

Hydrogen atom in the momentum representation

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The wave functions for the hydrogen atom are determined in the momentum representation, using momentum variables p_r , p_θ , p_ϕ which are associated with the spherical polar variables r , θ ($=e^{i\theta} \cos\theta$) and ϕ ($=e^{i\phi}$). The functions may be written as

$$\begin{aligned}\phi_{n,l,m}(p_r, p_\theta, p_\phi) &= \alpha_{n,l}(\beta_1^m(p_\theta) \delta(p_\phi + m), \\ \alpha_{n,l}(p_r) &= \left(\frac{n}{ip_0}\right)^{3l+2} \sum_{k=0}^{n-l-1} \binom{n-l-1}{k} \frac{2^{k-l+1}}{(2l+k+1)(2l+k) \cdots (l+k+2)} \left(\frac{ip_0/n}{p_r - ip_0/n}\right)^{l+k+2}, \\ \beta_1^m(p_\theta) &= \sum_{j=E(l/2)}^{E(l/2)} a_j p_\theta^{-(m+1)/2} J_{j-(m-1)/2}(p_\theta),\end{aligned}$$

where δ is the Dirac delta function and $p_0 = Za_0^{-1}$ (a_0 is the Bohr radius). $J_\nu(p_0)$ are Bessel functions of integer or half-integer order. The radial functions are shown to have poles up to order $n+1$ at $p_r = ip_0/n$.

INTRODUCTION

It is generally known that the solution to all quantum-mechanical problems may be expressed either as a function of q the position, or of p the momentum, where position and momentum are the appropriate conjugate variables.¹ Both representations are entirely equivalent and state functions expressed in either representation will suffice for calculations of the expectation value of any observable. The selection of the most appropriate representation depends merely on convenience. Generally, the position representation has been useful for most bound-state problems such as atomic and molecular structure as well as many scattering problems. With few exceptions, the momentum representation has been used almost exclusively to study scattering.²⁻⁴ Little work has been carried out on bound-state problems since Coulson and Duncanson published a series of articles on momentum distribution in molecular systems.^{5,6} These investigations were based on a derivation of a state function for the hydrogen atom originally obtained by Podolsky and Pauling,⁷ and later by Fock.⁸ A rather comprehensive discussion of these functions is given by Bethe and Salpeter.⁹

The functions of Podolsky and Pauling were determined by direct Fourier transformation from position space to a space in which the variables are P , Θ , and Φ . These are the total momentum, and its polar angular coordinates referred to the same axes as the position coordinates of the electron; r , θ , ϕ . While the functions derived by Podolsky and Pauling are perfectly good wave functions, useful for calculations of expectation values, they can not be considered truly expressed

in the momentum representation. Firstly, the variables used by Podolsky and Pauling are not conjugate to any of the relevant spatial variables. By this it is meant that they have not been selected so that a commutation relationship can be found with an appropriate spatial variable leading to a Heisenberg uncertainty relationship. Secondly, the angular coordinates are not chosen to be Hermitian, although they do represent observables. It is the purpose of this work to determine the wave functions for the hydrogen atom in a momentum space in which each of the three momentum variables are represented by Hermitian variables which are conjugate to appropriately chosen position space variables.

MOMENTUM REPRESENTATION

Quantum-mechanical calculations usually start with the determination of an appropriate Hamiltonian which is a function of the positions and momenta of all the particles. For a single particle in one dimension

$$H(p, q) = p^2/2\mu + V(q),$$

where μ is the mass of the particle and $V(q)$ is its potential energy function. Using units in which $\hbar=1$ we express the momentum as an operator

$$p \rightarrow -id/dq \quad (1)$$

and seek solutions of the resulting differential equation

$$H\psi(q) = E\psi(q),$$

where E is a constant and $\psi(q)$ is the state vector

expressed as a function of the position of the particle. The variables p and q are chosen to be continuous on the interval $(-\infty, \infty)$ and Hermitian conjugates, such that a relationship

$$[p, q] = i \quad (2)$$

may be written. It is an easy matter¹ to show that this relationship leads to an uncertainty expression of the form

$$\Delta p \Delta q \geq \frac{1}{2}. \quad (3)$$

Alternatively, we could seek solutions $\phi(p)$ as functions of the momentum variable. These two functions may be related by a transformation $S(p, q)$ such that

$$\phi(p) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} S(p, q) \psi(q) dq.$$

In order to preserve the magnitude of the probability amplitude we require that $S(p, q)$ be a unitary transformation, or that

$$\int_{-\infty}^{\infty} S^*(p', q) S(p, q) dq = 2\pi \delta(p' - p).$$

To determine the correct equation governing $\phi(p)$ we replace functions of q with operators, while p remains a variable,

$$q \rightarrow id/dp, \quad q^{-1} \rightarrow -i \int dp. \quad (4)$$

Depending on the form of $V(q)$ we obtain either a differential or integral equation which must be solved for $\phi(p)$. The extension of these ideas to more than one dimension is relatively straightforward, as long as the space is Cartesian. We shall see in the next section that for spherical polar coordinates, we can not simultaneously obtain Hermitian conjugates and a viable uncertainty relationship, unless some care is taken in the choice of variables.

THE HYDROGEN ATOM

Owing to the spherical symmetry of the potential energy of the hydrogen atom, considerable mathematical simplicity is obtained by transforming the equations to spherical polar coordinates r, θ, ϕ . We might then search for a set of conjugate variables p_r, p_θ, p_ϕ which are Hermitian, and for which acceptable uncertainty relations of the form³ may be obtained. This approach, unfortunately, leads to several mathematical difficulties which should be examined before deriving the equations to be solved.

We expect to require that our momentum operators be Hermitian. For p_r it has been shown that the choice¹

$$p_r = -i \left(\frac{\partial}{\partial r} + \frac{1}{r} \right)$$

is Hermitian only if we restrict ourselves to

square-integrable functions such that

$$\lim_{r \rightarrow 0} r \psi(r) = 0.$$

Nevertheless, questions as to the physical interpretation of p_r arise. It has been pointed out¹⁰ that although p_r is Hermitian, it is not an observable since no solution to the differential equation $p_r f(r) = cf(r)$ can satisfy the above condition. Despite the fact that p_r itself is not an observable, certain functions of p_r (such as the square of the total momentum) are observables, so that the choice of p_r as one of the momentum variables is of practical importance. We shall also see later that it is necessary to interpret p_r as a complex variable. The functions derived have singularities in the complex plane and the location and nature of these singularities have physical consequences.

The variables p_θ and p_ϕ also present difficulties. If, for example, we choose

$$p_\phi = -i\partial/\partial\phi$$

such that

$$[\phi, p_\phi] = i$$

we find that p_ϕ is only Hermitian in the space of functions with period 2π . However, ϕ itself is not periodic, but runs between $-\infty$ and ∞ . If we restrict ϕ to range only from 0 to 2π (making it in effect periodic over the range $\pm\infty$), then the commutation relation must be modified to include a series of δ functions.¹¹ In addition this restriction makes it difficult to find a physically meaningful uncertainty relation. Several authors¹²⁻¹⁶ have dealt with this paradox. It is clear that if we restrict ourselves in position space only to functions which are periodic in the angle, we may ensure the Hermitian character of the momentum variable, as well as maintain consistency with the uncertainty principle. The cost of this is that our position variables are no longer Hermitian, but unitary. However, Levy-Leblond¹⁵ has shown that a consistent formulation of quantum-mechanical relations can be established by abandoning the strict reliance on Hermitian operators, combined with a careful consideration of uncertainty relations. For an operator which is non-Hermitian, Levy-Leblond defines the spectral extension

$$(\Delta F)^2 = \langle \psi | F^* F | \psi \rangle - |\langle \psi | F | \psi \rangle|^2$$

which for a unitary operator U becomes,

$$(\Delta U)^2 = 1 - |\langle U \rangle|^2.$$

In keeping with these ideas we find it convenient to define the unitary operator $v = e^{i\phi}$. Then we choose

$$p_\phi = v \frac{\partial}{\partial v}$$

and the correct commutation relation becomes

$$[p_\phi, v] = v.$$

The operator p_ϕ is now Hermitian over the whole range of v ($|v| \leq 1$), and the uncertainty relation becomes

$$(\Delta p_\phi)^2 (\Delta v)^2 \geq \frac{1}{4} [1 - (\Delta v)^2].$$

In considering the variable θ the equations in position space may most easily be expressed in terms of the variable $u = \cos \theta$. If we then choose the unitary operator

$$t = e^{i\pi u} = e^{i\pi \cos \theta}$$

and

$$p_\theta = -i \frac{\partial}{\partial u} = \pi t \frac{\partial}{\partial t}.$$

The commutation relation in this case is

$$[p_\phi, t] = \pi t$$

and the uncertainty relation is

$$(\Delta p_\phi)^2 (\Delta t)^2 \geq \frac{1}{4} \pi^2 [1 - (\Delta t)^2].$$

We thus choose r, t, v as our position variables and p_r, p_θ, p_ϕ as their associated momentum variables. Note that p_θ and p_ϕ can not be considered conjugate to t and v in the strict sense as formulated by Gruber,¹⁷ or De Witt.¹⁸ They showed that for any coordinate system the conjugate momentum is the Hermitian part of $p = -id/dq$. As shown above this choice does not lead to consistent uncertainty relations, and we have chosen momenta in such a way as to have physically meaningful uncertainty relations with associated position variables, while maintaining Hermitian character of the momenta. This choice also has certain mathematical advantages as shown in the following sections.

The Hamiltonian for the hydrogen atom may be written

$$H = \tilde{p}^2 / 2\mu + V(\tilde{r}),$$

$$V(\tilde{r}) = -Ze^2/r.$$

Expressing \tilde{p} as a differential operator in spherical polar coordinates, we may show

$$H = -\frac{1}{2\mu} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{\mathcal{L}^2}{r^2} \right) - \frac{Ze^2}{r}, \quad (5)$$

where \mathcal{L}^2 is the square of the total angular momentum (written in terms of u, v)

$$\mathcal{L}^2 = (1 - u^2) \frac{\partial^2}{\partial u^2} - 2u \frac{\partial}{\partial u} + \frac{1}{1 - u^2} \left(v^2 \frac{\partial^2}{\partial v^2} + v \frac{\partial}{\partial v} \right). \quad (6)$$

If we seek solutions of this problem expressed as functions of the position variables, assuming separability:

$$\psi(r, u, v) = R(r)P(u)Z(v). \quad (7)$$

This leads to three one-dimensional equations,

$$v^2 \frac{\partial^2 Z(v)}{\partial v^2} + v \frac{\partial Z(v)}{\partial v} = m^2 Z(v), \quad (8)$$

$$\mathcal{L}^2 P(u) = -l(l+1)P(u), \quad (9)$$

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} + \frac{2\mu Ze^2}{r} + 2\mu E \right) R(r) = 0, \quad (10)$$

where m^2 and $l(l+1)$ are separation constants chosen in this form for mathematical convenience. To solve this problem in momentum space we shall also assume that the three-dimensional momentum function is also separable,

$$\phi(p_r, p_\theta, p_\phi) = \alpha(p_r)\beta(p_\theta)\rho(p_\phi).$$

The momentum function is related to the position function by the transformation $S(\tilde{p}, \tilde{q})$. The volume element in position space is

$$d\tau = r^2 (\pi v t)^{-1} dr dt dv = \pi^{-1} r^2 dr d \ln t d \ln v,$$

where we choose \ln to be the principal value. Then,

$$\phi(p_r, p_\theta, p_\phi) = (2\pi)^{-3/2} \times \int_0^\infty \int_{-1}^1 \int_1^{e^{i2\pi}} S(\tilde{p}, \tilde{q}) \psi(r, t, v) \pi^{-1} r^2 \times dr d \ln t d \ln v.$$

Imposing the unitary requirement we choose the transformation

$$S(\tilde{p}, \tilde{q}) = \sqrt{2/\pi} (1/r) \exp(i r p_r + \pi^{-1} p_\theta \ln t + p_\phi \ln v).$$

Note that we may write the transformation as a product of three separate one-dimensional transforms

$$S(p_r, r) = (\sqrt{2}/r) \exp(i r p_r),$$

$$S(p_\theta, t) = (1/\sqrt{\pi}) \exp[(1/\pi) p_\theta \ln t],$$

$$S(p_\phi, v) = \exp(p_\phi \ln v).$$

In the next sections we shall find the momentum representation analogs of Eqs. (8)–(10) and solve the resulting equations. In so doing we shall require numerous integrals. They are from a comprehensive set of tables compiled by Gradshteyn and Ryzhik.¹⁹ For the convenience of the readers, when we refer to these we shall indicate it by (GR), followed by the appropriate tabulated reference.

THE RADIAL EQUATION

We shall first examine the radial equation (10) in momentum space. If we make the transformation

$$\begin{aligned} -i\left(\frac{d}{dr} + \frac{1}{r}\right) &\rightarrow p_r, \\ \frac{1}{r} &\rightarrow -i \int dp_r \equiv I, \\ R(r) &\rightarrow \alpha(p_r), \end{aligned}$$

we obtain

$$[(p_r^2 - 2\mu E) + l(l+1)I^2 + 2\mu Ze^2 I] \alpha(p_r) = 0. \quad (11)$$

We may find the solution to this equation most easily by taking its $(l+1)$ th derivative. The resulting equation is

$$\left((p_r^2 - 2\mu E) \frac{d}{dp_r} + 2(l+1)p_r + 2\mu Ze^2 I\right) \chi(p_r) = 0, \quad (12)$$

where

$$\chi(p_r) = i^l \frac{d^l}{dp_r^l} \alpha(p_r). \quad (13)$$

Note that this is the equivalent of the substitution $U(r) = r^l R(r)$ in position space. Let $c = 2\mu Ze^2 I$:

$$-\frac{d\chi}{\chi} = \frac{2(l+1)p_r + c}{p_r^2 - 2\mu E} dp_r;$$

integrating both sides of the equation (GR, p. 57)

$$\begin{aligned} -\ln \chi &= (l+1) \ln(p_r^2 - 2\mu E) \\ &+ \frac{c}{2\sqrt{2\mu E}} \ln \left| \frac{p_r - \sqrt{2\mu E}}{p_r + \sqrt{2\mu E}} \right|, \end{aligned}$$

$$\alpha_{n,l}(p_r) = \left(\frac{n}{ip_0}\right)^{3l+2} \sum_{k=0}^{n-l-1} \begin{bmatrix} n-l-1 \\ k \end{bmatrix} \frac{2^{k-l-1}}{(2l+k+1)(2l+k) \cdots (l+k+2)} \left(\frac{ip_0/n}{p_r - ip_0/n}\right)^{l+k+2}. \quad (16)$$

ANGULAR FUNCTIONS

We first transform Eq. (8) into momentum space using

$$\begin{aligned} Z(v) &\rightarrow \rho(p_\phi), \\ -iv \frac{d}{dv} &\rightarrow p_\phi. \end{aligned}$$

The equation becomes simply

$$\begin{aligned} p_\phi^2 \rho(p_\phi) &= m^2 \rho(p_\phi), \\ \text{which has the solution} \\ \rho_m(p_\phi) &= \delta(p_\phi + m), \end{aligned} \quad (17)$$

where δ is the Dirac delta function.

We recognize that the lowest value of m^2 is zero. If we now examine matrix elements of the

$$\chi(p_r) = \frac{1}{(p_r^2 - 2\mu E)^{l+1}} \left(\frac{p_r + \sqrt{2\mu E}}{p_r - \sqrt{2\mu E}} \right)^{c/2\sqrt{2\mu E}}.$$

In order for $\chi(p_r)$ to be single valued we must require

$$c/2\sqrt{2\mu E} = n,$$

where n is a nonzero integer. Solving for E we obtain

$$E = -Z^2 \mu e^4 / 2n^2, \quad (14)$$

which is just the energy of the hydrogen atom. Defining $p_0 = \mu Ze^2 = Za_0^{-1}$, where a_0 is the Bohr radius, we have

$$\chi_{n,l}(p_r) = \frac{(p_r + ip_0/n)^{n-l-1}}{(p_r - ip_0/n)^{n+l+1}}. \quad (15)$$

With the aid of GR Eqs. (3.384-9) and (9.237-2) in Ref. 19 it is a simple matter to transform χ back to position space and obtain r^l times the usual hydrogenic radial functions. Note that in order to prevent the function $\chi_{n,l}$ from becoming infinite at $p_r = \pm\infty$ we must require that $n \geq l+1$. It is also easy to see that $\chi_{n,l} = \chi_{-n,l}$ so that no new degeneracy has been introduced and we may restrict ourselves to positive values of n with no loss of generality.

We may now obtain the functions $\alpha(p_r)$ by integrating Eq. (15) l times. The constant of integration is chosen so that $\alpha(p_r) = 0$ at $p_r = \pm\infty$:

commutator of p_ϕ with v , recognizing p_ϕ is Hermitian

$$\langle m | [p_\phi, v] | m' \rangle = \langle m | v | m' \rangle,$$

we obtain $m = m' \pm 1$, which shows that successive eigenvalues of p_ϕ must differ by an integer. Consequently the spectrum of p_ϕ consists of all positive and negative integers, including zero.

We now turn our attention to Eq. (9) which may be written

$$\left[(1-u^2) \frac{d^2}{du^2} - 2u \frac{d}{du} - \frac{m^2}{1-u^2} \right] P(u) = -l(l+1)P(u).$$

Substituting $P(u) = (1-u^2)^{-m/2} Q(u)$ we obtain

$$(1-u^2) \frac{d^2 Q}{du^2} + 2(m-1)u \frac{dQ}{du} - m(m-1)Q = -l(l+1)Q.$$

Transforming to the momentum representation

we take

$$Q(u) \rightarrow \omega(p_\theta),$$

$$u \rightarrow i \frac{d}{dp_\theta},$$

$$\frac{d}{du} \rightarrow ip_\theta,$$

$$\left[p_\theta^2 \frac{d^2}{dp_\theta^2} + 2(m+1)p_\theta \frac{d}{dp_\theta} + p_\theta^2 + m(m+1) - l(l+1) \right] \omega(p_\theta) = 0. \quad (18)$$

It is easy to show [GR Eq. (8.494-8)] that this equation has solutions

$$\omega_l^m(p_\theta) = N_\theta p_\theta^{-(m+1/2)} J_{l+1/2}(p_\theta), \quad (19)$$

where N_θ is a normalization constant given by [GR Eq. (6.574-2)]

$$N_\theta^2 = \frac{2^{2m}(m!)^2(l+m)!}{(2m)!(l-m-1)!}.$$

We may readily show that ω_l^m are indeed transforms of $Q(u)$ with the aid of GR's Eqs. (7.321) and (8.936-2). Note that to prevent $\omega(p_\theta)$ from diverging at $p_\theta = 0$ we must require $|m| \leq l$.

We are, however, interested in the functions $\beta(p_\theta)$ which are transforms of the associated Legendre polynomials $P_l^m(u)$. [well-known solutions to Eq. (9)] rather than ω_l^m which are transforms of $Q(u)$. However, remembering

$$P_l^m(u) = (1-u^2)^{-m/2} Q_l^m(u)$$

and since $|u| \leq 1$, we may write

$$(1-u^2)^{-m/2} = 1 + \frac{1}{2}mu^2 + (1/2!) \frac{1}{2}m(\frac{1}{2}m+1)u^4 + \dots$$

Transforming this operator to momentum space it becomes

$$(1-u^2)^{-m/2} = 1 - \frac{1}{2}mD^2 + (1/2!) \frac{1}{2}m(\frac{1}{2}m+1)D^4 + \dots,$$

where we have used $D \equiv d/dp_\theta$ and we may write symbolically

$$\beta_l^m(p_\theta) = (1+D^2)^{-m/2} \omega_l^m(p_\theta). \quad (20)$$

However, due to the requirement $l \geq |m|$ and the known properties of Bessel functions, it is easy to see that β_l^m may be written as a finite polynomial in ω_j^k . The highest-order ω_j^k in this sum will be $j = E(l/2)$ and all the terms will involve the index $k = \frac{1}{2}m$. Thus, in general,

$$\beta_l^m = \sum_{j=E(m/2)}^{E(l/2)} a_j \omega_{j-m/2}^{m/2}. \quad (21)$$

Clearly, for $m=0$, we have $\beta_l^0 = \omega_l^0$. By direct Fourier transformation it may also be shown that

$$\beta_l^1 = \omega_{l+1/2}^{1/2} = p_\theta^{-(l+1)/2} J_{(l+1)/2}(p_\theta),$$

$$\beta_{l-1}^1 = \omega_{(l-1)/2}^{1/2} = p_\theta^{-l/2} J_{(l-1)/2}(p_\theta).$$

Other functions may be derived by use of recursion relations:

$$(2l+1)(1+D^2)^{1/2} \beta_l^{m-1} = \beta_{l-1}^m - \beta_{l+1}^m, \quad (22)$$

$$-(2l+1)iD\beta_l^m = (l-m+1)\beta_{l+1}^m + (l+m)\beta_{l-1}^m. \quad (23)$$

For example, recognizing

$$\begin{aligned} \omega_l^1 &= (1+D^2)^{1/2} \beta_l^1 \\ &= (2l+1)^{-1} (\beta_{l-1}^2 - \beta_{l+1}^2), \end{aligned}$$

we obtain

$$\beta_l^2 = \begin{cases} -\sum_{j=1}^{l/2} (4j-1) \omega_{2j-1}^1 & (l \text{ even}) \\ -\sum_{j=1}^{(l-1)/2} (4j+1) \omega_{2j}^1 & (l \text{ odd}). \end{cases}$$

We may see generally that for even values of m , β_l^m will involve Bessel functions of integer order, while for odd m , there will be functions of half-integer order.

CONCLUSION

We may now collect the complete solution which may be written

$$\phi_{n,l,m}(p_r, p_\theta, p_\phi) = \alpha_{n,l}(p_r) \beta_l^m(p_\theta) \delta(p_\phi + m),$$

$$\alpha_{n,l}(p_r) = \left(\frac{n}{ip_0} \right)^{3l+2} \sum_{k=0}^{n-l-1} \binom{n-l-1}{k} \frac{2^{k-l+1}}{(2l+k+1)(2l+k) \cdots (l+k+2)} \left(\frac{ip_0/n}{p_r - ip_0/n} \right)^{l+k+2},$$

$$\beta_l^m(p_\theta) = \sum_{j=E(m/2)}^{E(l/2)} a_j p_\theta^{-(m+1/2)} J_{j-(m-1)/2}(p_\theta).$$

The lowest few functions may be written

$$\phi_{1,0,0} = \frac{1}{(p_r - ip_0)^2} \frac{1}{p_\theta^{1/2}} J_{1/2}(p_\theta) \delta(p_\phi),$$

$$\phi_{2,0,0} = \frac{(p_r + ip_0/2)}{(p_r - ip_0/2)^3} \frac{1}{p_\theta^{1/2}} J_{1/2}(p_\theta) \delta(p_\phi),$$

$$\phi_{2,1,0} = \frac{1}{(p_r - ip_0/2)^3} \frac{1}{p_\theta^{1/2}} J_{3/2}(p_\theta) \delta(p_\phi),$$

$$\phi_{2,1,1} = \frac{1}{(p_r - ip_0/2)^3} \frac{1}{p_\theta} J_1(p_\theta) \delta(p_\phi + 1).$$

In this representation it is clear that the radial momentum must be considered as a complex variable. The radial function is a sum of terms with poles of order $l+2$ through $n+1$, with the singularity at $p_r = ip_0/n$. It is easy to see that this point is related to the ionization potential I through $p_0 = \sqrt{2\mu I}$ and is characteristic of momentum eigenfunctions. This has been discussed in considerable detail recently by Lassettre.²⁰

The functions derived above differ considerably from those derived by Podolsky and Pauling. This may be attributed to the considerable difference

in representation used. Since most of the subsequent work on momentum representation for atoms and molecules was based on their functions it would be worthwhile to extend the present treatment as well to such systems. It is well known, for example, that an examination of the nature and location of singularities in functions of a complex variable is of considerable value in understanding the function elsewhere in the complex plane. Thus, even though we are interested in the radial function for real values of p_r , its functional form is dependent on the location of its complex poles, which in turn may be related to ionization potentials, as well as electronegativities, dipole moments, and possibly other important atomic and molecular properties.²⁰ This realization will enable us to invoke the powerful tools of complex variables in the examination of multielectron atoms and molecules. This will be the topic of future investigations.

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