Coherent States of the Hydrogen Atom

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Abstract

Coherent states of the hydrogen atom are constructed using Perelomov and Barut-Girardello methods. Quasiclassical properties of such states are discussed.

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Denote generators of the dynamical group $O(4,2)$ of the hydrogen atom as $a_{\alpha\beta}$ which are related to notation used in [1]: $a_{\alpha 1} = M_\alpha,\ a_{\alpha 2} = -\Gamma_\alpha,\ a_{\alpha 3} = A_\alpha,\ a_{01} = \Gamma_4,\ a_{02} = T,\ a_{03} = \Gamma_4$. We assume that the vectors of spherical $|n,l,m>$ and parabolic $|n,n_1,n_2,m>$ bases in a vectorial R space which are produced out of the physical space vectors by a hyperbolic "rotation" (the transformation $\psi \to \tilde{\psi}$ in [1]) are the eigenvectors of the operators a_{03} and a_{30} with the eigenvalues n and m $(n_1 + n_2 = n - m - 1)$.

Consider three types of reduction to a subgroup corresponding to a certain construction procedure of the R space (more accurately, subspaces $R^\pm$, their union produces R) starting from irreducible representations (IR) spaces of groups $O(3)$ and $O(2,1)$:

(a) $O(4,2) \supset O(4) \sim O(3) \otimes O(3)$
(b) $O(4,2) \supset O(2,2) \sim O(2,1) \otimes O(2,1)$
(c) $O(4,2) \supset O(3) \otimes O(2,1)$

with generating subalgebras have form:

(a) $p^+_\alpha \oplus p^-_\beta$
(b) $q^+_\alpha \oplus q^-_\beta$
(c) $a_{\alpha 0} \oplus a_{0\beta}$

where

$$p^\pm_\alpha = 1/2(a_{\alpha 0} \pm a_{\alpha 3}); q^\pm_\alpha = 1/2(a_{0\alpha} \pm a_{3\alpha}).$$

For these cases we may write:

$$\begin{aligned}
(a)\ R &= \oplus_{n\geq 1}\{R(+,n-1,(n_1)) \otimes R(+,n-1,(n_2))\},\\
(b)\ R^+ &= \oplus_{m\geq 0}\{R(-,m+1,(n_1)) \otimes R(-,m+1,(n_2))\},\\
R^- &= \oplus_{m\leq 0}\{R(-,1-m,(n_1+m)) \otimes R(-,1-m,(n_2+m))\},\\
(c)\ R &= \oplus_{l\geq 0}\{R(+,2l,(l-m)) \otimes R(-,2l+2,(n-1-l))\},
\end{aligned} \tag{1}$$

where $R(\epsilon,S,(K))$ denotes IR spaces of groups $O(3)$ and $O(2,1)$. Indicies of basis vectors $|(\epsilon,S),K\rangle$ are chosen in such a way that the operators E_3 and $E_1^2 + E_2^2 + \epsilon E_3^2$ have an

eigenvalues $S/2-\epsilon K$ and $S/2+\epsilon S^2/4$ correspondingly. Here E_α are generators of these groups; $\epsilon=\pm 1$ (or $\pm$); plus(minus) signs correspond to group $O(3)$ ($O(2,1)$); $s=1,2,\ldots$ denotes IR; $k=0,1,\ldots$ and not exceeds s for $O(3)$ and is unlimited for $O(2,1)$.

The vectorial subspaces with maximal $|n,0,0,n-1\rangle$ (minimal $|n,n-1,n-1,-n+1\rangle$) values of magnetic quantum number correspond to the circular orbits (CO) [2] which are the main vectors in the subspaces generating the diadic sums (2). The IR of group $O(2,1)$ for $s=1$ enters the subspaces of CO vectors: corresponding generators are

$$\chi_1^{\pm}=\frac{1}{2}(\pm a_{11}-a_{22});\ \chi_2^{\pm}=\frac{1}{2}(a_{21}\pm a_{12});\ \chi_3^{\pm}=\frac{1}{2}(\pm a_{03}\pm a_{30}),$$

where $\pm$ corresponds to the vectorial subspace with $m=\pm(n-1)$.

Using the methods discussed in [3] we construct coherent states (CS) in the subspace R in two stages – at the first one we introduce CS in the CO vectorial subspaces (using the operators $\chi_\alpha^{\pm}$), and then we construct CS in R using the generators of subgroups in (2). Consider the CS of groups $O(3)$ and $O(2,1)$ using the generating operators (we omit explicit expressions given in [4, 5]:

$$|(\epsilon,S),\omega\rangle=D_\nu((\epsilon,S),\omega,(K_\alpha))|(\epsilon,S),K=0\rangle, \tag{2}$$

where $\nu=1$ corresponds to CS introduced by Perelomov in [4] for $O(3)$ and $O(2,1)$; $\nu=2$ corresponds to CS by Barut and Girardello in [5] for $O(2,1)$. We call the CS $|\psi_i\rangle$ quasiclassical if they have a classical limit (CL) property $|\langle\psi_i|\psi_k\rangle|^2\to 0$ for $|\psi_i\rangle\neq|\psi_k\rangle$ ($\langle\psi_i|\psi_i\rangle=1$), and if the mean values of the operator products tend to the product of mean values. Perelomov's CS are quasiclassical at $s\to\infty$, and Barut-Girardello CS have this property at fixed s and $|\omega|\to\infty$. It should be underlined that there are different limiting operations to CL transformation for different types of CS.

The value of s is fixed for $O(2,1)$ IR in the CO vector spaces, hence at the first stage we use the Barut-Girardello method to produce the quasiclassical states arriving at:

$$|\omega^{\pm}\rangle=D_2((-,1),\omega,(\chi_\alpha^{\pm}))|1,0,0,0\rangle. \tag{3}$$

At $|\omega|\to\infty$ main contribution to mean values calculated with the states (3) comes out of CO vectors with large n. For each $O(3)$ and $O(2,1)$ IR space this number plays a role of the index s, so at the second stage we use the Perelomov method. Then each reduction scheme in (2) corresponds to a separate construction method of hydrogen atom CS:

$$|O(4),\omega^{\pm},\tau,\eta\rangle = D_1((+),\tau,(p_\alpha^+))D_1((+),\eta,(p_\alpha^-))|\omega^{\pm}\rangle, \tag{4}$$

$$|O(2,2),\omega^{\pm},\tau,\eta\rangle = D_1((-),\tau,(q_\alpha^+))D_1((-),\eta,(q_\alpha^-))|\omega^{\pm}\rangle, \tag{5}$$

$$|O(3)\otimes O(2,1),\omega^{\pm},\tau,\eta\rangle = D_1((+),\tau,(a_{\alpha 0}))D_1((-),\eta,(a_{0\alpha}))|\omega^{\pm}\rangle. \tag{6}$$

Consider a transition to CL for the CS of the type (4) with plus sign chosen. Consider the CS in the equivalent form using another parametrization

$$T(\alpha,\beta,\gamma)\exp(i\lambda a_{13})|\omega^{\pm}\rangle,$$

and find mean values in these CS. The rotation operator $T(\alpha,\beta,\gamma)$, determining an angular position of an electron density in a physical space, may be omitted. Considering

the mean values of the main quantum number, angular moment components, electron position vector components and its modulus calculated using the CS $\exp(i\lambda a_{13})|\omega^{\pm}\rangle$ one may deduce that in the limit $|\omega| \to \infty$ these CS describe a wave packet moving along an elliptic orbit with an eccentricity $\sin\lambda$ (the angular moment is equal to $\langle n\rangle \cos\lambda, \langle n\rangle \sim |\omega|$). The angular position of the packet center is determined by the parameter $\arg\omega$. Averaging Heisenberg equation for electron position using the CS and replacing averages of products by products of averages (this operation is valid in quasiclassical limit) one can produce classical Kepler equation of motion.

In conclusion, the suggested method of CS construction for hydrogen atom differs from that of described in [3], in which at both construction stages the Perelomov method was used. CS discussed there are not quasiclassical contrary to CS introduced in this communication.

References

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