. The strip I, maps into the physical sheet except for the "cardioid" region of $|E| < 2me^4 \sin^2(\varphi/2)$ which includes all bound states. Finally, the right-hand part of the ν plane, $\text{Re } \nu > 1/2$ has its image inside the cardioid

identity between Hermite and Langerre polynomials (see App. A)

$$\begin{aligned} & \frac{e^{-e}}{2^n \sqrt{(n+l)! (n-l)!}} H_{n+l} \left(\sqrt{e} \cos \frac{\theta}{2} \right) H_{n-l} \left(\sqrt{e} \sin \frac{\theta}{2} \right) \\ &= \sum_{M=-n}^n e^{iM\pi} d_{Ml}^n \left(-\frac{\pi}{2} \right) \sqrt{\frac{(n-|M|)!}{(n+|M|)!}} e^{-e} e^{iM\theta} (2e)^{|M|} L_{n-|M|}^{2|M|}(e) \end{aligned} \tag{45}$$

$$\begin{aligned} &= \sqrt{\frac{(n-|M|)!}{(n+|M|)!}} e^{-e} e^{iM\theta} (2e)^{|M|} L_{n-|M|}^{2|M|}(2e) \\ &= \sum_{l=0}^n e^{iM\pi} d_{Ml}^n \left(-\frac{\pi}{2} \right) \frac{e^{-e}}{2^n \sqrt{(n+l)! (n-l)!}} H_{n+l} \left(\sqrt{e} \cos \frac{\theta}{2} \right) H_{n-l} \left(\sqrt{e} \sin \frac{\theta}{2} \right) \end{aligned} \tag{46}$$

where $l \equiv (n_1 - n_2)/2$ and $d_{Ml}^n(\beta)$ are the usual representation functions of rotations. Thus we can express again the residue in the form:

$$\sum_{n_1+n_2=2n} \psi_{n_1 n_2}(\mathbf{u}_b) \psi_{n_1 n_2}^*(\mathbf{u}_a) = \sum_{M=-n}^n \psi_{nM}(\mathbf{x}_b) \psi_{nM}^*(\mathbf{x}_a) \quad (47)$$

with spherical wave functions

$$\psi_{nM}(x) = \frac{e^{iM\varphi}}{\sqrt{2\pi}} R_{nM}(r) = \frac{p_0}{\sqrt{n + \frac{1}{2}}} \sqrt{\frac{(n - |M|)!}{(n + |M|)!}} e^{-p_0 r} (2p_0 r)^{|M|} \frac{e^{iM\varphi}}{\sqrt{2\pi}} L_{n-|M|}^{2|M|}(2p_0 r). \quad (48)$$

If we Fourier transform the result, the Green's function can also be written as

$$K(\mathbf{p}_b, \mathbf{p}_a | E) = -\frac{m}{p_0^2} \sum_{n,M} \frac{i}{1 - \frac{\nu}{n + \frac{1}{2}}} \psi_{nM}(\mathbf{p}_b) \psi_{nM}^*(\mathbf{p}_a) \quad (49)$$

where the momentum space wave functions have the form

$$\psi_{nM}(\mathbf{p}) = \frac{e^{iM\varphi_p}}{\sqrt{2\pi}} \int_0^\infty dr r J_M(pr) R_{nM}(r) = (-i)^M \frac{2^{3/2} p_0^2}{(p^2 + p_0^2)^{3/2}} Y_{nM}(\xi) \quad (50)$$

in which $Y_{nM}(\xi)$ are the spherical harmonics evaluated on the three-dimensional unit sphere defined by Fock's stereographic projection

$$\xi_0 = \frac{p^2 - p_0^2}{p^2 + p_0^2}, \quad \xi = \frac{2pp_0}{p^2 + p_0^2}, \quad \xi^2 = 1. \quad (51)$$

Therefore the Green's function has the alternative representation

$$K(\mathbf{p}_b, \mathbf{p}_a | E) = -\frac{im}{p_0^2} \frac{2^3 p_0^4}{(p_a^2 + p_0^2)^{3/2} (p_b^2 + p_0^2)^{3/2}} \Gamma(\xi_b, \xi_a) \quad (52)$$

with

$$\Gamma(\xi_b, \xi_a) = \sum_{n,M} \frac{1}{1 - \frac{\nu}{n + \frac{1}{2}}} Y_{nM}(\xi_b) Y_{nM}^*(\xi_a) \quad (53)$$

being the analogue of the Green's function of the potential equation employed by SCHWINGER [9] in the case of the three-dimensional H atom [10]. It is useful to remove those parts of (53) which are singular for $\xi_b = \xi_a$ by expanding

$$\frac{1}{1 - \frac{\nu}{n + \frac{1}{2}}} = 1 + \frac{\nu}{n + \frac{1}{2}} + \frac{\nu^2}{\left(n + \frac{1}{2}\right)\left(n + \frac{1}{2} - \nu\right)} \quad (54)$$

and taking into account the completeness relation

$$\sum_{n,M} Y_{nM}(\xi_b) Y_{nM}^*(\xi_a) = \delta(\xi_b - \xi_a) \quad (55)$$

and the well-known summation formula

$$\sum_{n=0}^{\infty} \frac{1}{n + \frac{1}{2}} \sum_{M=-n}^n Y_{nM}(\xi_b) Y_{nM}^*(\xi_a) = \frac{1}{2\pi} \frac{1}{\sqrt{(\xi_b - \xi_a)^2}}. \quad (56)$$

Then I may be rewritten as

$$\Gamma(\xi_b, \xi_a) = \delta(\xi_b - \xi_a) + \frac{\nu}{2\pi \sqrt{(\xi_b - \xi_a)^2}} + \Gamma'(\xi_b, \xi_a) \quad (57)$$

with

$$\begin{aligned} \Gamma'(\xi_b, \xi_a) &= \nu^2 \sum_{n=0}^{\infty} \frac{1}{\left(n + \frac{1}{2}\right) \left(n + \frac{1}{2} - \nu\right)} \sum_{M=-n}^n Y_{nM}(\xi_b) Y_{nM}^*(\xi_a) \\ &= \frac{\nu^2}{2\pi} \sum_{n=0}^{\infty} \frac{1}{n + \frac{1}{2} - \nu} P_n(\xi_b \cdot \xi_a). \end{aligned} \quad (58)$$

This expression has the advantage of converging for all

$$\cos \chi \equiv \xi_a \cdot \xi_b \in (-1, 1) \quad (59)$$

as long as ν avoids the poles. This integral may be viewed as a degenerate form of the standard ‘‘Lehmann ellipse’’ of partial wave expansions [12] whose area shrinks to zero due to the long range of the Coulomb force.

The angle χ in Fock space depends on initial and final momenta p_a, p_b and the energy as follows:

$$\begin{aligned} \cos \chi = \xi_a \cdot \xi_b &= 1 - \frac{2p_0^2}{(\mathbf{p}_b^2 + p_0^2)(\mathbf{p}_a^2 + p_0^2)} (\mathbf{p}_b - \mathbf{p}_a)^2 \\ &= 1 + \frac{E}{\left(E - \frac{\mathbf{p}_b^2}{2m}\right) \left(E - \frac{\mathbf{p}_a^2}{2m}\right)} \frac{(\mathbf{p}_b - \mathbf{p}_a)^2}{m}. \end{aligned} \quad (60)$$

We have gone to expression (58) since it is the convenient starting point for a calculation of the continuum wave functions. Before doing this, let us first clarify the mapping from the energy plane to the complex $\cos \chi$ plane. For $E > 0$, $\cos \chi$ can become > 1 or < 1 . For definiteness, suppose that $p_a^2 > p_b^2 > p_0^2 > 0$. Then, as E is continued from negative values to above the continuum cut, $\cos \chi$ passes the point $\cos \chi = 1$. At $2mE = p_a^2$, $\cos \chi$ becomes positive infinite. For $p_a^2 < 2mE < p_b^2$, $\cos \chi$ comes in from $-\infty$, runs up to a maximum value

$$\cos \chi_{\max} = -1 - \frac{8p_a p_b}{(|\mathbf{p}_b| - |\mathbf{p}_a|)^2} \sin^2 \frac{\theta}{2} < -1 \quad (61)$$

where θ is the true two-dimensional scattering angle defined by:

$$\mathbf{p}_a \cdot \mathbf{p}_b = \cos \theta |\mathbf{p}_a| |\mathbf{p}_b| \quad (62)$$

and then turns back to $-\infty$. For $E > p_b^2$, finally, the curve returns from ∞ to $\cos \chi = 1$ (see Fig. 3). Due to the asymptotic behaviour, as $\text{Re } n \rightarrow \infty$ [11],

$$|P_n(\cos \chi)| < \frac{1}{\sqrt{n}} e^{|\text{Im}n \text{Re}\chi + \text{Re}n \text{Im}\chi|} f(\cos \chi) \tag{63}$$

the representation (58) does not converge as E runs along this contour. This can be improved by performing a Sommerfeld-Watson transformation on the sum

$$\Gamma''(\xi_b, \xi_a) = -\frac{\nu^2}{4\pi i} \int_C \frac{dn}{\sin \pi n} \frac{1}{n + \frac{1}{2} - \nu} P_n(-\cos \chi) \tag{64}$$

where the contour C in the complex n plane comes in from $+\infty - i\varepsilon$ runs along the real axis to the left, passing underneath all bound state poles at $n = 0, 1, 2, \dots$, and returns again to $\infty + i\varepsilon$ above the real axis. Since the integral behaves for $\text{Re } \chi \in (0, \pi)$

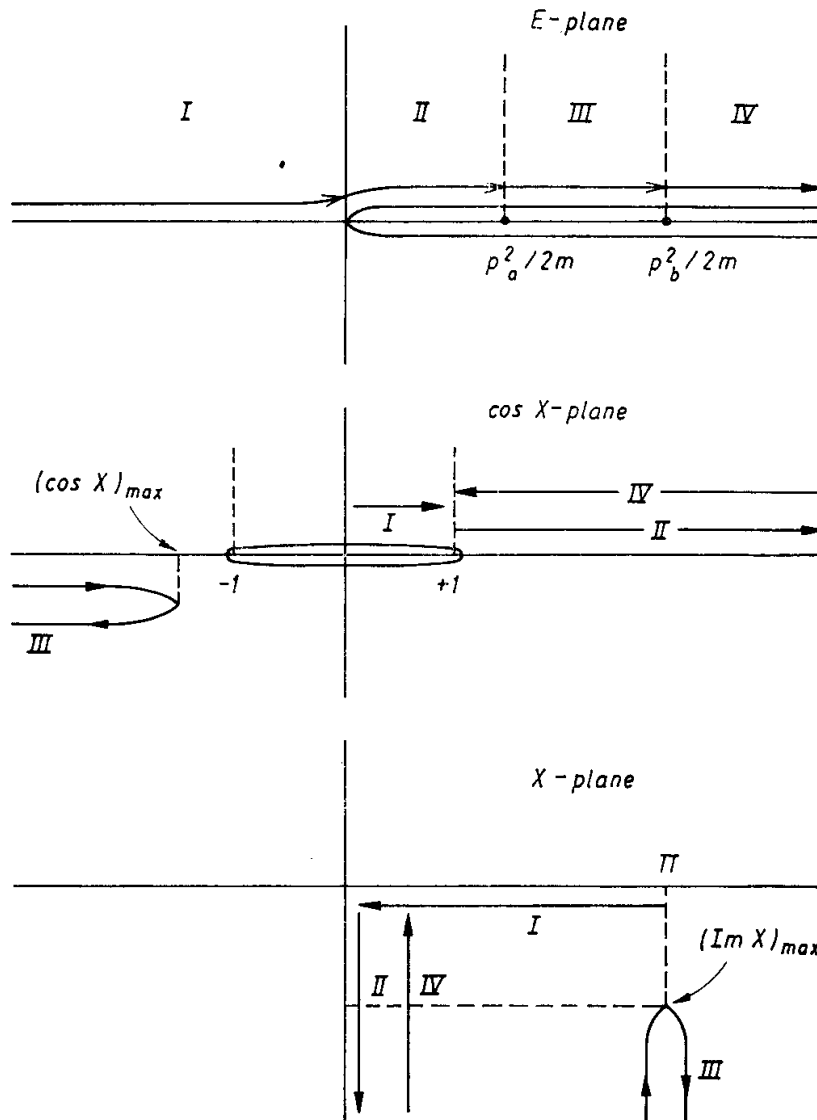


Fig. 3. The movement of the scattering angle χ as a function of the energy variable E for $P_a^2 < P_b^2$, say. As E is continued from $-\infty$ to ∞ along the portions I \rightarrow VI of the real axis, $\cos \chi$ and χ itself move as shown in the layer parts of the figure. The "Lehmann ellipse" consists of the interval $-1 < \cos \chi < 1$

as [12]

$$\left| \frac{P_{i\lambda-(1/2)}(-\cos \chi)}{\sin \pi \left(i\lambda - \frac{1}{2} \right)} \right| < \frac{1}{\sqrt{i\lambda - \frac{1}{2}}} \frac{e^{|-1/2\text{Im}\chi + (\pi - \text{Re}\chi)\lambda|}}{e^{\pi|\lambda|}} f(\cos \chi) \quad (65)$$

the contour may be opened up to run along $n = -\frac{1}{2} + i\lambda + \varepsilon$, $\lambda \in (-\infty, \infty)$:

$$\Gamma'(\xi_b, \xi_a) = \frac{\nu^2}{4\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\text{ch } \pi\lambda} \frac{1}{i\lambda - \nu + \varepsilon} P_{i\lambda-(1/2)}(-\cos \chi) \quad (66)$$

the circle at infinity can be neglected, and the final integral is convergent. (see again Fig. 3 for the range of χ).

We can now determine the continuum wave functions by factorizing the residues into the separate functions of ξ_b and ξ_a . For this it is convenient to introduce

$$\tilde{p}_0 = ip_0 = \sqrt{2mE} \quad (67)$$

as well as the analytically continued version of the Fock coordinates:

$$\tilde{\xi}_0 = \frac{\mathbf{p}^2 + \tilde{p}_0^2}{\mathbf{p}^2 - \tilde{p}_0^2}, \quad \xi = \frac{2\mathbf{p}\tilde{p}_0}{\mathbf{p}^2 - \tilde{p}_0^2}, \quad \tilde{\xi}_0^2 - \xi^2 = 1 \quad (68)$$

which now lie on a unit hyperboloid instead of a sphere. Both branches of the hyperboloid are needed; the upper for $\mathbf{p}^2 > \tilde{p}_0^2$ and the lower for $\mathbf{p}^2 < \tilde{p}_0^2$.

In terms of \tilde{p}_0 we have

$$\cos \chi = \tilde{\xi}_a \cdot \tilde{\xi}_b = 1 + \frac{2\tilde{p}_0^2}{(\mathbf{p}_b^2 - \tilde{p}_0^2)(\mathbf{p}_a^2 - \tilde{p}_0^2)} (\mathbf{p}_b - \mathbf{p}_a)^2 \quad (69)$$

such that the parts II, IV of the $\cos \chi$ region in Fig. 3 correspond to $\tilde{\xi}_b, \tilde{\xi}_a$ lying on the same branch, while for III they lie on opposite branches of the hyperboloid. Considering these different possibilities, we can expand $P_{i\lambda-(1/2)}(-\cos \chi)$ and rewrite $\Gamma'(\xi_b, \xi_a)$ as (see App. C)

$$\begin{aligned} \Gamma'(\xi_b, \xi_a) &= \frac{\nu^2}{4\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\text{ch } \pi\lambda} \frac{e^{-\pi\lambda}}{i\lambda - \nu} \sum_{M=-\infty}^{\infty} (-1)^M \frac{\Gamma\left(i\lambda - M + \frac{1}{2}\right)}{\Gamma\left(i\lambda + M + \frac{1}{2}\right)} \\ &\quad \times e^{iM(\varphi_b - \varphi_a)} \left(P_{i\lambda-(1/2)}^M(\tilde{\xi}_{0b}) \theta(\tilde{\xi}_{0b}) + (-1)^M P_{i\lambda-(1/2)}^M(\tilde{\xi}_{0b}) \theta(-\tilde{\xi}_{0b}) \right) \\ &\quad \times \left(P_{i\lambda-(1/2)}^M(\tilde{\xi}_{0a}) \theta(\tilde{\xi}_{0a}) + (-1)^M P_{i\lambda-(1/2)}^M(\tilde{\xi}_{0a}) \theta(-\tilde{\xi}_{0a}) \right)^* \end{aligned} \quad (70)$$

where the θ functions select the proper branches on the unit hyperboloids. Using (58) and (50) we can now identify the continuum wave functions in momentum space:

$$\begin{aligned} \psi_{i\lambda-(1/2)}(\mathbf{p}) &= \frac{2^{1/2}\tilde{p}_0^2}{(\mathbf{p}^2 - \tilde{p}_0^2)^{3/2}} \frac{\sqrt{\lambda} e^{-\pi\lambda/2}}{\pi} \left| \Gamma\left(i\lambda - M + \frac{1}{2}\right) \right| \\ &\quad \times e^{iM\varphi_p} \left[P_{i\lambda-(1/2)}(\tilde{\xi}_0) \theta(\tilde{\xi}_0) + (-1)^M P_{i\lambda-(1/2)}(\tilde{\xi}_0) \theta(-\tilde{\xi}_0) \right]. \end{aligned} \quad (71)$$

In \mathbf{x} -space, these take the well-known form (see App. D) [10]

$$\begin{aligned} \psi_{i\lambda-(1/2),M}(\mathbf{x}) &= \frac{(-i)^M}{\pi} \sqrt{\frac{me^2}{\lambda}} \frac{1}{\sqrt{\lambda}} e^{-i(\pi/2)(i\lambda-(1/2))} \frac{\left| \Gamma\left(i\lambda + M + \frac{1}{2}\right) \right|}{\Gamma(2M + 1)} \\ &\times e^{iM\varphi} \frac{1}{\sqrt{|\mathbf{x}|}} M_{i\lambda,M} \left(\frac{2me^2}{i\lambda} |\mathbf{x}| \right) \end{aligned} \quad (72)$$

when expressed in terms of Whittaker functions $M_{i\lambda,M}(\mathbf{x})$.

For completeness, we note that there is certainly the analogue of SCHWINGER'S [9] integral representation of the expansion (53) which can be obtained from the well-known formula

$$\frac{1}{2\pi} \frac{1}{\sqrt{(1-\varrho)^2 + \varrho(\xi_b - \xi_a)^2}} \sum_{n=0}^{\infty} \frac{\varrho^n}{n + \frac{1}{2}} \sum_M Y_{nM}(\xi_b) Y_{nM}^*(\xi_a). \quad (73)$$

Inserting this into equ. (53) one finds

$$\begin{aligned} \Gamma(\xi_b, \xi_a) &= \delta(\xi_b - \xi_a) + \frac{\nu}{2\pi} \frac{1}{|\xi_b - \xi_a|} + \frac{\nu^2}{2\pi} \int_0^1 d\varrho \varrho^{-\nu-(1/2)} \frac{1}{\sqrt{(1-\varrho)^2 + \varrho(\xi_b - \xi_a)^2}} \\ &= \delta(\xi_b - \xi_a) + \frac{\nu}{2\pi} \int_0^1 d\varrho \varrho^{-\nu} \frac{d}{d\varrho} \frac{\varrho^{1/2}}{\sqrt{(1-\varrho)^2 + \varrho(\xi_b - \xi_a)^2}}. \end{aligned} \quad (74)$$

From this it is easy to derive the scattering amplitude (see App. E):

$$T(\mathbf{p}_b, \mathbf{p}_a) = \frac{e^2}{|\mathbf{p}_b - \mathbf{p}_a|} e^{-\nu \log(4\tilde{p}_0^2 / (p_b^2 - p_a^2))}. \quad (75)$$

IV. The Three-Dimensional H-Atom

Consider now the three-dimensional problem. Just as before, we can write the Fourier transformed amplitude as

$$K(\mathbf{x}_b, \mathbf{x}_a | E) = |\mathbf{x}_b| \int_{s_a}^{\infty} ds_b \mathcal{K}^E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) \quad (76)$$

where \mathcal{K}^E is the auxiliary propagator given by the path integral

$$\mathcal{K}^E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = e^{ie^2(s_b - s_a)} \int \mathcal{D}\mathbf{x} \frac{\mathcal{D}\mathbf{p}}{(2\pi)^3} \exp \left\{ i \int_{s_a}^{s_b} ds \left(\mathbf{p}\mathbf{x}' - \frac{r\mathbf{p}^2}{2m} - rE \right) \right\}. \quad (77)$$

Again we shall transform the exponent into Gaussian form. For this we need a generalization of the change of variables (17) to "square root coordinates". A transformation of this type does indeed exist: It has been used a long time ago in astronomy [13] for the purpose of regularizing the Kepler problem. There one chooses new variables

u_1, u_2, u_3, u_4 to satisfy

$$\begin{aligned} x_1 &= 2(u_1u_3 + u_2u_4) \\ x_2 &= -2(u_1u_2 - u_3u_4) \\ x_3 &= -u_1^2 + u_2^2 + u_3^2 - u_4^2 \end{aligned} \quad (78)$$

thereby embedding the three-dimensional physical space into a four-dimensional auxiliary space. Because of

$$r \equiv u^2 = u_1^2 + u_2^2 + u_3^2 + u_4^2 \quad (79)$$

the transformation maps spherical shells of x space into those of u space. We now see an important difference with respect to the two dimensional case: There the mapping of points in x space into those in u space was ambiguous only as far as the sign of the image $u = \pm\sqrt{|x|} \hat{x}$ was concerned. Here we have a whole continuous set of possible image points. The freedom in this mapping may be parametrized by using an angular variable $\alpha \in [0, 4\pi)$ in addition to the polar coordinates (r, θ, φ) of (x_1, x_2, x_3) and writing

$$\begin{aligned} u_1 &= \sqrt{r} \sin \frac{\theta}{2} \cos \frac{\alpha + \varphi}{2} \\ u_2 &= \sqrt{r} \cos \frac{\theta}{2} \sin \frac{\alpha - \varphi}{2} \\ u_3 &= \sqrt{r} \cos \frac{\theta}{2} \cos \frac{\alpha - \varphi}{2} \\ u_4 &= \sqrt{r} \sin \frac{\theta}{2} \sin \frac{\alpha + \varphi}{2}. \end{aligned} \quad (80)$$

If we use this mapping of points to transform paths in x space into paths in u space we have the freedom of choosing an arbitrary angle $\alpha(s)$ for every point along the path. Thus the mapping can be made unique only by specifying a whole path in the redundant angle $\alpha(s)$:

$$x(s) \rightarrow u(x(s), \alpha(s)). \quad (81)$$

At the initial pseudo time we may choose $\alpha(s_a) = \alpha_a = 0$, for simplicity. The variable $\alpha(s)$ is cyclic such that it remains in the strip $\alpha(s) \in [0, 4\pi)$. Since the point 0 is identical with 4π there may be n jumps down from 4π to zero or \bar{n} jumps in the opposite direction at arbitrary intermediate places (see Fig. 4). Instead of distinguishing the paths $\alpha(s)$ according to their jumps, it is more economical to picture them continuously in an extended zone scheme (see Fig. 4) in which the final $\alpha(s)$ is not α_b but $\alpha_b + 4\pi(n - \bar{n})$ with arbitrary integers n, \bar{n} . In this way the mapping of paths can be made unique by adding such a continuous path $\alpha(s)$ in the extended zone scheme as a functional label

$$x(s) \xrightarrow{\alpha(s)} u(x(s)). \quad (82)$$

We are now confronted with the problem in rewriting the path integral in x space into one in u space in such a way that the freedom in the choice of $\alpha(s)$ becomes irrelevant. Let us recall that a very similar problem arises in path integrals of gauge fields. Also there the description in terms of potentials A_μ is ambiguous up to an arbitrary function of a space-time. Paths in the functional space of fields map into those

of potentials with the same type of ambiguity. Due to this, there are infinitely many ways of rewriting the path integral of gauge fields, depending on what dynamics one chooses to attribute to the physically irrelevant content in A_μ .

For the problem at hand we choose to take advantage of the same freedom. We shall introduce some trivial dynamics depending on the movement along the irrelevant path $\alpha(s)$. Actually, this angle is not the most symmetric variable to express the addi-

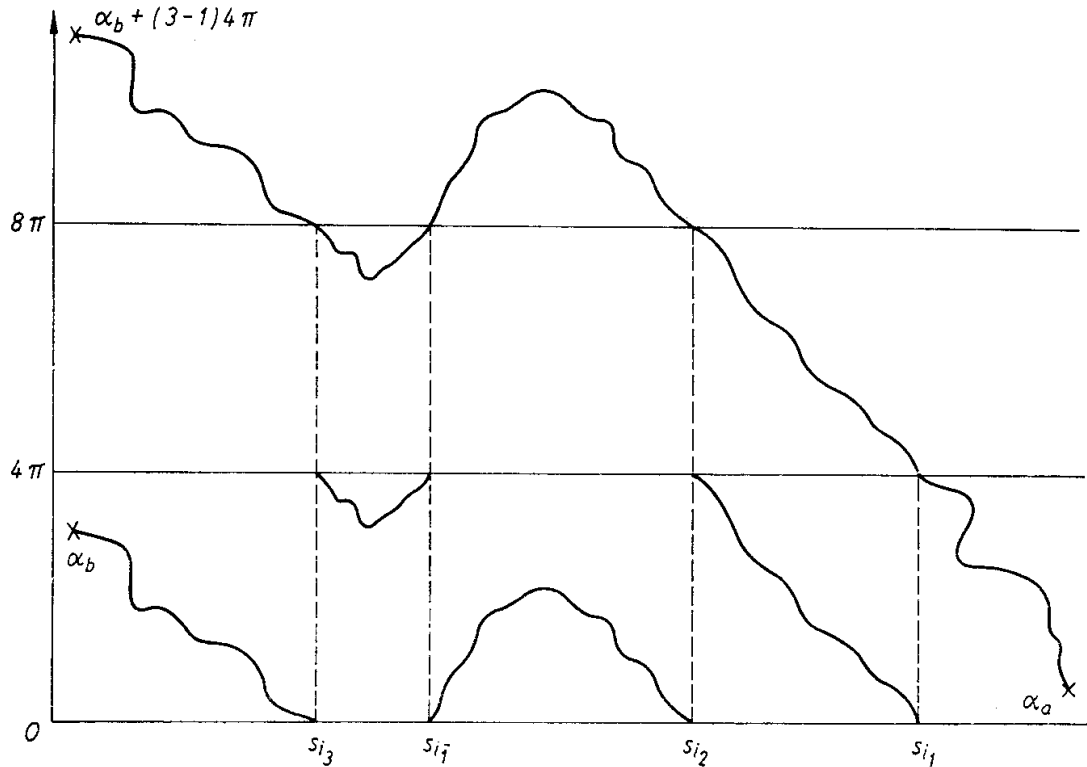


Fig. 4. A curve with 3 jumps from 4π to zero (at $S_{i_{1,2,3}}$) and 1 jump from 0 to 4π (at S_{i_1}) can be drawn as a smooth curve in the extended zone scheme arriving at $\alpha_b^{(n,\bar{n})} = \alpha_b + (n - \bar{n}) 4\pi$ where n and \bar{n} count the numbers of jumps down and up, respectively

tional dynamics. A better way is based on a fictitious dummy fourth component x_4 in addition to the three space components \mathbf{x} to describe $\alpha(s)$. In fact, due to the four-component nature of u , there exists quite a natural choice also for such a fourth component for \mathbf{x} .

Consider the differential change of dx as u proceeds along an arbitrary path. From (78) we find

$$\begin{pmatrix} dx_1 \\ dx_2 \\ dx_3 \end{pmatrix} = 2 \begin{pmatrix} u_3 & u_4 & u_1 & u_2 \\ -u_2 & -u_1 & u_4 & u_3 \\ -u_1 & u_2 & u_3 & -u_4 \end{pmatrix} \begin{pmatrix} du_1 \\ du_2 \\ du_3 \\ du_4 \end{pmatrix}. \tag{83}$$

For symmetry reasons this equation calls for a completion by means of a fourth row.

$$dx_4 = 2(u_4 \quad -u_3 \quad u_2 \quad -u_1) \begin{pmatrix} du_1 \\ du_2 \\ du_3 \\ du_4 \end{pmatrix}. \tag{84}$$

This permits a unique definition of the dummy coordinate x_4 as

$$x_4(s) = 2 \int_{s_a}^s ds (u_4 u_1' - u_3 u_2' + u_2 u_3' - u_1 u_4') \quad (85)$$

where we have chosen $x_4(s_a) = 0$ for the initial point of the path. The relation with $\alpha(s)$ can be obtained by inserting (80) as

$$x_4(s) = - \int_{s_a}^s ds (\alpha' - \cos \theta \varphi') r(s). \quad (86)$$

In this way we have established a one to one correspondence between paths in x space and those in u space. The freedom in $\alpha(s)$ may now be characterized by the motion of the path along the fourth axis in x space.

We now have to search for some trivial dynamics for this additional motion in such a way that the path integral remains unchanged and becomes soluble. Since we work in the phase space formulation, we shall search for convenient path integrals involving also a momentum variable p_4 associated with x_4 . If there is no dynamics at all, the basic canonical relation is expressed by

$$\int_{x_4(s_a)}^{x_4(s_b)} \mathcal{D}x_4 \frac{\mathcal{D}p_4}{(2\pi)} e^{i \int_{s_a}^{s_b} ds p_4 x_4'} = \delta(x_4(s_b) - x_4(s_a)). \quad (87)$$

This corresponds to the propagator of a particle moving through the dummy phase space x_4, p_4 with vanishing Hamiltonian. One may integrate in $x_4(s_b)$ and obtain the identity

$$\int_{-\infty}^{\infty} dx_4(s_b) \int_{x_4(s_a)}^{x_4(s_b)} \mathcal{D}x_4 \frac{\mathcal{D}p_4}{(2\pi)} e^{i \int_{s_a}^{s_b} ds p_4 x_4'} = 1. \quad (88)$$

Certainly, such a factor can be multiplied with formula (77) thereby expressing again the original dynamical problem in the extended x_μ, p_μ phase space. Actually, there exists a great variety of such extensions. For example, we may use a free particle Hamiltonian

$$H^{\text{ext}} = \frac{p_4^2}{2m}. \quad (89)$$

In this case the integral

$$\int \mathcal{D}x_4 \frac{\mathcal{D}p_4}{(2\pi)} e^{i \int_{s_a}^{s_b} ds (p_4 x_4' - (p_4^2/2m))} \quad (90)$$

becomes the propagator

$$\frac{1}{\sqrt{2\pi i \hbar (s_b - s_a) / m}} e^{(i/2)(m/(s_b - s_a))(x_{4b} - x_{4a})^2} \quad (91)$$

such that (88) holds again with $p x_4' - H^{\text{ext}}$ in the exponent. Moreover, we can multiply with H^{ext} an arbitrary s dependent factor $\varrho(s)$ and still find

$$\int_{-\infty}^{\infty} dx_4(s_b) \int_{x_4(s_a)}^{x_4(s_b)} \mathcal{D}x_4 \frac{\mathcal{D}p_4}{(2\pi)} \exp \left\{ i \int_{s_a}^{s_b} ds \left(p_4 x_4' - \varrho(s) \frac{p_4^2}{2m} \right) \right\} = 1. \quad (92)$$

This can easily be seen by going to the grated version (thereby dropping the inessential subscript 4 and using $\varepsilon \equiv (s_b - s_a)/(N + 1)$):

$$\int_{-\infty}^{\infty} dx_{N+1} \left(\prod_{n=1}^N \int_{-\infty}^{\infty} dx_n \right) \left(\prod_{n=1}^{N+1} \int_{-\infty}^{\infty} \frac{dp_n}{2\pi} \right) \exp \left\{ i \sum_{n=1}^{N+1} \left(p_n(x_n - x_{n-1}) - \varepsilon \varrho(s_n) \frac{p_n^2}{2m} \right) \right\}. \quad (93)$$

Performing successively the integrals over $\int_{-\infty}^{\infty} dx_n$ and then over $dp_n/2\pi$ gives

$$\begin{aligned} & \int_{-\infty}^{\infty} dx_{N+1} \prod_{n=1}^{N+1} \int_{-\infty}^{\infty} \frac{dp_n}{2\pi} \prod_{n=1}^N 2\pi \delta(p_{n+1} - p_n) e^{i(p_{N+1}x_{N+1} - p_1x_0)} \exp \left\{ -i \sum_{n=1}^{N+1} \varepsilon \varrho(s_n) \frac{p_n^2}{2m} \right\} \\ &= \int_{-\infty}^{\infty} dx_{N+1} \int_{-\infty}^{\infty} \frac{dp_{N+1}}{2\pi} e^{ip_{N+1}(x_{N+1} - x_0)} \exp \left\{ -i \left(\sum_{n=1}^{N+1} \varepsilon \varrho(s_n) \right) \frac{p_{N+1}^2}{2m} \right\} = 1. \end{aligned} \quad (94)$$

The basic idea which renders the path integral (77) soluble consists in taking the last identity (92) as the additional dynamics in the extended part of phase space $x_\mu, p_\mu (\mu = 1, \dots, 4)$. This yields the new representation for the Green's function

$$\begin{aligned} \mathcal{N}^E(x_b, s_b; x_a, s_a) &= \int_{-\infty}^{\infty} dx_4(s_b) e^{ie^2(s_b - s_a)} \int_{x_a}^{x_b} \mathcal{D}x \mathcal{D}x_4 \int \frac{\mathcal{D}^3p}{(2\pi)^3} \frac{\mathcal{D}p_4}{(2\pi)} \\ &\quad \times \exp \left\{ i \int_{s_a}^{s_b} ds \left(p x' + p_4 x_4' - \frac{r p^2}{2m} - \frac{\varrho(s) p_4^2}{2m} - rE \right) \right\}. \end{aligned} \quad (95)$$

Here the function $\varrho(s)$ is completely arbitrary. In particular it may depend explicitly on the spatial coordinates $x(s)$ which were not involved in formula (92). It is this freedom which allows for an immediate transformation to the four-dimensional oscillator form. All we have to do is choose $\varrho(s) = r(s)$.

Let us see that this really achieves our goal. Consider the matrix of (83), (84):

$$A = 2 \begin{pmatrix} u_3 & u_4 & u_1 & u_2 \\ -u_2 & -u_1 & u_4 & u_3 \\ -u_1 & u_2 & u_3 & -u_4 \\ u_4 & -u_3 & u_2 & -u_1 \end{pmatrix}. \quad (96)$$

It is obvious that A is orthogonal up to a factor

$$A^{-1} = \frac{1}{4u^2} A^T = \frac{1}{4r} A^T \quad (97)$$

such that we obtain directly

$$\det A = \sqrt{\det A \cdot \det A^T} = \sqrt{\det 4r} = 16r^2$$

and

$$d^4x = 16r^2 d^4u. \quad (98)$$

We now introduce momenta canonical to the coordinate u by

$$p = \frac{1}{4r} A p_u.$$

It can be verified that the transformation $x \rightarrow u, p \rightarrow p_u$ is really canonical. With the volume elements in momentum space being related as

$$\frac{d^4 p}{(2\pi)^4} \Big|_{u=\text{const}} = \frac{1}{16r^2} \frac{d^4 p_u}{(2\pi)^4}$$

we verify the measure in the phase space to remain invariant.

$$d^4 x \frac{d^4 p}{(2\pi)^4} = d^4 u \frac{d^4 p_u}{(2\pi)^4} \tag{99}$$

as it should. Also, $p \cdot x' + p_4 x_4'$ goes over into $p_u \cdot u_a'$ and

$$p^2 + p_4^2 = \frac{1}{16r^2} p_u^T A^T A p_u = \frac{1}{4r} p_u^2.$$

We now see that formula (95) with $\varrho(s) = r(s)$ does indeed turn into the Green's function of a harmonic oscillator.

$$\mathcal{K}^E(x_b, s_b; x_a, s_a) = \frac{1}{16r_b^2} \int_{-\infty}^{\infty} dx_4(s_b) e^{ie^2(s_b-s_a)} \int_{u_a}^{u_b} \mathcal{D}u \frac{\mathcal{D}p_u}{(2\pi)^4} \exp \left\{ i \int_{s_a}^{s_b} ds \left(p_u u' - \frac{p_u^2}{8m} - u^2 E \right) \right\} \tag{100}$$

where the factor in front has its origin in there being one more p_u than u integration, just as in the derivation of equ. (24). Inserting (100) into (76) we obtain

$$K(x_b, x_a | E) = \frac{1}{16r_b} \int_{s_a}^{\infty} ds_b e^{ie^2(s_b-s_a)} \int_{-\infty}^{\infty} dx_4(s_b) K(u_b(x_b, \alpha_b), s_b; u_a(x_a, \alpha_a), s_a) \tag{101}$$

with

$$K(u_b(x_b, \alpha_b), s_b; u_a(x_a, \alpha_a), s_a) = \int \mathcal{D}u \frac{\mathcal{D}p_u}{(2\pi)^4} \exp \left\{ i \int_{s_a}^{s_b} ds \left(p_u u' - \frac{p_u^2}{2\mu} + \frac{1}{2} \omega^2 \mu u^2 \right) \right\} \tag{102}$$

where μ and ω^2 are defined as before: $\mu = 4m, \omega^2 = \sqrt{-E/2m}$.

Notice that this expression is not yet identical with the usual Green's function $K(u_b, s_b; u_a, s_a)$ of the four dimensional harmonic oscillator due to the explicit occurrence of the cyclic variable α . As discussed before, for a given final point $u_b(x_b, \alpha_b)$ there are infinitely many final angles α_b modulo 4π which have to be summed in order to account for *all* paths, with any number of jumps, going from u_a to u_b . Consequently, when expressed in terms of the angular variable α the oscillator Green's function consists of an infinite sum of amplitudes (102)

$$K(u_b, s_b; u_a, s_a) = \sum_{n=-\infty}^{\infty} K(u_b(x_b, \alpha_b + 4\pi n), s_b; u_a(x_a, \alpha_a), s_a). \tag{103}$$

If we now remember the relation (86) we see that $dx_4(s_b)$ in (101) can be rewritten as an integral over α_b :

$$\int_{-\infty}^{\infty} \frac{dx_4(s_b)}{r} \Big|_{x=\text{fixed}} = \int_{-\infty}^{\infty} d\alpha_b. \tag{104}$$

If we split this according to

$$\int_{-\infty}^{\infty} d\alpha_b = \int_0^{4\pi} \alpha_b \sum_{\alpha_b \rightarrow \alpha_b + 2\pi n} \tag{105}$$

we find the final result

$$K(\mathbf{x}_b, \mathbf{x}_a | E) = \int_0^{\infty} ds_b e^{ie^2(s_b - s_a)} \left(\frac{1}{4} \int_{s_a}^{2\pi} d\alpha_b \right) \frac{1}{4} (K(u_b, s_b; u_a, s_a) + K(-u_b, s_b; u_a, s_a)) \tag{106}$$

where we have used the fact that the shift $\alpha_b \rightarrow \alpha_b + 2\pi$ amounts to a reflection in u_b . In this way we have reached a symmetrized form thereby establishing the closest possible connection with the two-dimensional formulas (25), (26), (28).

The explicit form of the four-dimensional oscillator Green's function is

$$K(u_b, s_b; u_a, s_a) = F^4(s) \exp \{ -\pi F^2(S) [\cos \omega S (u_b^2 + u_a^2) - 2u_b \cdot u_a] \} \tag{107}$$

where $F(S)$ denotes again the fluctuation factor (31).

Therefore (106) becomes

$$K(\mathbf{x}_b, \mathbf{x}_a | E) = \int_0^{\infty} dS e^{ie^2 S} \frac{1}{4} F^4(S) e^{-\pi F^2(S) \cos \omega S (r_b + r_a)} \frac{1}{2} \int_0^{4\pi} d\alpha_b e^{2\pi F^2(S) u_b \cdot u_a}. \tag{108}$$

The integral over $d\alpha_b$ can be done by observing that

$$u_b u_a = \sqrt{\frac{1}{2} (\mathbf{x}_b \mathbf{x}_a + r_b r_a)} \cos (\alpha_b - \alpha_a - \beta) / 2$$

where β depends only on $\theta_b, \theta_a, \varphi_b, \varphi_a$ *) such that

$$\frac{1}{2} \int_0^{4\pi} d\alpha_b e^{2\pi F^2(S) u_b \cdot u_a} = 2\pi I_0 \left(2\pi F^2(S) \sqrt{\frac{1}{2} (\mathbf{x}_b \mathbf{x}_a + r_b r_a)} \right).$$

We now proceed just as in the two dimensional case: We rotate the contour of integration to run from $S = 0$ to $S = i\infty$, let $\varrho = e^{-2i\omega S} \in (0, 1)$ and use (32) to find

$$K(\mathbf{x}_b, \mathbf{x}_a | E) = -i \frac{mp_0}{\pi} \int_0^1 d\varrho \frac{e^{-\nu}}{(1-\varrho)^2} I_0 \left(2p_0 \frac{\sqrt{2\varrho}}{1-\varrho} \sqrt{\mathbf{x}_b \mathbf{x}_a + r_b r_a} \right) e^{-p_0(1+e/(1-\varrho))(r_b+r_a)} \tag{109}$$

as the integral representation of the Green's function of the three dimensional Coulomb problem.

*) $\cos \frac{\beta}{2} = \cos \left(\frac{\theta_b - \theta_a}{2} \right) \cos \left(\frac{\varphi_b - \varphi_a}{2} \right) / \left[\frac{1}{2} (1 + \cos \theta_b \cos \theta_a + \sin \theta_b \sin \theta_a \cos (\varphi_b - \varphi_a)) \right]^{1/2}$

For the explicit determination of the wave functions we shall again resort to the direct expansion of the oscillator Green's functions which reads for $\omega^2 > 0$, $E < 0$:

$$K^E(u_b, s_b; u_a, s_a) = \frac{1}{8} e^{ie^2(s_b-s_a)^2} \int_0^{2\pi} d\alpha_b \sum_{\substack{n_1 n_2 \\ n_3 n_4}} \psi_{n_1 n_2}(u_b) \psi_{n_3 n_4}^*(u_a) e^{-i\omega(n_1+n_2+n_3+n_4+2)(s_b-s_a)} \quad (110)$$

where $\psi_{n_1 n_2}$ are the 4 dimensional oscillator wave functions

$$\psi_{n_1 n_2}(u) = \frac{\mu\omega}{\pi} \frac{e^{-\mu\omega u^2/2}}{2^{(\sum n_i)/2}} \prod_{i=1}^4 \frac{1}{\sqrt{n_i!}} H_{n_i}(\sqrt{\mu\omega} u_i). \quad (111)$$

Due to the final symmetrization in u_b , only states with an even total number of oscillator quanta contribute. We may therefore introduce a principal quantum number $n = 1, 2, 3, \dots$ as

$$n_1 + n_2 + n_3 + n_4 = 2(n - 1). \quad (112)$$

Such that (106) becomes

$$K(x_b, x_a | E) = \frac{1}{8} \sum_{n=0}^{\infty} \frac{1}{e^2 - 2n\omega} \sum_{\substack{\sum n_i = 2(n-1) \\ n_i = 1, 2, 3, \dots}} \int_0^{2\pi} d\alpha_b \psi_{n_1 n_2}(u_b) \psi_{n_3 n_4}^*(u_a) \quad (113)$$

$$= -\frac{m}{p_0^2} \sum_{n=1}^{\infty} \frac{i}{1 - \frac{v}{n}} \sum_{\substack{\sum n_i = 2(n-1) \\ n_i = 1, 2, 3, \dots}} \frac{p_0}{8n} \int_0^{2\pi} d\alpha_b \psi_{n_1 n_2}(u_b) \psi_{n_3 n_4}^*(u_a). \quad (114)$$

This from displays poles at E_n of the form

$$\frac{i}{E - E_n} \sum_{\sum n_i = 2(n-1)} \int_0^{2\pi} d\alpha_b \sqrt{\frac{p_0}{8n}} \psi_{n_1 n_2}(u_b) \sqrt{\frac{p_0}{8n}} \psi_{n_3 n_4}^*(u_a). \quad (115)$$

The residues are the atomic bound state wave functions with unconventional quantum numbers. In order to establish contact with standard forms we use $p_0|_{\text{pole}} = me^2/n$ to rewrite the residue as (see App. F)

$$\sum_{m=0}^{n-1} \sum_{\substack{n-|m| \\ n_1' = n - n_2' - |m| - 1}} \psi_{n_1' n_2' m}(x_b) \psi_{n_1' n_2' m}^*(x_a) \quad (116)$$

where

$$\begin{aligned} \psi_{n_1' n_2' m}(x) &= \frac{1}{\sqrt{\pi n}} \sqrt{p_0^3} \sqrt{\frac{n_1'! n_2'!}{(n_1' + |m|)! (n_2' - |m|)!}} e^{im\varphi} (p_0 r \sin \theta)^{|m|} \\ &\quad - e^{-p_0 r} L_{n_1'}^{|m|} \left(2p_0 r \cos^2 \frac{\theta}{2} \right) L_{n_2'}^{|m|} \left(2p_0 r \sin^2 \frac{\theta}{2} \right) \end{aligned} \quad (117)$$

are the parabolic wave functions used on the description of the Stark effect. For fixed m , the quantum numbers n_1' , n_2' take all integers from 0 to $n - |m|$ subject to the condition

$$n_1' + n_2' + |m| + 1 = n. \quad (118)$$

These wave functions in parabolic coordinates are related to the spherical wave functions by Clebsch-Gordon coefficients [16] (see App. G)

$$\psi_{n_1' n_2' m}(\mathbf{x}) = \sum_{l=m}^{n-1} (-1)^{n_1'} \sqrt{2l+1} \begin{pmatrix} \frac{n-1}{2} & \frac{n-1}{2} & l \\ \frac{2m-n+2n_1'+1}{2} & \frac{n-2n_1'-1}{2} & -m \end{pmatrix} \times \psi_{nlm}(r, \theta, \varphi). \quad (119)$$

Then the residue (116) can be written as

$$\sum_{\pm m=1}^{n-1} \sum_{n_1'=0}^{n-|m|} \psi_{n_1' n_2' m}(\mathbf{x}_b) \psi_{n_1' n_2' m}^*(\mathbf{x}_a) = \sum_{l=m}^{n-1} \sum_{m=-l}^l \psi_{nlm}(\mathbf{x}_b) \psi_{nlm}^*(\mathbf{x}_a) \quad (120)$$

where $\psi_{nlm}(\mathbf{x})$ are the usual spherical wave functions of H atom:

$$\psi_{nlm}(\mathbf{x}) = \frac{1}{\sqrt{\pi n}} \sqrt{p_0^3} \sqrt{\frac{(2l+1)(l-|m|)!(n-l-1)!}{(l+|m|)!(n+l)!}} e^{im\varphi} P_l^m(\cos \theta) \times (2p_0 r)^l e^{-p_0 r} L_{n-l-1}^{2l+1}(2p_0 r). \quad (121)$$

For the continuum states (i.e. for $E > 0$) the sum (120) diverges and a resummation is necessary which can be continued analytically, just as in the two-dimensional case. For this purpose let us again Fourier transform the Green's function of (116). The wave functions (120) become (normalized to $\int d^3x |\psi(\mathbf{x})|^2 = 1$):

$$\psi_{nlm}(\mathbf{p}) = \frac{2}{\sqrt{p_0^3}} \sqrt{\frac{n}{\pi}} \sqrt{\frac{(2l+1)(l-|m|)!(n-l-1)!}{(l+|m|)!(n+l)!}} \times e^{im\varphi_p} P_l^m(\cos \theta_p) \frac{1}{\left(\frac{p^2}{p_0^2} + 1\right)^2} \left(\frac{\frac{2|p|}{p_0}}{\frac{p^2}{p_0^2} + 1}\right)^2 T_{n-l-1}^{l+(1/2)}\left(\frac{\frac{p^2}{p_0^2} - 1}{\frac{p^2}{p_0^2} + 1}\right) \quad (122)$$

where $T_m^n(x)$ are Gegenbauer polynomials (see App. B). They can be written in terms of the spherical harmonics evaluated on the four dimensional unit sphere [16]:

$$\psi_{nlm}(\mathbf{p}) = \frac{4p_0^{5/2}}{(p^2 + p_0^2)^2} y_{nlm}(\xi) \quad (123)$$

with ξ being defined by Fock's stereographic projection:

$$\xi_0 = \frac{p^2 - p_0^2}{p^2 + p_0^2}, \quad \xi = \frac{2pp_0}{p^2 - p_0^2}, \quad \xi^2 = 1. \quad (124)$$

Thus the Green's function has the form

$$K(\mathbf{p}_b, \mathbf{p}_a | E) = -\frac{im}{p_0^2} \frac{2^4 p_0^5}{(p_b^2 + p_0^2)(p_a^2 + p_0^2)} \Gamma(\xi_b, \xi_a) \quad (125)$$

where

$$\Gamma(\xi_b, \xi_a) = \sum_{n,l,m} \frac{1}{1 - \frac{\nu}{n}} Y_{nlm}(\xi_b) Y_{nlm}^*(\xi_a) \quad (126)$$

is the Green's function of the four dimensional potential equation of SCHWINGER [8]. Using again the expression (53), the completeness relation analogous to (55) and the sum rule

$$\sum_{n=1}^{\infty} \frac{1}{n} \sum_{l,m} Y_{nlm}(\xi_b) Y_{nlm}^*(\xi_a) = \frac{1}{2\pi^2(\xi_b - \xi_a)^2} \tag{127}$$

we find

$$\Gamma(\xi_b, \xi_a) = \delta(\xi_b - \xi_a) + \frac{\nu}{2\pi^2(\xi_b - \xi_a)^2} + \Gamma'(\xi_b, \xi_a) \tag{128}$$

with

$$\Gamma'(\xi_b, \xi_a) = \nu^2 \sum_{n=1}^{\infty} \frac{1}{n(n-\nu)} \sum_{l,m} Y_{nlm}(\xi_b) Y_{nlm}^*(\xi_a) = \frac{\nu^2}{2\pi^2} \sum_n \frac{1}{n-\nu} \frac{\sin n\chi}{\sin \chi}. \tag{129}$$

which converges for all real $\chi \in (0, \pi)$. The angle χ is defined as before (see (59)). We can now perform a Sommerfeld-Watson transform of (129) and obtain

$$\Gamma'(\xi_b, \xi_a) = \frac{\nu^2}{(2\pi)^2} \int \frac{d\lambda}{\text{sh } \pi\lambda} e^{\pi\lambda} \frac{1}{i\lambda - \nu} \frac{\text{sh } \lambda\chi}{\sin \chi}. \tag{130}$$

This representation converges for all complex ν to the left of the line $\text{Re } \nu = 1$. The continuum wave functions may be obtained by factorizing the integrand into separate functions of ξ_b, ξ_a which are defined in four dimensions just as in (68). Setting $\chi = i\tilde{\chi}$ we can use a well-known addition relation for "hyperbolic harmonics"

$$\frac{\text{sh } \lambda\chi}{\sin \chi} = -\frac{1}{\lambda} \frac{d(\cos \lambda\tilde{\chi})}{d \text{ch } \tilde{\chi}} = \frac{2\pi^2}{\lambda} \sum_{l,m} H_{i\lambda lm}^{(4)}(\xi_b) H_{i\lambda lm}^{(4)*}(\xi_a) \tag{131}$$

If ξ_b, ξ_a lie on opposite branches of the hyperboloid. For $\xi_0 > 1$, the $H^{(4)}$ functions are given explicitly as [10]

$$\begin{aligned} H_{i\lambda lm}^{(4)}(\tilde{\xi}) &= \left\{ \frac{\sqrt{2}}{\sqrt{\lambda \text{sh } \pi\lambda}} \frac{1}{\Gamma(l + i\lambda + 1)} (\text{sh } \theta)^l \left(\frac{d}{d \text{ch } \theta} \right)^{l+1} \cos \lambda\theta \right\} Y_{lm}(\hat{\xi}) \\ &= \sqrt{\frac{2}{n}} \frac{1}{\sqrt{\lambda^2(\lambda^2 + 1) \dots (\lambda^2 + l^2)}} (\text{sh } \theta)^l \left(\frac{d}{d \text{ch } \theta} \right)^{l+1} \cos \lambda\theta Y_{lm}(\hat{\xi}) \end{aligned} \tag{132}$$

where we have decomposed the four vector $\tilde{\xi}$ as

$$\tilde{\xi} \equiv (\text{ch } \theta, \hat{\xi} \text{sh } \theta), \quad \text{ch } \theta \equiv \xi_0, \quad \hat{\xi} \text{sh } \theta = \xi$$

such that the four dimensional scattering angle is directly

$$\chi = \theta_b - \theta_a.$$

For $\xi_0 < -1$ we replace [10] $H_{i\lambda lm}^{(4)}(\xi_0, \xi) \rightarrow e^{\pi\lambda} H_{i\lambda lm}^{(4)}(-\xi_0, \xi)$. The continuum wave functions in momentum space can then be identified from (129) and (131) as:

$$\psi_{i\lambda, lm}(\mathbf{p}) = \frac{4\tilde{p}_0^{5/2}}{(\mathbf{p}^2 - p_0^2)^2} \frac{e^{i\pi\lambda/2}}{\sqrt{2 \text{sh } \pi\lambda}} \{ \theta(\xi_0) H_{i\lambda lm}^{(4)}(\xi_0, \xi) - \theta(-\xi_0) e^{-\pi\lambda} H_{i\lambda lm}^{(4)}(-\xi_0, \xi) \}. \tag{133}$$

The x space wave functions are then obtained by Fourier transforming (133) (see App. H):

$$\begin{aligned} \psi_{i\lambda lm}(\mathbf{x}) = & \frac{(-1)^{l+m}}{\sqrt{2\tilde{p}_0 r}} \sqrt{\frac{(2l+1)(n-|m|)!}{4\pi \cdot (n+|m|)!}} \frac{\Gamma(l+i\lambda+1)}{(2l+1)!} \\ & \times e^{im\varphi} P_l^m(\cos\theta) e^{\pi\lambda/2} M_{-i\lambda, l+1/2}(2\tilde{p}_0 r). \end{aligned} \quad (134)$$

Both bound and continuous wave functions are included in a single integral representation which is obtained by summing up the Green's function (126) via the relation [9]

$$\frac{1}{2\pi^2} \frac{1}{(1-\varrho)^2 + \varrho(\xi_b - \xi_a)^2} = \sum_{n=1}^{\infty} \varrho^{n-1} \frac{1}{n} \sum_{l,m} Y_{nlm}(\xi_b) Y_{nlm}^*(\xi_a) \quad (135)$$

and employing the trivial identity

$$\frac{1}{n-\nu} = \int_0^1 d\varrho \varrho^{-\nu} \varrho^{n-1}, \quad \nu < 1. \quad (136)$$

Equ. (126) can be written as

$$\Gamma(\xi_b, \xi_a) = \delta(\xi_b - \xi_a) + \frac{\nu}{2\pi^2} \int_0^1 d\varrho \varrho^{-\nu} \frac{d}{d\varrho} \frac{\varrho}{(1-\varrho)^2 + \varrho(\xi_b - \xi_a)^2}. \quad (137)$$

Then, after inserting the values of ξ_b, ξ_a vectors in terms of $\mathbf{p}_b, \mathbf{p}_a$, the Green's function (125) becomes

$$\begin{aligned} & K(\mathbf{p}_b, \mathbf{p}_a | E) \\ & = \frac{i}{E-T} \delta^{(3)}(\mathbf{p}_b - \mathbf{p}_a) - \frac{e^2}{2\pi^2} \frac{i}{E-T_b} \\ & \quad \times \left[\int_0^1 d\varrho \varrho^{-\nu} \frac{d}{d\varrho} \frac{\varrho}{(\mathbf{p}_b - \mathbf{p}_a)^2 \varrho - \frac{m}{2E} (E-T_b)(E-T_a)(1-\varrho^2)} \right] \frac{i}{E-T_a}. \end{aligned} \quad (138)$$

with $E = \tilde{p}_0^2/2m$ and $T = \mathbf{p}^2/2m$. In order to find the scattering amplitude, we look at the asymptotic form of (138) which is determined from the neighborhood of the energy shell

$$E - T_a \sim 0, \quad E - T_b \sim 0$$

as well as the $\varrho \approx 0$ part of the integral. Thus (138) becomes

$$K(\mathbf{p}_b, \mathbf{p}_a | E) \sim G^0(\mathbf{p}_a | E) \frac{1}{4\pi^2 m} T(\mathbf{p}_b, \mathbf{p}_a | E) G^0(\mathbf{p}_a | E) \quad (139)$$

where $G^0(\mathbf{p} | E)$'s are the free particle Green's functions modified by the long-range Coulomb interaction:

$$G^0(\mathbf{p} | E) = \frac{i}{E-T} (e^{-\nu \ln(E-T/4E)}) \sqrt{\frac{-2\pi i \nu}{e^{-2\pi i \nu} - 1}} \quad (140)$$

and $T(\mathbf{p}_b, \mathbf{p}_a | E)$ is the scattering amplitude

$$T(\mathbf{p}_b, \mathbf{p}_a | E) = \frac{2me^2}{(\mathbf{p}_b - \mathbf{p}_a)^2} e^{-\nu \log(4\bar{p}_0^2/(\mathbf{p}_b - \mathbf{p}_a)^2)}. \quad (141)$$

Thus the Coulomb problem in three dimensions has been solved completely.

V. Conclusion

On the basis of a few simple manipulations it has been possible to bring the path integral for a Coulomb potential to a gaussian form. We hope that our methods developed along the way may be applicable in other circumstances permitting a transformation of complicated looking problems into simple ones.

The H atom has fascinated researchers for many years due to the great beauty and high symmetry [16] of its dynamics. It is interesting to discover while performing the sum over its fluctuating paths that it also furnishes a simple example of a gauge theory in u space which becomes soluble by choosing a specific gauge in which the dynamics reduces to that of a four-dimensional harmonic oscillator.

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Appendix A: Laguerre versus Hermite Polynomials

Since $H_{n_1}(\sqrt{\varrho} \cos \varphi/2) H_{2n-n_1}(\sqrt{\varrho} \sin \varphi/2)$ and $L_{n-|M|}^{2|M|}(\varrho)$ are independent polynomials of n^{th} order, there is certainly an expansion

$$H_{n_1}(\sqrt{\varrho} \cos \varphi/2) H_{2n-n_1}(\sqrt{\varrho} \sin \varphi/2) = \sum_{M=-n}^n L_{n-|M|}^{2|M|}(\varrho) e^{iM\varphi} (2\varrho)^{|M|} B_M^{nn_1}. \quad (\text{A.1})$$

Collecting on both sides coefficients of the same power in ϱ gives

$$B_M^{nn_1} = (n - |M|)! (-i)^{n_1} \sum_{k=0}^{n-M} (-)^{n_1+k} \binom{n_1}{k} \binom{2n - n_1}{n - M - k}. \quad (\text{A.2})$$

This result can be derived more algebraically by noticing that $H_n(u_1)$ can be generated by

$$\left(u_1 - \frac{\partial}{\partial u_1}\right)^n e^{-u_1^2/2} = H_n(u_1) e^{-u_1^2/2} \quad (\text{A.3})$$

while

$$\varrho^{|M|} e^{iM\varphi} L_{n-|M|}^{2|M|}(u^2) \text{ arises from} \quad (\text{A.4})$$

$$\begin{aligned} & \frac{1}{\sqrt{(n + |M|)! (n + |M|)!}} \left(\frac{u_1 + iu_2}{\sqrt{2}} - \frac{\partial}{\partial(u_1 + iu_2)/\sqrt{2}} \right)^{n+|M|} \\ & \times \left(\frac{u_1 - iu_2}{\sqrt{2}} - \frac{\partial}{\partial(u_1 + iu_2)/\sqrt{2}} \right)^{n-|M|} e^{-(u_1^2 + u_2^2)/2} \\ & = (u^2)^{|M|} e^{iM\varphi} L_{n-|M|}^{2|M|}(2u^2) e^{-(u_1^2 + u_2^2)/2}. \end{aligned}$$

But

$$\begin{aligned} \frac{u_1 + iu_2}{\sqrt{2}} - \frac{\partial}{\partial(u_1 - iu_2)/\sqrt{2}} &= \frac{1}{\sqrt{2}} \left[\left(u_1 - \frac{\partial}{\partial u_1}\right) + i \left(u_2 - \frac{\partial}{\partial u_2}\right) \right] \\ \frac{u_1 - iu_2}{\sqrt{2}} - \frac{\partial}{\partial(u_1 + iu_2)/\sqrt{2}} &= \frac{1}{\sqrt{2}} \left[\left(u_1 - \frac{\partial}{\partial u_1}\right) - i \left(u_2 - \frac{\partial}{\partial u_2}\right) \right]. \end{aligned} \quad (\text{A.5})$$

Hence, the expansion of functions (A.4) into products of Hermite polynomials is equivalent to expanding

$$\frac{1}{\sqrt{(n - |M|)!}} \frac{1}{\sqrt{(n + |M|)!}} \left(\frac{a_1^+ + ia_2^+}{\sqrt{2}} \right)^{n+|M|} \left(\frac{a_1^+ - ia_2^+}{\sqrt{2}} \right)^{n-|M|} \quad (\text{A.6})$$

in powers of $1/\sqrt{(n_1! n_2!) a_1^{+n_1} (-i a_2^+)^{n_2}}$. But this is exactly what defines the rotation matrices of angular momentum $j = n$:

$$d_{(n_1-n_2/2), M}^n \left(\frac{\pi}{2} \right).$$

Hence

$$\begin{aligned} & \sqrt{\frac{(n-|M|)!}{(n+|M|)!}} L_{n-|M|}^{2|M|}(\mathbf{u}^2) e^{iM\varphi} (2\mathbf{u}^2)^{|M|} \\ &= \sum_{n_1+n_2=2n} \frac{1}{2^n \sqrt{n_1! n_2!}} H_{n_1}(u_1) H_{n_2}(u_2) (-i)^{n_2} d_{(n_1-n_2/2), M}^n \left(\frac{\pi}{2} \right). \end{aligned} \quad (\text{A.7})$$

This relation can be inverted such that

$$B_M^{nn_1} = d_{M, (n_1-n_2/2)}^n \left(-\frac{\pi}{2} \right) (-i)^{n_2} 2^n \sqrt{n_1! n_2!} \sqrt{\frac{(n-|M|)!}{(n+|M|)!}}. \quad (\text{A.8})$$

In fact, putting $\beta = -\pi/2$, $m' = n_1 - n_2/2$, $n = n_1 + n_2/2$ into

$$\begin{aligned} d_{M, m'}^n(\beta) &= \sqrt{\frac{(n+M)!(n-M)!}{(n+m')!(n-m')!}} \sum_k \binom{n+m'}{n+M-k} \binom{n-m'}{k} (-1)^{n+m'-k} \\ &\quad \times \left(\cos \frac{\beta}{2} \right)^{2k-m'-m} \left(\sin \frac{\beta}{2} \right)^{2n-2k+m'+m} \end{aligned} \quad (\text{A.9})$$

and using the symmetry relations of d -functions:

$$\begin{aligned} d_{|M|, (n_1-n_2/2)}^n \left(-\frac{\pi}{2} \right) &= (-1)^{M-(n_1-n_2/2)} d_{-|M|, (n_2-n_1/2)}^n \left(-\frac{\pi}{2} \right) \\ &= \sqrt{\frac{(n-|M|)!(n+|M|)!}{n_1! n_2!}} \sum_k (-1)^k \binom{n_1}{k} \binom{2n-n_1}{n-|M|-k} \frac{(-1)^{n_1}}{2^n}. \end{aligned} \quad (\text{A.10})$$

Together with (A.8) we recover (A.2).

Appendix B: Fourier Transform of the Bound State Wave Functions

Consider first the bound states $\psi_{nM}(\mathbf{x})$ of (48). Their Fourier transform

$$\psi_{nM}(\mathbf{p}) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \int_0^\infty dr r e^{-i\mathbf{p}\mathbf{r}} \psi_{nM}(\mathbf{r}) \quad (\text{B.1})$$

involves, after the angular integral,

$$\frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{-i\mathbf{p}r \cos(\varphi_p - \varphi) + iM\varphi} = i^M e^{iM\varphi_p} J_M(pr), \quad (\text{B.2})$$

the following expression

$$\begin{aligned} \psi_{nM}(p) = & i^M e^{iM\varphi_p} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{(n-|M|)!}{(n+|M|)!}} \left(\frac{2me^2}{n+\frac{1}{2}}\right)^{M+(1/2)} \frac{1}{\sqrt{2n+1}} \\ & \times \sqrt{\frac{2me^2}{n+\frac{1}{2}}} \int_0^\infty dr r^{|M|+1} e^{-(me^2/n+(1/2)r} J_M(pr) L_{n-M}^{2M} \left(\frac{2me^2}{n+\frac{1}{2}} r\right). \end{aligned} \quad (\text{B.3})$$

Using the integral

$$\int_0^\infty du u^{M+1} e^{-u/2} J_M\left(\frac{1}{2}u\omega\right) L_{n-M}^{2M}(u) = 8\left(n+\frac{1}{2}\right) \frac{(2\omega)^M}{(\omega^2+1)^{M+3/2}} T_{n-M}^M\left(\frac{\omega^2-1}{\omega^2+1}\right)$$

where $T_m^n(x)$ are the Gegenbauer polynomials which can be expressed terms of Legendre polynomials as

$$T_{n-M}^M(x) = \frac{1}{(1-x^2)^{M/2}} P_n^M(x) \quad (\text{B.4})$$

the integral (B.3) reduces to equ. (50) of the text. (see Ref. [8] p. 1680, p. 738, and equ. (5. 3. 38)).

Appendix C: Decomposition of $P_{i\lambda-(1/2)}(-\cos\theta)$

Consider

$$P_{i\lambda-(1/2)}(-\cos\theta) = P_{i\lambda-(1/2)}(-\tilde{\xi}_0\tilde{\xi}'_0 + \sqrt{\tilde{\xi}_0^2-1}\sqrt{\tilde{\xi}'_0^2-1}\cos\psi) \quad (\text{C.1})$$

where ψ is the angle between $\tilde{\xi}, \tilde{\xi}'$. We distinguish four different cases:
For $\text{Re } \tilde{\xi}_0 > 0, \text{Re } \tilde{\xi}'_0 < 0$

$$P_{i\lambda-(1/2)}(-\cos\theta) = P_{i\lambda-(1/2)}(\tilde{\xi}_0(-\tilde{\xi}'_0) - \sqrt{\tilde{\xi}_0^2-1}\sqrt{(-\tilde{\xi}'_0)^2-1}\cos(\psi+\pi)) \quad (\text{C.2})$$

using the addition theorem we obtain

$$P_{i\lambda-(1/2)}(-\cos\theta) = \sum_{M=-\infty}^{\infty} \frac{\Gamma\left(i\lambda - M + \frac{1}{2}\right)}{\Gamma\left(i\lambda + M + \frac{1}{2}\right)} P_{i\lambda-(1/2)}^M(\tilde{\xi}_0) P_{i\lambda-(1/2)}^M(-\tilde{\xi}'_0) e^{iM(\varphi_p - \varphi'_p)}. \quad (\text{C.3})$$

For $\text{Re } \tilde{\xi}_0 < 0, \text{Re } \tilde{\xi}'_0 > 0$ we obtain the same formula with $\tilde{\xi}_0 \leftrightarrow \tilde{\xi}'_0$.

For $\text{Re } \tilde{\xi}_0 > 0, \text{Re } \tilde{\xi}'_0 > 0$ choosing $\tilde{\xi}_0 = \xi_0 - i0, \tilde{\xi}'_0 = \xi'_0 - i0$ and making use of

$$P_\nu^\mu(-z) = e^{i\pi\nu} P_\nu^\mu(z) - \frac{2}{\pi} e^{-i\pi\nu} \sin\pi(\nu+\mu) Q_\nu^M(z)$$

we get

$$\begin{aligned}
 & P_{i\lambda-(1/2)}(-\cos\theta) \\
 &= e^{i\pi(i\lambda-(1/2))} P_{i\lambda-(1/2)}(\xi_0\xi_0' - \sqrt{\xi_0^2-1}\sqrt{\xi_0'^2-1}\cos\psi) \\
 &\quad - \frac{2}{\pi} \sin\pi\left(i\lambda - \frac{1}{2}\right) Q_{i\lambda-(1/2)}(\xi_0\xi_0' - \sqrt{\xi_0^2-1}\sqrt{\xi_0'^2-1}\cos\psi) \\
 &= \sum_{M=-\infty}^{\infty} (-1)^M \frac{\Gamma\left(i\lambda - M + \frac{1}{2}\right)}{\Gamma\left(i\lambda + M + \frac{1}{2}\right)} \left\{ e^{i\pi(i\lambda-(1/2))} P_{i\lambda-(1/2)}^M(\xi_0) - \frac{2}{\pi} \sin\pi\left(i\lambda - \frac{1}{2}\right) Q_{i\lambda-(1/2)}^M(\xi_0) \right\} \\
 &\quad \times P_{i\lambda-(1/2)}^M(\xi_0') e^{iM(\varphi_p - \varphi_p')}. \tag{C.4}
 \end{aligned}$$

Similarly for $\text{Re } \xi_0 < 0, \text{Re } \xi_0' < 0$ we get

$$\begin{aligned}
 P_{i\lambda-(1/2)}(-\cos\theta) &= \sum_{M=-\infty}^{\infty} (-1)^M \frac{\Gamma\left(i\lambda - M + \frac{1}{2}\right)}{\Gamma\left(i\lambda + M + \frac{1}{2}\right)} \\
 &\quad \times \left\{ e^{-i\pi(i\lambda-(1/2))} P_{i\lambda-(1/2)}^M(-\xi_0) - \frac{2}{\pi} \sin\pi\left(i\lambda - \frac{1}{2}\right) Q_{i\lambda-(1/2)}^M(-\xi_0) \right\} \\
 &\quad \times P_{i\lambda-(1/2)}^M(-\xi_0') e^{iM(\varphi_p - \varphi_p')}. \tag{C.5}
 \end{aligned}$$

When these expansions are put into (66), terms with $Q_{i\lambda-(1/2)}^M$ do not contribute since they are multiplied by $\sin\pi(i\lambda - 1/2)$, such that we obtain (70).

Appendix D: Fourier Transform of the Continuum State Wave Function $\psi_{i,\lambda,M}(\mathbf{x})$

Fourier transform of the continuum wave function of (65) is

$$\psi_{i\lambda,M}(\mathbf{p}) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \int_0^\infty dr r e^{-i\mathbf{p}\cdot\mathbf{x}} \psi_{i\lambda,M}(\mathbf{x}). \tag{D.1}$$

After calculating the angular integral

$$\begin{aligned}
 \psi_{i\lambda,M}(\mathbf{p}) &= \frac{(-1)^M}{\pi} \sqrt{\frac{me^2}{v}} \frac{1}{\sqrt{\lambda}} e^{-i(\pi/2)(i\lambda-(1/2))} \frac{\left| \Gamma\left(M + \frac{1}{2} + i\lambda\right) \right|}{\Gamma(2M+1)} \\
 &\quad \times e^{iM\varphi_p} \int_0^\infty dr r^{1/2} J_M(pr) M_{i\lambda,M}\left(\frac{2me^2}{i\lambda} r\right). \tag{D.2}
 \end{aligned}$$

To calculate the radial integral, we use the integral representation for the Whittaker function $M_{i\lambda,M}$ [10]:

$$\begin{aligned}
 M_{i\lambda,M}\left(\frac{2me^2}{iv} r\right) &= \frac{1}{2^{2M}} \frac{\Gamma(2M+1)}{\left| \Gamma\left(M + \frac{1}{2} + i\lambda\right) \right|} \left(\frac{2me^2}{i\lambda}\right)^{M+(1/2)} \\
 &\quad \times r^{M+(1/2)} \int_0^\pi dt e^{-(me^2/i\lambda)rcost} (\sin t)^{2M} \left(\cos \frac{t}{2}\right)^{2i\lambda}. \tag{D.3}
 \end{aligned}$$

Then we have

$$\psi_{i\lambda, M}(\mathbf{p}) = N \int_0^\pi dt (\sin t)^{2M} \left(\cot \frac{t}{2} \right)^{2i\lambda} \int_0^\infty dr r^{M+1} e^{-(me^2/i\lambda)r \cos t} J_M(pr) \quad (\text{D.4})$$

where N collects all the numerical factors. If we add a small imaginary part $-i\varepsilon$ ($\varepsilon > 0$) to t we obtain for the radial integral [8]

$$\begin{aligned} & \int_0^\infty dr r^{M+1} e^{-(me^2/i\lambda)\cos(t-i\varepsilon)} J_M(pr) \\ &= 2 \frac{me^2}{i\lambda} \frac{1}{\sqrt{\pi}} (2p)^M \Gamma\left(M + \frac{3}{2}\right) \frac{\cos(t-i\varepsilon)}{\left[\left(\frac{me^2}{i\lambda}\right)^2 \cos^2(t-i\varepsilon) + p^2\right]^{M+(3/2)}}. \end{aligned} \quad (\text{D.5})$$

After performing a variable change and using the integral representation for the Legendre functions

$$\begin{aligned} P_{i\lambda-(1/2)}^M(\xi_0) &= 2^M \operatorname{ch} \pi\lambda (-1)^M \frac{q^M (1-q^2)^{3/2}}{\pi i\lambda \sqrt{2}} \prod_{s=0}^{M-1} \left(\frac{3}{2} + s\right) \\ &\times \int_{-\infty}^{\infty} dx e^{ix} \operatorname{sh} x [q^2(1 - \operatorname{ch}(x-i\varepsilon)) + (1 + \operatorname{ch}(x-i\varepsilon))]^{-M-3/2} \end{aligned} \quad (\text{D.6})$$

with

$$\xi_0 = \frac{1+q^2}{1-q^2}, \quad q = \frac{p}{p_0}, \quad p_0 \equiv \frac{me^2}{i\nu}$$

we obtain $\psi(\mathbf{p})$:

$$\begin{aligned} \psi_{i\lambda-(1/2), M}(\mathbf{p}) &= \frac{i^{M+(1/2)}}{\pi} \frac{2^{1/2} \tilde{p}_0^2}{(\tilde{p}_0^2 - p^2)^{3/2}} \sqrt{\lambda} e^{-\pi\lambda/2} e^{iM\varphi_p} \\ &\times \left| \Gamma\left(i\lambda - M + \frac{1}{2}\right) \right| \{P_{i\lambda-(1/2)}^M(\xi_0) \theta(\xi_0) + (-1)^M P_{i\lambda-(1/2)}^M(\xi_0) \theta(-\xi_0)\}. \end{aligned} \quad (\text{D.7})$$

Appendix E: Derivation of the Scattering Amplitude

The asymptotic form of (74) is dominated by $\varrho \sim 0$, $(\xi_b - \xi_a)^2 \gg 1$

$$\begin{aligned} \Gamma(\xi_b, \xi_a) &= \delta(\xi_b - \xi_a) + \frac{\nu}{2\pi} \int_0^1 d\varrho \varrho^{-\nu} \frac{d}{d\varrho} \frac{\varrho^{1/2}}{\sqrt{(1-\varrho)^2 + \varrho(\xi_b - \xi_a)^2}} \\ &\sim \delta(\xi_b - \xi_a) + \frac{\nu}{2\pi} \int_0^1 \frac{\varrho^{-\nu-1/2}}{2(1 + \varrho(\xi_b - \xi_a)^2)^{3/2}} \\ &\sim \delta(\xi_b - \xi_a) + \frac{\nu^2}{2\sqrt{\pi}} \frac{1}{\cos \pi\nu} \frac{\Gamma(\nu)}{\Gamma\left(\nu + \frac{1}{2}\right)} [(\xi_b - \xi_a)^2]^{\nu-(1/2)}. \end{aligned} \quad (\text{E.1})$$

Using the value of

$$(\xi_b^2 - \xi_a^2) = 4p_0^2(\mathbf{p}_b - \mathbf{p}_a)^2 / [(p_0^2 + p_b^2)(p_0^2 + p_a^2)]$$

we obtain for the asymptotic form of $K(\mathbf{p}_b, \mathbf{p}_a)$:

$$\begin{aligned} K(\mathbf{p}_b, \mathbf{p}_a) &\sim \frac{i\delta(\mathbf{p}_b - \mathbf{p}_a)}{E - T_a} - i \frac{i}{E - T_a} \\ &\times \left\{ \sqrt{\frac{\nu\Gamma(\nu)}{\operatorname{ch} \pi\nu \Gamma\left(\nu + \frac{1}{2}\right)}} e^{-\nu \ln(E - T_b/4E)} \frac{e^2}{2\sqrt{\pi} (\mathbf{p}_b - \mathbf{p}_a)} e^{-\nu \ln(4\bar{p}_0^2/(p_b^2 - p_a^2)^2)} \right. \\ &\times \left. \sqrt{\frac{\nu\Gamma(\nu)}{\operatorname{ch} \pi\nu \Gamma\left(\nu + \frac{1}{2}\right)}} e^{-\nu \ln(E - T_a/4E)} \right\} \frac{i}{E - T_b} \end{aligned} \quad (\text{E.2})$$

where $T = \mathbf{p}^2/2m$ and $E = p_0^2/2m$. Here we identify the long-range Coulomb propagator

$$G(\mathbf{p}) \sim \frac{i}{E - T} \sqrt{\frac{\nu\Gamma(\nu)}{\operatorname{ch} \pi\nu \Gamma\left(\nu + \frac{1}{2}\right)}} e^{-\nu \ln(E - T/4E)}$$

and the scattering amplitude

$$T(\mathbf{p}_b, \mathbf{p}_a) = \frac{e^2}{|\mathbf{p}_b - \mathbf{p}_a|} e^{-\nu \log(4\bar{p}_0^2/(p_b - p_a)^2)}. \quad (\text{E.3})$$

Appendix F: Derivation of Wave Functions of the Three Dimensional H-Atom in Parabolic Coordinates

We first express the products

$$\begin{aligned} H_{n_1}(\sqrt{\mu\omega} u_1) H_{n_4}(\sqrt{\mu\omega} u_4) &= H_{n_1}(\sqrt{2p_0} u_1) H_{n_4}(\sqrt{2p_0} u_4) \\ &= H_{n_1}\left(\sqrt{2p_0} r \sin \frac{\theta}{2} \cos \frac{\alpha + \varphi}{2}\right) H_{n_4}\left(\sqrt{2p_0} r \sin \frac{\theta}{2} \sin \frac{\alpha + \varphi}{2}\right) \end{aligned} \quad (\text{F.1})$$

via formula (45) as

$$\begin{aligned} &\frac{e^{-p_0 r \cos^2 \theta/2}}{2^{(n_1+n_4)/2} \sqrt{n_1! n_4!}} H_{n_1}(\sqrt{\mu\omega} u_1) H_{n_4}(\sqrt{\mu\omega} u_4) \\ &= \sum_{m_{14} = -n_1+n_4/2}^{n_1+n_4/2} d_{m_{14}, n_1-n_4/2}^{n_1+n_4/2} \left(-\frac{\pi}{2}\right) \sqrt{\frac{\left(\frac{n_1+n_4}{2} - |m_{14}|\right)!}{\left(\frac{n_1+n_4}{2} + |m_{14}|\right)!}} \\ &\times e^{im_{14}(\alpha+\varphi+\pi)} e^{-p_0 r \cos^2 \theta/2} (2p_0 r)^{|m_{14}|} \left(\sin^2 \frac{\theta}{2}\right)^{|m_{14}|} L_{\left(\frac{n_1+n_4}{2}\right)-|m_{14}|}^{2|m_{14}|} \left(2p_0 r \sin^2 \frac{\theta}{2}\right) \end{aligned} \quad (\text{F.2})$$

and write the product

$$H_{n_3}(\sqrt{\mu\omega} u_3) H_{n_2}(\sqrt{\mu\omega} u_2)$$

in a similar way in terms of Laguerre functions by replacing $(n_1 \rightarrow n_3, n_4 \rightarrow n_2$ and $\cos \theta/2 \leftrightarrow \sin \theta/2)$. The the full wave function (111) becomes:

$$\begin{aligned} & \frac{2p_0}{\pi} \sum_{m_{14} = -n_1 + n_4/2}^{n_1 + n_4/2} \sum_{m_{32} = -n_3 + n_2/2}^{n_3 + n_2/2} e^{im_{14}(\alpha + \varphi + \pi)} e^{im_{32}(\alpha - \varphi + \pi)} \\ & \times \sqrt{\frac{\left(\frac{n_1 + n_4}{2} - |m_{13}|\right)! \left(\frac{n_3 + n_2}{2} - |m_{32}|\right)!}{\left(\frac{n_1 + n_4}{2} + |m_{14}|\right)! \left(\frac{n_3 + n_2}{2} + |m_{32}|\right)!}} d_{m_{14}, n_1 - n_4/2}^{n_1 + n_4/2} \left(-\frac{\pi}{2}\right) d_{m_{32}, n_3 - n_2/2}^{n_3 + n_2/2} \left(-\frac{\pi}{2}\right) \\ & \times e^{-p_0 r} (2p_0 r)^{|m_{14}| + |m_{32}|} \left(\cos \frac{\theta}{2}\right)^{2|m_{32}|} \left(\sin \frac{\theta}{2}\right)^{2|m_{14}|} \\ & \times L_{n_1 - n_4/2 - |m_{14}|}^{2|m_{14}|} \left(2p_0 r \sin^2 \frac{\theta}{2}\right) L_{n_3 - n_2/2 - |m_{32}|}^{2|m_{32}|} \left(2p_0 r \cos^2 \frac{\theta}{2}\right). \end{aligned} \tag{F.3}$$

The integral over $d\alpha_b$ in (110) from zero to 2π enforces $m_{14} = -m_{32}$ and gives a factor 2π . The wave functions become:

$$\begin{aligned} & 4p_0 \sum_{m_{14}} e^{2im_{14}\varphi} \\ & \times \sqrt{\frac{\left(\frac{n_1 + n_4}{2} - |m_{14}|\right)! \left(\frac{n_3 + n_2}{2} - |m_{32}|\right)!}{\left(\frac{n_1 + n_4}{2} + |m_{13}|\right)! \left(\frac{n_3 + n_2}{2} + |m_{32}|\right)!}} d_{m_{14}, n_1 - n_4/2}^{n_1 + n_4/2} \left(-\frac{\pi}{2}\right) d_{-m_{14}, n_3 - n_2/2}^{n_3 + n_2/2} \left(-\frac{\pi}{2}\right) \\ & \times e^{-p_0 r} (p_0 r \sin \theta)^{2|m_{14}|} L_{n_1 - n_4/2 - |m_{14}|}^{2|m_{14}|} \left(2p_0 r \sin^2 \frac{\theta}{2}\right) L_{n_3 - n_2/2 - |m_{14}|}^{2|m_{14}|} \left(2p_0 r \cos^2 \frac{\theta}{2}\right) \end{aligned} \tag{F.4}$$

where m_{14} runs from the minimum of $(-n_1 + n_4/2, -n_3 + n_2/2)$ to the opposite value. At the residue (116) the d -functions occur on the form

$$\begin{aligned} & d_{m_{14}, n_1 - n_4/2}^{n_1 + n_4/2} \left(-\frac{\pi}{2}\right) d_{-m_{14}, n_3 - n_2/2}^{n_3 + n_2/2} \left(-\frac{\pi}{2}\right) \\ & d_{m_{14}, n_1 - n_4/2}^{n_1 + n_4/2} \left(-\frac{\pi}{2}\right) d_{-m_{14}, n_3 - n_2/2}^{n_3 + n_2/2} \left(-\frac{\pi}{2}\right) \end{aligned} \tag{F.5}$$

with the indices $(n_1 - n_4)/2$ running for every fixed $(n_1 + n_4)/2$ from $-n_1 + n_4/2$ to $n_1 + n_4/2$ (similarly for $(n_3 - n_2)/2$).

Due to the orthogonality of the d -functions we obtain $\delta_{m_{14}^a, m_{14}^b} \delta_{m_{14}^a, m_{14}^b}$. Thus the residue takes the form of (116). The quantum number $n_1 + n_4/2 - |m_{14}|$ is always integer and may be denoted by

$$n_1' = \frac{n_1 + n_4}{2} - |m_{14}|$$

and similarly we have the integer

$$n_2' = \frac{n_3 + n_2}{2} - |m_{14}|$$

thus we have

$$n_1' + n_2' = n - 2|m_{14}|$$

with $m = 2|m_{14}|$ always being integer.

Appendix G: Relation Between the Parabolic and Spherical Wave Functions

Here we will calculate the coefficients C_{sl}^{nm} defined in the following way ($n = n_1' + n_2' + |m| + 1$)

$$\psi_{n_1'n_2'm}(x) = \sum_{l=m}^{n-1} C_{n_1'l}^{nm} \psi_{nlm}(x) \tag{G.1}$$

where $\psi_{n_1'n_2'm}$ is the parabolic wave functions and ψ_{nlm} is the spherical wave functions of H-Atom given by (117) and (121), respectively. Using the power series representation for the Laguerre polynomials

$$L_n^\alpha(x) = \sum_{m=0}^n (-1)^m \binom{n+\alpha}{n-m} \frac{x^m}{m!} \tag{G.2}$$

(G.1) becomes:

$$\begin{aligned} & \sum_{p=0}^{n_1'} \sum_{q=0}^{n-n_1'-|m|-1} B \frac{(-1)^{p+q}}{p!q!} \binom{n_1'+|m|}{n_1'-p} \binom{n-n_1'-1}{n-n_1'-|m|-q-1} \\ & \times \left(\cos \frac{\theta}{2}\right)^{2p} \left(\sin \frac{\theta}{2}\right)^{2q} \varrho^{|m|+p+q} \\ & = \sum_{t=0}^{n-l-1} \sum_{l=m}^{n-1} A C_{n_1't}^{nm} \frac{1}{t!} P_l^m(\cos \theta) \binom{n+l}{n-t-l-1} \varrho^{l+t} \end{aligned} \tag{G.3}$$

where

$$B = \sqrt{\frac{n_1'!(n-n_1'-|m|-1)!}{(n_1'+|m|)!(n-n_1-1)!}} \tag{G.4}$$

and

$$A = \sqrt{\frac{(2l+1)(l-|m|)!(n-l-1)!}{(l+|m|)!(n+l)!}} \tag{G.5}$$

and $\varrho = 2p_0r$. Equating the coefficients of the highest powers of ϱ in (G.3) which occur for $p = n_1'$, $q = n - n_1' - |m| - 1$ and $t = n - l - 1$ we obtain:

$$\begin{aligned} & \frac{B}{2^{|m|}} (-1)^{n-|m|-1} \frac{\left(\cos^2 \frac{\theta}{2}\right)^{n_1'} \left(\sin^2 \frac{\theta}{2}\right)^{n-n_1'-|m|-1} \sin^{|m|} \theta}{n_1'!(n-n_1'-|m|-1)!} \\ & = \sum_{l=m}^{n-1} A C_{n_1'l}^{nm} \frac{1}{(n-l-1)!} P_l^m(\cos \theta). \end{aligned} \tag{G.6}$$

Multiplying both sides by $\sin \theta P_l^m(\cos \theta)$, and integrating over $\theta \in (0, 2\pi)$ and using the orthogonality of the polynomials P_l^m , $C_{n_1'l}^{nm}$ can be expressed as ($x \equiv \cos \theta$)

$$C_{n_1'l}^{nm} = \frac{(-1)^{n+l-|m|-1}}{l! 2^{n+l}} \sqrt{\frac{(2l+1)(l+|m|)!(n+l)!(n-l-1)!}{(n_1'+|m|)!(n-n_1'-1)!(l-|m|)!n_1'!(n-n_1'-|m|-1)!}}$$

$$\times \int_{-1}^1 dx (1-x)^{n-n_1'-|m|-1} (1+x)^{n_1'} \frac{d^{l-|m|}}{dx^{l-|m|}} ((1-x)^l (1+x)^l). \tag{G.7}$$

From this last expression we can see that $C_{n_1'l}^{nm}$ is equal to the Clebsch-Gordon coefficients up to a phase [15]:

$$C_{n_1'l}^{nm} = (-1)^{n_1'-|m|} (-1)^m \sqrt{2l+1} \begin{pmatrix} \frac{n-1}{2} & \frac{n-1}{2} & l \\ \frac{2|m|-n+2n_1'+1}{2} & \frac{n-2n_1'-1}{2} & -m \end{pmatrix}.$$

Appendix H: Fourier Transform of $\psi_{i\lambda lm}(\mathbf{p})$

Fourier transform of (133) is

$$\psi_{i\lambda lm}(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \int_0^{2\pi} d\varphi_p \int_0^\pi d\theta_p \sin \theta_p \int_0^\infty dp p^2 e^{i\mathbf{p}\cdot\mathbf{x}} \psi_{i\lambda lm}(\mathbf{p}) \tag{H.1}$$

from which we obtain after taking the angular integrals and changing the variable p to $q = |\mathbf{p}|/\tilde{p}_0$

$$\psi_{i\lambda lm}(\mathbf{x}) = -\frac{i^l}{\sqrt{\pi}} \tilde{p}_0^{3/2} \left[\frac{\pi}{2} (1 - e^{-2\pi\lambda}) \lambda^2 (\lambda^2 + 1^2) \dots (\lambda^2 + l^2) \right]^{-1/2}$$

$$\times \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos \theta) e^{im\varphi}$$

$$\times \left[\int_0^1 dq q^2 j_l(\tilde{p}_0 r q) \left(\frac{2}{1-q^2}\right)^2 (\text{sh } \theta_-)^l \left(\frac{d}{d \text{ch } \theta_-}\right)^{l+1} \text{ch } \lambda \theta_- \right.$$

$$\left. - e^{-\varphi\lambda} \int_1^\infty dq q^2 j_l(\tilde{p}_0 r q) \left(\frac{1}{1-q^2}\right)^2 (\text{sh } \theta_+)^l \left(\frac{d}{d \text{ch } \theta_+}\right)^{l+1} \text{ch } \lambda \theta_+ \right] \tag{H.2}$$

where $\text{th}(\theta_-/2) = q$ for $q \in (0, 1)$ and $\text{th}(\theta_+/2) = 1/q$ for $q \in (1, \infty)$. To handle the singularity at $q = 1$, following reference [10], we introduce

$$F_l(\lambda, \theta) = -\frac{1}{\text{sh } \pi\lambda} \left(\frac{d}{d \text{ch } \theta}\right)^{l+1} \frac{\cos \lambda\theta}{\text{sh } \theta}$$

and

$$\tilde{F}_l(t, \theta) = \int_{-\infty}^\infty d\lambda e^{i\lambda t} F_l(\lambda, \theta) = i \frac{\text{sh } t (-1)^l (l+1)!}{(\text{ch } \theta + \text{ch } t)^{l+2}}.$$

Then we get

$$\begin{aligned}
 \psi_{i\lambda lm}(\mathbf{x}) = & -\frac{i^l}{\sqrt{\pi}} e^{im\varphi} \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos\theta) \\
 & \times \tilde{p}_0^{3/2} \left[\frac{\pi}{2} (1 - e^{-2\pi\lambda}) \lambda^2(\lambda^2 + 1^2) \dots (\lambda^2 + l^2) \right]^{-1/2} \\
 & \times \frac{1}{i} (-1)^l (l+1)! 2^{l+1} \int_{-\infty}^{\infty} dt e^{-i\lambda t} \text{sh } t \\
 & \times \int_{-\infty}^{\infty} dq j_l(\tilde{p}_0 r q) \left(\frac{q}{q^2 [1 - \text{ch}(t - i\varepsilon)] + [1 + \text{ch}(t - i\varepsilon)]} \right)^{l+2}. \quad (\text{H.3})
 \end{aligned}$$

Then using the relation between $j_l(z)$ and the Hankel functions

$$j_l(z) = \frac{1}{2i} (h_l^{(+)}(z) - h_l^{(-)}(z))$$

we obtain [10]

$$\begin{aligned}
 \psi_{i\lambda, lm}(\mathbf{x}) = & -\frac{(-i)^l}{\sqrt{\pi}} \sqrt{2\tilde{p}_0^3} \frac{1}{2\tilde{p}_0 r} \frac{e^{im\varphi}}{\sqrt{\lambda}} \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} \\
 & \times P_l^m(\cos\theta) \frac{|\Gamma(l+i\lambda+1)|}{(2l+1)!} e^{\pi\lambda/2} M_{-i\lambda, l+(1/2)}(2i\tilde{p}_0 r). \quad (\text{H.4})
 \end{aligned}$$