Dynamical symmetries and well-localized hydrogenic wave packets

Vladimir ZVEREV † and Boris RUBINSTEIN ‡
† Ural State Technical University, Ekaterinburg, 620002, Russia
zverev@dpt.ustu.ru
‡ Department of Mathematics, University of California, Davis, CA 95616, USA
boris@math.ucdavis.edu

Abstract

A new method for constructing of composite coherent states of the hydrogen atom, based on the dynamical group approach and various schemes of reduction to subgroups, is presented. A wide class of well-localized (Gaussian) hydrogenic wave packets for circular and elliptic orbits is found using the saddle-point method.

1 Introduction

In recent years, new experimental techniques opened way to creation and study of high energy (Rydberg) states in atoms. These states are described by approximate hydrogenic wave functions with very large principal quantum numbers. Some new effects, as the dynamical localization and the dynamical chaos, have attracted considerable interest. Explanation of these phenomena uses classical equations of motion \[. \] It is reasonable to look for an alternative quantum description on the basis of semi-classical approximations, which is naturally provided by a coherent states (CS) formalism.

In Section 2, starting from the O(4, 2) dynamical group approach \[ and using three schemes of reduction to subgroups \[ : O(4, 2) \supset O(4) \sim O(3) \otimes O(3), O(4, 2) \supset O(2, 2) \sim O(2, 1) \otimes O(2, 1), O(4, 2) \supset O(3) \otimes O(2, 1), \] we construct composite CS in physical and auxiliary (“tilted”) representations \[. \] We use two types of generating operators of CS with different procedures of transition to a classical limit. In particular, the generating operators for Perelomov SO(3) and SO(2, 1) CS \[, Barut-Girardello SO(2, 1) CS \[, \] generalized hypergeometric CS \[, Brif SO(3) and SO(2, 1) algebra eigenstates \[, may be used for this purpose. The CS are separated into two classes with different semi-classical behavior.

The hydrogenic CS wave functions have complicated form, so it is reasonable to use simplified asymptotic expressions. In Section 3 we describe a method for asymptotic estimate and obtain well-localized hydrogenic wave packets for circular and elliptic orbits. A similar asymptotic estimate method is used in the theory of CS path integrals. We believe that the approach discussed in this paper can be applied to computation of the CS path integrals for the hydrogen atom and other systems with known dynamical symmetry.

2 The hydrogen atom: O(4, 2) dynamical group and reductions to subgroups

Denote generators of the dynamical group O(4, 2) of the hydrogen atom \[ (the group of rotations in six-dimensional pseudo-Euclidean space with a metric \( g = \text{diag}(1, 1, 1, 1, -1, -1) \)) as \( \mathcal{L}_{\alpha \beta} \) (in the notation used in \[): \n
\[
\mathcal{L}_{\alpha 0} = (\mathbf{r} \times \mathbf{p})_\alpha, \quad \mathcal{L}_{\alpha 1} = (r_\alpha p^2 - 2p_\alpha \mathbf{r} \cdot \mathbf{p} + r_\alpha)/2.
\]

\[ Submitted to Proceedings of Institute of Mathematics of NAS of Ukraine.\]
\[
\mathcal{L}_{\alpha 2} = -r p_\alpha, \quad \mathcal{L}_{\alpha 3} = (r_\alpha p^2 - 2 p_\alpha r_\alpha) / 2, \\
\mathcal{L}_{0 1} = (r p^2 - r) / 2, \quad \mathcal{L}_{0 2} = r p - i, \quad \mathcal{L}_{0 3} = (r p^2 + r) / 2.
\]

The Schrödinger equation for the hydrogen atom reads \( (\mathcal{H} - E) |\Psi\rangle = 0 \) with \( \mathcal{H} = p^2 / 2 - a / r \).
After multiplication by \( r \) it can be rewritten in terms of the generators \( \mathfrak{P}_1, \mathfrak{P}_2, \mathfrak{P}_3, \mathfrak{P}_4, \mathfrak{P}_5, \mathfrak{P}_6, \mathfrak{P}_7, \mathfrak{P}_8 \):
\[
 r(\mathcal{H} - E) |\Psi\rangle = ((\mathcal{L}_{0 3} + \mathcal{L}_{0 1}) / 2 - E(\mathcal{L}_{0 3} - \mathcal{L}_{0 1}) - a) |\Psi\rangle = 0.
\]

The unitary transformation
\[
|\Psi\rangle = \exp(i \theta \mathcal{L}_{0 2}) |\Psi\rangle, \quad \tanh \theta = (1 + 2E) / (1 - 2E),
\]
reduces \( \mathfrak{P} \) to
\[
(\mathcal{L}_{0 3} - a / \sqrt{-2E}) |\Psi\rangle = 0.
\]

The eigenstates of \( \mathcal{L}_{0 3} \) may be chosen in this auxiliary representation (AR) as \( |n, l, m\rangle_{sph} \) or \( |n, n_1, n_2, m\rangle_{par} \) with \( n = a / \sqrt{-2E} \), in the spherical or parabolic coordinates. An inverse transformation
\[
\left\{ \begin{array}{c} |n, l, m\rangle_{sph} \vspace{1mm} \\ |n, n_1, n_2, m\rangle_{par} \end{array} \right\} = \exp(-i \theta \mathcal{L}_{0 2}) \left\{ \begin{array}{c} |n, l, m\rangle_{sph} \vspace{1mm} \\ |n, n_1, n_2, m\rangle_{par} \end{array} \right\},
\]
produces the physical representation (PR) of the eigenvectors.

Consider three types of reduction to subgroups and corresponding Lie algebras:

\[
\begin{align*}
(\text{a}) & \quad O(4, 2) \supset O(4) \sim O(3) \otimes O(3), \quad o(3) \oplus o(3) = \{ \mathfrak{P}_\alpha^{(+)} \} \oplus \{ \mathfrak{P}_\alpha^{(-)} \}, \\
(\text{b}) & \quad O(4, 2) \supset O(2, 2) \sim O(2, 1) \otimes O(2, 1), \quad o(2, 1) \oplus o(2, 1) = \{ \mathfrak{Q}_\alpha^{(+)} \} \oplus \{ \mathfrak{Q}_\alpha^{(-)} \}, \\
(\text{c}) & \quad O(4, 2) \supset O(3) \otimes O(2, 1), \quad o(3) \oplus o(2, 1) = (\mathcal{L}_{0 a} \oplus \mathcal{L}_{0 a}),
\end{align*}
\]

where
\[
\mathfrak{P}_\alpha^{(+)} = (\mathcal{L}_{0 a} \pm \mathcal{L}_{0 a}) / 2, \quad \mathfrak{Q}_\alpha^{(+)} = (\mathcal{L}_{0 a} \pm \mathcal{L}_{0 a}) / 2.
\]

For these cases the space \( R \) of bound states of the hydrogen atom is decomposed as follows:

\[
\begin{align*}
(\text{a}) & \quad R = \oplus_{n \geq 1} \left( R(O(3), n-1, (n_1)) \otimes R(O(3), n-1, (n_2)) \right), \\
(\text{b}) & \quad R = \oplus_{m \in \mathbb{Z}} \left( R(O(2,1), n, (n_1 + 1/2 (m - |m|))) \otimes R(O(2,1), n, (n_2 + 1/2 (m - |m|))) \right), \\
(\text{c}) & \quad R = \oplus_{l \geq 0} \left( R(O(3), l, (l - m)) \otimes R(O(2,1), (l - 1), (n - 1 - l)) \right),
\end{align*}
\]

where \( R(G, S, (K)) = \{ \mathcal{G} S, (K) \} \) denotes the irreducible representation space of a group \( G = O(3) \) or \( O(2, 1) \) with generators \( \{ E_n \} \), for which we have
\[
E_3 |\mathcal{G} S, (K)\rangle = (S/2 - \epsilon G K) |\mathcal{G} S, (K)\rangle, \\
(E_1^2 + E_2^2 + \epsilon G E_3^2) |\mathcal{G} S, (K)\rangle = (S/2 - \epsilon G S^2/4) |\mathcal{G} S, (K)\rangle,
\]
where \( \epsilon_{O(3)} = 1 \), \( \epsilon_{O(2,1)} = -1 \), and the representation space \( R(G, S, (K)) \) is spanned by the set of orthonormal eigenvectors \( |\mathcal{G} S, (K)\rangle \). The vector subspaces
\[
R_0^{[+]} = \{ |n, n, -n-1, -n+1\rangle_{sph} \} = \{ |n, 0, 0, n-1\rangle_{par} \}, \\
R_0^{[-]} = \{ |n, n, -n-1, n+1\rangle_{sph} \} = \{ |n, n-1, n-1, -n+1\rangle_{par} \},
\]
with maximal \( m = n-1 \) or minimal \( m = -n+1 \) values of the magnetic quantum number correspond to the circular orbits \( \{ 3 \} \). The vectors from \( R_0^{[\pm]} \) play the role of reference vectors in decompositions \( \{ 4 \} \). On the other hand, \( R_0^{[-]} \) and \( R_0^{[+] \pm} \) are irreducible spaces of \( O(2, 1) \) \( (S = 1) \). The corresponding \( O(2, 1) \) Lie algebras have the form
\[
\mathcal{H}_1^{[\pm]} = (\pm \mathcal{L}_{12} - \mathcal{L}_{22}) / 2, \quad \mathcal{H}_2^{[\pm]} = (\mathcal{L}_{21} \pm \mathcal{L}_{12}) / 2, \quad \mathcal{H}_3^{[\pm]} = (\pm \mathcal{L}_{03} \pm \mathcal{L}_{30}) / 2,
\]

2
where $\pm$ corresponds to the subspace $R_0^{[\pm]}$ with $m = \pm(n - 1)$. Following [12], we construct coherent states in two stages. At first, using the operators $\{H_0^{[\pm]}\}$, we construct the circular orbits CS in $R_0^{[\pm]}$. Next, we construct CS in the global space $R$ using one of the generator sets from [3]. Each reduction scheme corresponds to a specific construction method of the hydrogen atom CS:

\[(a)\] \[|O^{(3)}(\omega^{[\pm]}, \tau, \eta) = D_{\xi}(O^{(3)}(\tau, (P_{\alpha}^{(+)})|D_{\xi}(O^{(3)}(\eta, (P_{\alpha}^{(-)}))|\omega^{[\pm]}),\]

\[(b)\] \[|O^{(2,1)}(\omega^{[\pm]}, \tau, \eta) = D_{\xi}(O^{(2,1)}(\tau, (Q_{\alpha}^{(+)})|D_{\xi}(O^{(2,1)}(\eta, (Q_{\alpha}^{(-)}))|\omega^{[\pm]}),\]

\[(c)\] \[|O^{(3)}\otimes O^{(2,1)}(\omega^{[\pm]}, \tau, \eta) = D_{\xi}(O^{(3)}(\tau, (L_{\alpha}))|D_{\xi}(O^{(2,1)}(\eta, (L_{\alpha}))|\omega^{[\pm]}),\]

where

\[|\omega^{[\pm]} = D_{\xi}(O^{(2,1)}(\omega, (H_0^{[\pm]}))|1, 0, 0, 0)_{par}\]

is the circular orbit CS. We use an uniform notation for the generating operator of CS:

\[|G_S(\omega) = D_{\xi}(G_\omega, (E_{\alpha}))|G_S(0)),\]

where $G = O(3)$ or $O(2,1)$, and $\Omega = \mathbb{I}$ or $\mathbb{II}$. An important point is that one should use two types of generating operators of CS, with different procedures for transition to the classical limit: $S \to \infty (\Omega = \mathbb{I}); |\omega| \to \infty (\Omega = \mathbb{II})$.

There exist many algorithms to construct coherent states of dynamical groups and quantum physical systems (see review [13]). In most cases these CS provide a transition to the "classical limit" in some sense. However, a selection of the CS for a specific physical system must be done with great care. It is essential to take into account not only the symmetry of a model, but also the type of semiclassical behavior. We consider some special types of CS and clarify conditions of quantum-classical correspondence.

Usually CS $|\xi\rangle$ is called semiclassical if an overlapping distribution function $|\langle \xi | | \xi + \delta \xi\rangle|^2$ has a sharp peak for small $|\delta \xi\rangle$, and becomes singular delta-shaped function in the classical limit, which can be written in the form

\[\langle \xi | \eta \rangle_{cl.lim.} \to 0, \quad \xi \neq \eta; \quad \langle \xi | \xi \rangle = 1.\]

Satisfaction of the condition

\[\langle \xi | E^2 \rangle / (\langle \xi | E_{\alpha} \rangle)^2_{cl.lim.} \to 1,\]

where $E_{\alpha}$ are elements of the Lie algebra $L$, gives another evidence of semiclassical properties of the CS $|\xi\rangle$. The conditions (7), (8) are satisfied in the cases: the Barut-Girardello $O(2, 1)$ CS, $|\xi| \to \infty, L = o(2, 1)$; the Perelomov $O(2, 1)$ CS, $S \to \infty, L = o(2, 1)$; the Perelomov $O(3)$ CS, $S \to \infty, L = o(3)$.

An extended class of semiclassical CS follows from a definition of the generalized hypergeometric CS [7]:

\[|\xi\rangle = N^{-1}_\xi \sum_{n=0}^{\infty} \sqrt{\frac{\prod_{i=1}^{p} (\alpha_i)_n}{\prod_{j=1}^{p} (\beta_j)_n}} \frac{\xi^n}{\sqrt{n!}} |n\rangle,\]

where $(\alpha)_n$ is the Pochhammer symbol and $pF_q$ denotes the generalized hypergeometric function; $\xi$ is a complex argument; integers $\alpha_i$ are negative for $i = 1, ..., l$ and positive for $i = l + 1, ..., p$; $0 \leq l \leq p$; $\rho_j$ are positive real numbers. The overlapping function for these states has the form:

\[\langle \xi | \xi \rangle = N^{-1}_\xi N^{-1}_\xi pF_q((\alpha_p), (\rho_q), (-1)^l \xi^*, \zeta), \quad \langle \xi | \xi \rangle = 1.\]

Starting from the definition (9), let us consider a number of special realizations:

(i) $p = q + 1 \geq 1$, $\rho_j = 1$, $\alpha_j = S$, $S = 1, 2, ...$; in the special case $p = 1$ the state (9) is the Perelomov $O(2, 1)$ CS [3];

(ii) $p = q + 1 \geq 1$, $\rho_j = 1$, $\alpha_j = -S$, $S = 1, 2, ...$; in the special case $p = 1$ the state (9) is the Perelomov $O(3)$ CS [3];

(iii) $q \geq p$, $\rho_j = 1$, $\alpha_j = S$, $S = 1, 2, ...$; in the case $p = q = 0$ the state (9) is the CS of a harmonic oscillator [14]; in the case $p = -1, q = 0$ this is the Barut-Girardello CS [6].
We use the standard saddle-point method of asymptotic estimate for integrals

\[ F(\lambda, x) = \int_c \exp\{\lambda f(x, t)\} \phi(x, t) dt, \]

where \( \lambda \gg 1 \), \( x = \{x_1, x_2, \ldots, x_n\} \) and \( t = \{t_1, t_2, \ldots, t_m\} \); \( f(x, t) \) and \( \phi(x, t) \) are holomorphic functions; \( c \) is a \( n \)-dimensional smooth manifold deformed to reach a minimax (a saddle point is nonsingular). The asymptotic formula reads [15]

\[ F(\lambda, x) \sim (2\pi/\lambda)^{m/2} \exp\{\lambda f(x, t_0(x))\} \phi(x, t_0(x))/\sqrt{\det [\mu(x, t_0(x))]}, \]

where \( t = t_0(x) \) is a solution of the system of equations \( \partial f/\partial t_i = 0, i = 1, \ldots, m \), for a stationary point, and \( \mu_{ij} = \partial^2 f/\partial t_i \partial t_j \). We also assume that \( |F(\lambda, x)| \) has the delta-shaped peak near the point \( x = x_{00} \). Since \( |F(\lambda, x)| \sim |\exp\{\lambda f(x, t_0(x))\}| \sim \exp\{\text{Re} f(x, t_0(x))\} \), we can find \( x_{00} \) as an extremal point of the real part of the exponent. The supplementary equations for the stationary point have the form

\[ \frac{\partial f(x, t_0(x))}{\partial x_i} + c.c. = \frac{\partial f(x, t)}{\partial x_i} \Big|_{t = t_0(x)} + c.c. = 0. \]

Substituting the second order expansion of \( f(x, t_0(x)) \) at \( x = x_{00} \) into [10], we find the desired expression for the asymptotic estimate

\[ F(\lambda, x) \sim (2\pi/\lambda)^{m/2} \sqrt{\det [-\mu_{00}]}^{-1} \phi_{00} \exp \{\lambda f_{00} + i\hbar h^T \delta x \}
+ (\lambda/2) \delta x^T \left( \sigma_{00} - \gamma_{00}^T \mu_{00}^{-1} \gamma_{00} \right) \delta x \],

with

\[ \sigma_{00} = \left\{ \frac{\partial^2 f_{00}}{\partial x_k \partial x_l} \right\}, \qquad \gamma_{00} = \left\{ \frac{\partial^2 f_{00}}{\partial x_k \partial t_l} \right\}, \qquad h = \left\{ \text{Im} \left[ \frac{\partial f_{00}}{\partial x_k} \right] \right\}, \]

where we use the notation \((\cdot)|_{x = x_{00}, t = t_{00}}\) for different functions given in the point \((x_{00}, t_{00})\), \( t_{00} \equiv t_0(x_{00}) \).

Consider in detail a special case of hydrogenic CS wave function. Using the formulae [5] and [8] with generating operators for the Perelomov CS (P) and the Barut-Girardello CS (BG), we obtain

\[ |\omega, 0, \eta \rangle = D_1^{(O(2, 1))} \eta \{(L_{00}) \} D_1^{(O(2, 1))} \Omega \{(H_{BG}^{(3)})\}|1, 0, 0\rangle_{sph}. \]
Performing the summation we arrive at

\[ (r|n, l, m) = \frac{2}{(2l + 1)!} \sqrt{\frac{(n + l)!}{(n - l - 1)!}} (2r)^l e^{-r} F_1(l + 1 - n, 2l + 1, 2r) Y_{lm}(\theta, \phi), \]

and in the physical representation

\[ (r|n, l, m) = \frac{1}{n^2} \langle n|l, m\rangle, \]

we obtain the explicit form for the CS:

\[ (r|\omega, 0, \eta) = \frac{1}{\sqrt{\pi I_0(2|\omega|)}} \sum_{l=0}^{\infty} \sum_{n=l+1}^{\infty} \frac{\omega^l}{l!} (1 - |\eta|^2)^{l+1} \sqrt{\frac{(n + l)!}{(n - l - 1)!}} \eta^{n-l-1} \langle r|n, l, m\rangle. \]

Performing the summation we arrive at

\[ (r|\omega, 0, \eta) = \frac{1}{\sqrt{\pi I_0(2|\omega|)}} \frac{1 - |\eta|^2}{(1 - |\eta|^2)^2} e^{-r(1 + \eta)/1 - \eta} I_0 \left( \frac{2\sqrt{-\omega r_+ (1 - |\eta|^2)}}{1 - \eta} \right), \]

where \( r_+ = r \exp(i\phi) \), \( r = |r| \) and \( I_0 \) denotes the modified Bessel function. The asymptotic estimate (obtained directly or by the saddle-point method) for the absolute value of the CS wave function has the form:

\[ |(r|\omega, 0, \eta)|^2 \approx \frac{1}{2\pi^{3/2}|\omega|^{1/2}} \left( \frac{1 - |\eta|^2}{1 - |\eta|^4} \right) \exp \left\{ \frac{1}{2} \frac{(1 - |\eta|^2)}{|1 - |\eta|^4|} (\Delta x^2 + \Delta y^2 + 2\Delta z^2) \right\}, \]

where \( \Delta x = x - x_0 \), \( \Delta y = y - y_0 \); the point with coordinates \( x_0 = \langle n \rangle_\infty (e - \cos \theta) \), \( y_0 = \langle n \rangle_\infty \sqrt{1 - e^2} \sin \theta \) lies on the elliptic orbit with an eccentricity \( e \):

\[ \langle n \rangle_\infty = \frac{|\omega|(1 + |\eta|^2)}{1 - |\eta|^2}, \quad e = \frac{2|\eta|}{1 + |\eta|^2}. \]

In a similar way one can find the asymptotic estimate for the physical CS wave function, but it is omitted here due to its complexity. In this case only the saddle-point method with interchange of summation and integration can be used. It is remarkable that in this case the system of equations for the saddle point admits analytical solution. In a special case of circular orbits the asymptotic estimate for auxiliary and physical representations simplifies to

\[ (r_0 + \Delta r|\omega, 0, 0) \approx \frac{1}{\sqrt{2\pi^{3/4}|\omega|^{1/4}}} e^{-z_1^2/2|\omega|} \exp \left\{ i|\omega|\Delta \phi - z_1^2 \frac{|\Delta \phi|^2}{2|\omega|} - \frac{\Delta \rho^2}{4|\omega|^2} + \frac{i\Delta \rho \Delta \phi}{2} \right\}, \]

where \( r = (\rho \cos \phi, \rho \sin \phi, z) \), \( \Delta \phi = \phi - \phi_0 \), \( \Delta \rho = \rho - |\omega| \), and

\[ (r_0 + \Delta r|\omega, 0, 0) \approx \frac{1}{\sqrt{5\pi^{3/4}|\omega|^{9/4}}} e^{-z_1^2/2|\omega|^3} \exp \left\{ i|\omega|\Delta \phi - z_1^2 \frac{|\Delta \phi|^2}{10|\omega|^3} - \frac{\Delta \rho^2}{10|\omega|^3} + \frac{i\Delta \rho \Delta \phi}{5|\omega|} \right\}, \]

where \( r = (\rho \cos \phi, \rho \sin \phi, z) \), \( \Delta \phi = \phi - \phi_0 \), \( \Delta \rho = \rho - |\omega|^2 \). The functions [11] and [12] are related by the following equation:

\[ \langle r_1|\omega, 0, 0 \rangle = \int \frac{dr_2}{r_2^2} K(r_1, r_2)(r_2|\omega, 0, 0), \]

where

\[ K(r_1, r_2) \approx \frac{1}{\sqrt{10\pi^3 \rho_0^2}} e^{-z_2^2/2\rho_2} - \frac{z_1^2}{2\rho_2} - \frac{\Delta \phi^2}{10\rho_2^2} + \frac{i\Delta \rho \Delta \phi}{5\rho_2}, \]

and \( \Delta \phi = \phi_1 - \phi_2 \), \( \Delta \rho = \rho_1 - \rho_2^2 \).
References

[1] Bellomo P., Stroud C.R., Farrelly D. and User T., Quantum-classical correspondence in the hydrogen atom in weak external fields, Phys. Rev. A, 1998, 58, 3896.

[2] Barut A.O. and Raczka R., Theory of Group Representations and Applications, Singapore, World Scientific, 1986.

[3] Zverev V.V. and Rubinstein B.Ya., Coherent states of the hydrogen atom, Soviet Physics – Lebedev Institute Reports, 1982, 11, 4.

[4] Bechler A., Group theoretic approach to the screened Coulomb problem, Ann. Phys., 1977, 108, 49.

[5] Perelomov A.M., Coherent states for arbitrary Lie group, Commun. Math. Phys., 1972, 26, 222.

[6] Barut A.O. and Girardello L., New coherent states associated with noncompact groups, Commun. Math. Phys., 1971, 21, 41.

[7] Zverev V.V., Semiclassical description of quantum systems by means of hypergeometric coherent states, Abstract book of EASTMAG-2001, Institute of Metal Physics, Ekaterinburg, 2001, 345.

[8] Brif C., SU(2) and SU(1,1) algebra eigenstates: a unified analytic approach to coherent and intelligent states, Int. J. Theor. Phys., 1997, 36, 1651.

[9] Fock V., Zür theorie des Wasserstoffatoms, Z. Phys., 1935, 98, 145.

[10] Bednar M., Algebraic treatment of quantum-mechanical models with modified Coulomb potentials, Ann. Phys., 1973, 75, 305.

[11] Brown L.S., Classical limit of the hydrogen atom, Am. Journ. Phys., 1973, 41, 525.

[12] Mostowski J., On the classical limit of the Kepler problem, Lett. Math. Phys., 1977, 2, 1.

[13] Wei-Min Zhang, Da Hsuan Feng and Gilmore E., Coherent states: theory and some applications, Rev. Mod. Phys., 1990, 62, 867.

[14] Glauber R., Photon correlations, Phys. Rev. Lett., 1963, 10, 84.

Sudarshan E.C.G., Equivalence of semiclassical and quantum mechanical description of statistical light beams, Phys. Rev. Lett., 1963, 10, 277.

[15] Fedorjuk M.V., Asymptotics: Integrals and Series, Moscow, Nauka, 1987.