An algebraic construction of the coherent states of the Morse potential based on SUSY QM

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(August 23, 2016)

By introducing the shape invariant Lie algebra spanned by the SUSY ladder operators plus the unity operator, a new basis is presented for the quantum treatment of the one-dimensional Morse potential. In this discrete, complete orthonormal set, which we call the pseudo number states, the Morse Hamiltonian is tridiagonal. By using this basis we construct coherent states algebraically for the Morse potential in a close analogy with the harmonic oscillator. We also show that there exists an unitary displacement operator creating these coherent states from the ground state. We show that our coherent states form a continuous and overcomplete set of states. They coincide with a class of states constructed earlier by Nieto and Simmons by using the coordinate representation.

3.65.Fd, 02.20.Sv, 42.50.-p

I. INTRODUCTION

Coherent states [1] for systems other than the harmonic oscillator have attracted great attention for several years [2–8]. There are a number of different approaches to this problem and the one presented here is based on the methods of supersymmetric quantum mechanics (SUSY QM). It is well-known that this method allows the algebraic treatment of the eigenvalue problems of Hamiltonians associated with shape invariant potentials [9–12]. Since the SUSY description combined with the concept of shape invariance can be regarded as a generalization of the ladder operator method of the harmonic oscillator, one might think that the SUSY ladder operators will play an important role in the construction of coherent states for other, non-harmonic potentials, too. Based on this idea an algebraic construction of coherent states were proposed by Fukui and Aizawa [3] for the class of shape invariant potentials having an infinite number of bound energy eigenstates. Their definition, however, does not work for potentials, where the number of normalizable energy eigenstates is finite. Among these latter problems a particular attention deserves the Morse potential, because it plays an important role in applications like molecular vibrations and laser chemistry.

In this paper we present a new algebraic method by using the SUSY ladder operators and shape invariance to obtain coherent states for the one-dimensional Morse potential. Considering the shape invariant Lie group spanned by the SUSY ladder operators and the identity, we will introduce a new orthonormal basis set in the state space, called pseudo number states, having in a certain extent similar properties with respect of the Morse potential as the stationary states for the harmonic oscillator. In contrast with the set of energy eigenstates of the Morse Hamiltonian, this basis is a complete discrete set of normalizable states. However, this basis does not diagonalize the Hamilton operator, but tridiagonalizes it. By the help of these pseudo number states we will define our coherent states in a similar form as it is usual in the case of harmonic oscillator:

$$|β⟩ = g(β) ∏ \sum_{n=0}^{∞} \frac{β^n}{n!} |n⟩,$$

where β is a complex number, |n⟩ is an element of the above mentioned basis, {n}! is a later specified generalized factorial and g(β) is a normalization term. We will show that these states satisfy the minimal requirements established by Klauder (see in Ref. [4]) to be termed as coherent: they are continuous functions of the label β, and form an (over)complete set in the Hilbert space. It will be also shown that an unitary displacement operator exits in a quite similar form as in the case of the harmonic oscillator, so that the coherent states are generated by this operator from the ground state as: |β⟩ = D(β)|0⟩. We note that the coordinate representation wave functions corresponding to our coherent states have been obtained earlier by Nieto and Simmons [2] in an entirely different way.

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II. THE LIE ALGEBRA AND THE PSEUDO NUMBER STATES OF THE MORSE HAMILTONIAN

In this work we consider the Morse Hamiltonian:

\[
\hat{H}(s) = \frac{\hat{P}^2}{2m} + V_0 \left(s + \frac{1}{2} - \exp(-\gamma \hat{X})\right)^2,
\]

where \(s\), \(V_0\) and \(\gamma\) are real parameters depending on the shape of the potential, while the position and the momentum operators obey the commutation relation \([\hat{X}, \hat{P}] = i\hbar\). Introducing the dimensionless operators \(X = \gamma \hat{X}\) and \(P = \frac{1}{\sqrt{2mV_0}} \hat{P}\), and choosing the units so that \(\sqrt{\hbar} = 1\), we have \([X, P] = i\) and \(\hat{H} = V_0 H(s)\) with

\[
H(s) = P^2 + \left(s + \frac{1}{2} - \exp(-X)\right)^2.
\]

From now on we consider this latter \(H(s)\) as the Hamiltonian. If \(s > 0\), then there exists a normalizable ground state \(|\Psi_0(s)\rangle\) with energy \(E_0(s)\). As it is known from the theory of SUSY QM one can introduce the SUSY ladder operators \(A(s), A^\dagger(s)\) so that \(A(s)\) annihilates the ground state:

\[
A(s) |\Psi_0(s)\rangle = 0,
\]

and the Hamiltonian can be factorized as:

\[
H(s) = A^\dagger(s)A(s) + E_0(s).\]

In the case of Morse potential the ladder operators \(A(s)\) and \(A^\dagger(s)\) can be written as [10]:

\[
A(s) = s - \exp(-X) + iP,
\]

\[
A^\dagger(s) = s - \exp(-X) - iP.
\]

Considering the partner Hamilton operator, \(H^p(s) = A(s)A^\dagger(s) + E_0(s)\), one finds that the Morse potential is shape invariant [9], which means:

\[
H^p(s) = H(f(s)) + R(f(s)),
\]

with \(f(s) = s - 1\) and \(R(s) = 2(s+1)\). Due to this shape invariance property one can determine the energy eigenstates in an algebraic manner by generating them from the ground state, as well as the eigenvalues in the following way:

\[
|\Psi_n(s)\rangle \propto A^\dagger(s) \cdots A^\dagger(s-n+1) |\Psi_n(s-n)\rangle,
\]

\[
E_n(s) = E_0(s) + \sum_{k=1}^{n} R(s-k).
\]

The Morse potential has only a finite number of bound states (the integer part of \(s+1\)), which cannot form a complete set of states in the Hilbert space. Hence the full quantum description of the Morse potential is impossible by restricting oneself only to these bound states. One can of course use the continuous part of the spectrum of \(H\), but instead let us introduce here the following infinite series of states:

\[
|0\rangle \equiv |\Psi_0(s)\rangle,
\]

\[
|1\rangle \equiv C^{-1} A^\dagger(s) |0\rangle
\]

\[
|n\rangle \equiv C^{-1} A^\dagger(s+n-1) |n-1\rangle
\]

where \(n\) is a positive integer \((n \in \mathbb{N}^+)\) and \(C_n = \sqrt{n(2s+n-1)}\) is a normalization coefficient. We would like to emphasize here that the direction of the parameter shift in (8) is opposite to that of \(f(s)\) appearing in Eqs. (7), and (9). As one can easily check, the SUSY ladder operators \(A(s), A^\dagger(s)\) and the identity operator span a Lie algebra. Since for any \(n (n \in \mathbb{Z})\) we have:

\[
A(s + n) = A(s) + nI \quad (n \in \mathbb{Z}),
\]
the Lie algebra is invariant under the shift of the shape parameter $s$. An easy calculation shows that the SUSY ladder operators satisfy the following commutation relations:

\[
[A(s + m), A(s + n)] = 0 \quad \quad (n, m \in \mathbb{Z}),
\]

\[
[A(s + m), A^\dagger(s + n)] = 0,
\]

\[
[A(s + m), A^\dagger(s + n)] = 2sI - (A(s) + A^\dagger(s)).
\]

Eqs. (10-11), are valid for any complex $n$, but we shall exploit this property only for real, integer $n$. Using these relations and the fact that $A(s)$ annihilates the ground state: $A(s)|\Psi_0(s)\rangle = 0$, one can verify that the states defined in (3) are mutually orthogonal:

\[
\langle m| n \rangle = \delta_{m,n}.
\]

We are going to call these states as pseudo number states of the Morse potential.

To find the wave functions of our pseudo number states let us introduce a function of the coordinate variable as $y = 2 \exp(-x)$. By the help of (3) and (4) we find that the wave functions in question obey the following recursion relation:

\[
\varphi_0(y) := \langle y| 0 \rangle = \frac{1}{\sqrt{\Gamma(2s)}} y^s \exp(-y/2),
\]

\[
\varphi_n(y) := \langle y| n \rangle = C_n^{-1}(y \frac{\partial}{\partial y} + (s + n - 1) - \frac{1}{2}) \varphi_{n-1}(y).
\]

Using the Rodrigues’ formula for the Laguerre polynomials [13] one can verify that the wave functions appropriate to our pseudo number states are:

\[
\varphi_n(y) = \left( \Gamma(2s) \left( \frac{n + 2s - 1}{n} \right) \right)^{-\frac{1}{2}} y^s \exp(-y/2)L_n^{2s-1}(y).
\]

Here $L_n^{2s-1}(y)$ denote the generalized Laguerre-polynomials, which obey the following ortho-normalization relation [13]:

\[
\int_0^{\infty} L_n^{2s-1}(y)L_m^{2s-1}(y) \exp(-y)y^{2s-1}dy = \left( \Gamma(2s) \left( \frac{n + 2s - 1}{n} \right) \right) \delta_{n,m}.
\]

Due to the completeness of the Laguerre polynomials with respect of the weight function $\exp(-y)y^{2s-1}$ [13], the wave functions in (13) form a complete orthonormal set in the function space $L^2((0, \infty), \frac{dy}{y})$, (the square integrable functions on the $(0, \infty)$ interval, with respect of the measure $dy/y$ ), and therefore the set of the pseudo number states is a complete, orthonormal basis in the Hilbert space.

Calculating the matrices of the SUSY ladder operators shifted by an arbitrary integer $k$, one finds the following matrix elements:

\[
\langle m|A(s + k)| n \rangle = \sqrt{n(2s + m)d_{m+1,n} - (m - k)d_{m,n}},
\]

\[
\langle m|A^\dagger(s + k)| n \rangle = \sqrt{m(2s + n)d_{m,n+1} - (n - k)d_{m,n}},
\]

\[
\langle m|H(s)| n \rangle = \left( 2n(n + s - \frac{1}{2}) + E_0(s) \right) d_{m,n} - (n - 1)\sqrt{n(2s + n - 1)}d_{m+1,n} - (m - 1)\sqrt{n(2s + n - 1)}d_{m,n+1}.
\]

We see that the fundamental SUSY operators have simple matrices in this new basis and therefore they can be easily applied in calculations. The matrix of the Hamilton operator is not diagonal, although it is quite close to that, it has nonvanishing elements only in, above and below the diagonal, it is tridiagonal. As we have noted earlier, in the case of the Morse potential there is no complete set of normalizable states belonging to the Hilbert space in which the Hamiltonian would be diagonal.

### III. The Coherent States of the Morse Potential

Let us use now the SUSY operator analogy with the harmonic oscillator, and define the coherent states of the Morse potential as

\[
|\beta\rangle = g(\beta) \left\{ I + \sum_{n=1}^{\infty} \frac{\beta^n}{n!} A^\dagger(s + n - 1) \cdots A^\dagger(s) \right\} |0\rangle,
\]

(17)
where $\beta$ is a complex number and $g(\beta)$ is a normalization function to be determined below. Introducing a generalized factorial with the definition and notation

$$\{0\}! = 1, \quad \text{and} \quad \{n\}! = \frac{n!}{2^s \cdot (2s + n - 1)!} = \left(\frac{n + 2s - 1}{n}\right)^{-1} (n > 0), \quad (18)$$

the coherent states in [17] can be written by the help of (11) as:

$$|\beta\rangle = g(\beta) \sum_{n=0}^{\infty} \frac{\beta^n}{\sqrt{\{n\}!}} |n\rangle. \quad (19)$$

To obtain the explicit form of $g(\beta)$ and to find the label space (the set of allowed $\beta$-s) we set:

$$1 = \langle \beta | \beta \rangle = g^2(\beta) \sum_{n=0}^{\infty} \frac{|\beta|^{2n}}{\{n\}!} = g^2(\beta) \left\{ 1 + \sum_{n=1}^{\infty} \frac{2s \cdots (2s + n - 1)}{n!} |\beta|^{2n} \right\}. \quad (20)$$

The sum in the above expression is convergent if and only if $|\beta| < 1$, i.e. the label space is the complex open unit disk, and then the sum in the braces in Eq. (20) yields $\left(1 - |\beta|^2\right)^{-2s}$. So we have finally for the coherent states of the Morse potential:

$$|\beta\rangle = \left(1 - |\beta|^2\right)^{s} \sum_{n=0}^{\infty} \sqrt{\binom{n + 2s - 1}{n}} \beta^n |n\rangle \quad (\beta \in \mathbb{C}, |\beta| < 1). \quad (21)$$

The various sets of coherent states that have been introduced in the past for an arbitrary system have two fundamental common properties established in Ref. [4]: strong continuity in the label space and completeness in the sense that there exists a positive measure on the label space such that the unity operator admits the resolution of unity. Let us investigate whether our new states introduced in (21) satisfy these requirements. The first property follows obviously from the definition: if $\beta \to \beta'$, where $\beta, \beta'$ are complex numbers $|\beta|, |\beta'| < 1$, then $||\beta| - |\beta'||^2 \to 0$. To verify the second property, valid for $s > 1/2$, we consider the measure $\delta\beta = (2s - 1)/ \left(1 - |\beta|^2\right)^2 d\text{Re}\beta d\text{Im}\beta$ ($|\beta| < 1$) and find:

$$\int_{|\beta|<1} |\beta\rangle \langle \beta | \delta\beta = (2s - 1) \sum_{n,m=0}^{\infty} \frac{|n\rangle \langle m|}{\sqrt{\{n\}! \{m\}!}} \int_{|\beta|<1} (\beta^*)^m \beta^n \left(1 - |\beta|^2\right)^{2s-2} d\text{Re}\beta d\text{Im}\beta. \quad (22)$$

If we introduce polar coordinates in the label space, the integral above can be calculated easily, and we find that our coherent states form a complete set and the appropriate form of the resolution of unity is

$$\int_{|\beta|<1} |\beta\rangle \langle \beta | \delta\beta = \pi \sum_{n=0}^{\infty} |n\rangle \langle n| = \pi I. \quad (23)$$

Therefore these states can be regarded as coherent states in the sense of Ref. [4] too.

We also present here the wave functions corresponding to the coherent states of the Morse potential. Let us recast Eq. (19) in coordinate representation in the variable $y = 2 \exp(-x)$ by using the expression (14):

$$\varphi_\beta(y) := \langle y | \beta \rangle = \left(1 - |\beta|^2\right)^{s} \sum_{n=0}^{\infty} \frac{\beta^n}{\sqrt{\{n\}!}} \langle y | n\rangle =
$$

$$= \left(1 - |\beta|^2\right)^{s} \sum_{n=0}^{\infty} \frac{\beta^n}{\sqrt{\{n\}!}} \left(\Gamma(2s)(\frac{n+2s-1}{n})\right)^{-\frac{1}{2}} y^s \exp(-y/2) L_n^{2s-1}(y) = \quad (24)$$

$$= \left(\frac{1 - |\beta|^2}{\sqrt{\Gamma(2s)}}\right) y^s \exp(-y/2) \sum_{n=0}^{\infty} \beta^n \frac{d}{dz} L_n^{2s-1}(y).$$

Using the identity for the Laguerre polynomials [13]:

$$\sum_{n=0}^{\infty} w^n L_n^\alpha(y) = (1 - w)^{-\alpha-1} \exp(-\frac{yw}{1-w}), \quad (w \in \mathbb{C}, |w| < 1), \quad (25)$$


one obtains that the corresponding wave functions in the $y$ coordinate are:

$$
\varphi_\beta(y) = \frac{(1 - |\beta|^2)^s}{\sqrt{\Gamma(2s)(1 - \beta)^{2s}}} y^s \exp(-\frac{y (1 + \beta)}{2(1 - \beta)}),
$$

(26)

Here we would like to note that the wave functions above are essentially the same which have been discovered by Nieto and Simmons [2] in another way, who called them as generalized minimal uncertainty coherent states (MUCS) of the Morse potential. They introduced certain special coordinates in the classical phase space transforming the trajectories of the bound motions into ellipses. According to [3], the MUCS type coherent states are those which minimize the uncertainty relation of the quantum operators corresponding to these new classical coordinates called “natural classical variables” in Ref [2]. It is interesting that our algebraic approach has lead to the same states. Often the eigenvalue equation that defines the MUCS amounts to the ladder operator coherent states, if the ground state is a member of the minimum uncertainty set. Here we have found that to be the case. Otherwise the minimum uncertainty defining equation often yields the defining equation for lowering operator squeezed states [4].

IV. THE DISPLACEMENT OPERATOR GENERATING $|\beta\rangle$

In this section we present another interpretation for the coherent states considered in this paper, by giving the physical meaning of the parameter $\beta$. We will show here, that there exists an unitary operator generating the coherent states from the ground state, thus - according to the classification of [2] - they can be regarded as displacement operator coherent states (DOCS), too. Let us consider the wave functions of the coherent state $|\beta\rangle$ from the ground state, thus - according to the classification of [2] - they can be regarded as displacement operator coherent states, if the ground state is a member of the minimum uncertainty set. Here we have found that to be the case. Otherwise the minimum uncertainty defining equation often yields the defining equation for lowering operator squeezed states [4].

In this section we present another interpretation for the coherent states considered in this paper, by giving the physical meaning of the parameter $\beta$. We will show here, that there exists an unitary operator generating the coherent states from the ground state, thus - according to the classification of [2] - they can be regarded as displacement operator coherent states (DOCS), too. Let us consider the wave functions of the coherent state $|\beta\rangle$ in the original coordinate variable $x$. Substituting $y = 2 \exp(-x)$ in (20), one has:

$$
\varphi_\beta(x) := \langle x |\beta\rangle = \frac{e^{-i\varphi} 2^s}{\Gamma(2s)} e^{-s(x - \bar{x})} \exp\left\{-e^{-(x - \bar{x})}\right\} \exp\left\{-\frac{i}{s} \bar{p} e^{-(x - \bar{x})}\right\},
$$

(27)

where $e^{-i\varphi} = \left(\frac{1 - |\beta|^2}{1 - \beta}\right)^{2s}$ is a phase term and $\bar{x}$ and $\bar{p}$ are real numbers depending on $\beta$:

$$
\bar{x} \equiv \ln(\text{Re}\frac{1 + \beta}{1 - \beta}),
$$

$$
\bar{p} \equiv s \frac{\text{Im}\frac{1 + \beta}{1 - \beta}}{\text{Re}\frac{1 + \beta}{1 - \beta}}.
$$

(28)

Calculating the expectation values of the operators $X$ and $P$ in the state $|\beta\rangle$ one obtains:

$$
\langle \beta | X |\beta\rangle = \bar{x} + 0 | X | 0 \rangle,
$$

$$
\langle \beta | P |\beta\rangle = \bar{p}.
$$

(29)

We can realize that apart from an additive constant the position and momentum operator expectation values are equal to the numbers $\bar{x}$ and $\bar{p}$, respectively. (The additive constant is the expectation value of position in the ground state.) Hence we can introduce a new labeling for the coherent states by the help of the two numbers $\bar{x}$ and $\bar{p}$, as the position and momentum expectation values, instead of the original complex $\beta$. Therefore this coherent state can be written as $|\bar{x}, \bar{p}\rangle$ and the appropriate label space is $\mathbb{R}^2$ with the measure $d\bar{x}d\bar{p}$ on it. Then the resolution of unity (24) has the similar form as in the case of the HO:

$$
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\bar{x}, \bar{p}\rangle \langle \bar{x}, \bar{p}| \pi I = \frac{2s - 1}{4s} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle \bar{x}, \bar{p}| \langle \bar{x}, \bar{p}| \pi I
$$

(30)

It is not hard to see that the square of the modulus of the wave function in (27) is equal to the square of the modulus of the ground state function shifted along the $x$-axis. Eq. (27) also implies that our coherent states can be written as

$$
|\bar{x}, \bar{p}\rangle = e^{-i\varphi} \exp(-i\bar{x} P) \exp(-\frac{i}{s} \bar{p} e^{-X}) |\bar{x} = 0, \bar{p} = 0\rangle =
$$

$$
e^{-i\varphi} \exp(-\frac{i}{s} \bar{p} e^{X}) \exp(-\frac{i}{s} \bar{p} e^{-X}) \exp(-i\bar{x} P) |\bar{x} = 0, \bar{p} = 0\rangle,
$$

(31)
where \(|\vec{x} = 0, \vec{p} = 0\) is identical to the ground state \(|\beta = 0\) being itself a coherent state, as well. Writing the definitions \([3]\) of the \(A(s)\) and \(A^\dagger(s)\) into the above expression one obtains:

\[
|\vec{x}, \vec{p}\rangle = e^{-i\vec{p} \cdot \vec{x}} \exp (-i\vec{p}I) \exp (\frac{\vec{x}}{2s} \left( A^\dagger(s) - A(s) \right)) \exp \left( \frac{i}{2s} \vec{p} \left( A(s) + A^\dagger(s) \right) \right) |0\rangle,
\]

\[
|\vec{x}, \vec{p}\rangle = e^{-i\vec{p} \cdot \vec{x}} \exp (-i\vec{p}I) \exp \left( \frac{i}{2s} \vec{p} \left( A(s) + A^\dagger(s) \right) \right) \chi_{\vec{x}}(s) \left( A^\dagger(s) - A(s) \right) |0\rangle.
\]

Consideration of the case of the harmonic oscillator it inspires to introduce a displacement operator in the following way

\[
D(\vec{x}, \vec{p}) = e^{-i\vec{p} \cdot \vec{x}} \exp (-i\vec{p}I) \exp \left( \frac{i}{2s} \vec{p} \left( A^\dagger(s) - A(s) \right) \right) \exp \left( \frac{i}{2s} \vec{p} \left( A(s) + A^\dagger(s) \right) \right).
\]

Then according to \([3]\) the coherent states are created by this \(D(\vec{x}, \vec{p})\) operator from the ground state:

\[
|\beta\rangle \equiv |\vec{x}, \vec{p}\rangle = D(\vec{x}, \vec{p}) |0\rangle.
\]

From the definition in \([3]\), which is the obvious generalization of the case of the oscillator, it follows that the \(D(\vec{x}, \vec{p})\) operators are unitary for arbitrary \(\vec{x}, \vec{p}\) and it also proves that our states belong to the DOCS category according to \([2]\).

V. CONCLUSIONS AND FINAL REMARKS

By using the set of generalized creation and annihilation operators we have introduced the complete orthonormal set of pseudo number states for the Morse potential. Then, with a construction similar to the case of the harmonic oscillator, we have introduced the set of coherent states depending on the complex parameter \(\beta\). We have shown how this parameter is connected with the expectation values of the coordinate and the momentum, and have determined the unitary displacement operator generating our coherent states from the ground state.

In our construction of the states \(|\beta\rangle\) the fundamental role has been played by the shape invariant Lie algebra \([1]\) spanned by the SUSY ladder operators plus the identity. The pseudo number states have been are generated by its elements \(A^\dagger(s + n)\), while The unitary displacement operators, \(D(\vec{x}, \vec{p})\), that create the coherent states, are the elements of the corresponding Lie group obtained by exponentiating of the SUSY ladder algebra. As it can be simply shown, this algebra, which is solvable, but not nilpotent, is not isomorphic to the Heisenberg-Weyl algebra of the harmonic oscillator. Moreover our new SUSY ladder algebra is not isomorphic either to the class of \(so(2,1) \cong su(1,1) \cong sp(1,\mathbb{R})\), which has been applied to the various recent treatments of the Morse potential \([13]\). Therefore the SUSY ladder operator algebra and the coherent states presented here can be regarded as a new algebraic viewpoint for the description of the one-dimensional Morse potential.

We also think that our construction will be useful in describing molecular interactions with the electromagnetic field.

VI. ACKNOWLEDGEMENTS

The authors thank F. Bartha, F. Bogár, L. Fehér and G. Lévai for the useful discussions and remarks. This work was supported by the National Research Foundation of Hungary (OTKA) under contract No. T22281.

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[13] G. Szegő, Orthogonal Polynomials, (Am. Math. Soc., New York, 1959); M. Abramowitz, I. Stegun, Handbook of Mathematical Functions (Dover, 1965). The generalized Laguerre polynomials used here are defined as:
\[ L_n^\alpha(x) = \frac{1}{n!} e^x x^{-\alpha} \frac{d^n}{dx^n} e^{-x} x^{n+\alpha}, \]
(note that certain authors omit the factor \(1/n!\)). These are not to be confused with the associated Laguerre polynomials, \( \tilde{L}_n^\alpha(x) = \frac{d^n}{dx^n} e^x e^{-x} x^n \), appearing in the solution of the Coulomb problem.
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