Quantization of the charge in Coulomb plus harmonic potential

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We consider two models where the wave equation can be reduced to the effective Schrödinger equation whose potential contains both harmonic and the Coulomb terms, \( \omega^2 r^2 - a/r \). The equation reduces to the biconfluent Heun’s equation, and we find that the charge as well as the energy must be quantized and state dependent. We also find that two quantum numbers are necessary to count radial degrees of freedom and suggest that this is a general feature of differential equation with higher singularity like the Heun’s equation.

1. Introduction: Since Schrödinger established the equation in his name, it has been believed that for any confining potential, there exists discrete energy levels although we may not write the analytic solution explicitly. However, recent experience [1, 2] told us that it may not be the case. When the potential has higher singularity, we need higher regularity condition. As a consequence, there is no normalizable solution unless potential itself is quantized.

In this paper, we consider two models where the wave equation can be reduced to the effective Schrödinger equation whose potential contains both harmonic term \( \omega^2 r^2 \) and the Coulomb term \(-a/r\). The equation of motion reduces to the biconfluent Heun’s equation, and we find that the charge as well as the energy must be quantized. That is, both energy and charge must depend on the states.

We also find that due to the higher singularity, new quantum number appears. For example, in spherically symmetric case, apart from the radial quantum number \( N \) and two angular ones \( L, m \), one more quantum number \( K \) appears. It turns out that only when we combine two quantum numbers \( N, K \), the full radial degree of freedom can be counted. We suggest that the presence of extra quantum numbers to count correct radial degrees of freedom is a general feature of differential equation with higher singularity like the Heun’s equation.

2. A quark model with Coulomb and linear scalar potential

Lichtenberg et al. [3] found a semi-relativistic Hamiltonian which leads to a Krollkowsi type second order differential equation [4–9] in order to calculate meson and baryon masses. In the center-of-mass system, the total energy \( H \) of two free particles of masses \( m_1, m_2 \), is

\[
H = \sqrt{p^2 c^2 + m_1^2 c^4} + \sqrt{p^2 c^2 + m_2^2 c^4} \tag{1}
\]

Let \( S \) be the Lorentz scalar interaction and \( V \) be the interaction which is a time component of a 4-vector. Then it is natural to incorporate the \( V \) and \( S \) into (1) by making the replacements

\[
H \to H + V, \quad m_i \to m_i + \frac{1}{2} S, \quad i = 1, 2. \tag{2}
\]

We set \( m_1 = m_2 = 0 \) and introduce \( V = -a/r \) and study its effect for the spin-free Hamiltonian which was proposed for the meson \((\bar{q}q)\) system in [10–13]. Then we have

\[
\left( E + \frac{a}{r} \right)^2 \psi(r) = 4 \left[ c^4 \left( \frac{1}{2} b r \right)^2 + \epsilon^2 \left( \frac{P_r^2}{2} + \frac{\hbar^2 L(L+1)}{2 r^2} \right) \right] \psi(r) \tag{3}
\]

where \( b \) is a real positive constant and we used \( \bar{p}^2 = P_r^2 + \frac{\hbar^2 L(L+1)}{2 r^2} \) with \( P_r^2 = -\hbar^2 \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \). The linear scalar potential is for the confinement of the quarks bound by a QCD flux string with constant string tension \( b \). Previously, we investigated the model in the case \( V = 0 \) [1] and concluded that for the consistency of the spectrum the current quark should have zero mass. Here we want to introduce \( V = -a/r \) and understand its effect in the presence of the confining potential.

Factoring out the behavior near \( r = 0 \) by \( \psi(r) = \rho^L f(r) \), above equation becomes

\[
\frac{d^2 f(r)}{dr^2} + \frac{2(\tilde{L} + 1)}{r} \frac{df(r)}{dr} + \left( \frac{\epsilon^2}{4} - \frac{b^2}{4 r^2} + \frac{\epsilon a_0}{2 r} \right) f(r) = 0, \tag{4}
\]

where \( a_0 = a/hc, b_0 = be/h, \epsilon = E/hc \) and \( \tilde{L} = -1/2 + \sqrt{(L + 1/2)^2 - a_0^2/4} \). If we further factor out the near-infinity behavior by \( f(r) = \exp\left(-\frac{\epsilon}{2} r^2\right) y(r) \) and introduce \( \rho = \sqrt{b_0/2r} \), we get

\[
\rho^2 \frac{d^2 y}{d\rho^2} + \left( \mu \rho^2 + \epsilon \rho + \nu \right) \frac{dy}{d\rho} + \Omega \rho + \beta) y = 0. \tag{5}
\]

with \( \mu = -2, \epsilon = 0, \nu = 2(\tilde{L} + 1), \beta = \epsilon a_0 \) and

\[
\Omega = \epsilon^2 - (2\tilde{L} + 3), \quad \text{with} \quad \epsilon = \frac{\epsilon}{\sqrt{2b_0}}. \tag{6}
\]

This equation is a biconfluent Heun’s equation which has a regular singularity at the origin and an irregular singularity of rank two at the infinity [2, 3].

Substituting \( y(\rho) = \sum_{n=0}^{\infty} a_n \rho^n \) into (5), we obtain the recurrence relation:

\[
d_{n+1} = A_n d_n + B_n d_{n-1} \quad \text{for} \quad n \geq 1, \text{ with} \tag{7}
\]

\[
A_n = -\frac{\epsilon n + \beta}{(n+1)(n+\nu)}, \quad B_n = -\frac{\Omega + \mu(n-1)}{(n+1)(n+\nu)} \tag{8}
\]

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For \( n = 0 \) term, only \( d_1, d_0 \) appear and give \( d_1 = A_0 d_0 \).

Notice that when \( a_0 = 0 \), we have

\[
A_n = \frac{\beta}{(n+1)(n+\nu)} = \frac{\epsilon a_0}{(n+1)(n+2(L+1))} = 0, \quad (9)
\]

so that the three term recurrence relation given in eq. \([7]\) is reduced to two term recurrence relation between \( d_{n+1} \) and \( d_{n-1} \) and the Heun’s equation is reduced to hypergeometric one. That is, in this scaling, the Coulomb parameter is precisely the term increasing the singularity order. Similarly, if \( b_0 = 0 \), the system can also be mapped to a hypergeometric type. The problem rises only when both potential terms are present.

Now, unless \( y(\rho) \) is a polynomial, \( \psi(r) \) is divergent as \( \rho \to \infty \). Therefore we need to impose regularity conditions by which the solution is normalizable. If we impose two conditions \([5,6]\),

\[
B_{N+1} = d_{N+1} = 0 \quad \text{where} \quad N \in \mathbb{N}_0, \quad (10)
\]

the series expansion becomes a polynomial of degree \( N \): as one can see from eq. \([7]\), eq. \([10]\) is sufficient to give \( d_{n+2} = d_{n+3} = \cdots = 0 \) recursively. Then the solution is a polynomial of order \( N \), \( y_N(\rho) = \sum_{i=0}^{N} d_i \rho^i \). The question whether imposing both equations in eq.\([10]\) is really necessary for the finite solution was studied numerically and was concluded affirmatively in our earlier work \([7]\).

In general, \( d_{N+1} = 0 \) will define a \( N+1 \)-th order polynomial \( P_{N+1} \) in \( a_0 \), so that Eq. \([10]\) gives

\[
\epsilon_{N,L} = \sqrt{2N + 2L + 3}, \quad P_{N+1}(a_0) = 0. \quad (11)
\]

where the first comes from \( B_{N+1} = 0 \), and it is nothing but the usual energy quantization condition. Below we will examine the meaning of the second condition by constructing explicitly the expressions of a few low order polynomial \( P_{N+1} \), which are given in the appendix.

One surprising fact is that for a given \( N, L \), there are many solutions which we can index by an integer \( K \) which is smaller than \( N \). Depending on whether \( N \) is even or odd, the distribution of solutions of \( P_{N+1}(a_0) = 0 \) is different. For low lying \( L \), the number of roots increases with \( L \) but not regularly. However, for \( L \geq \lfloor N/2 \rfloor - 1 \) the number of roots is given by \( \lceil N/2 \rceil + 2 \). Here, \( \lfloor x \rfloor \) is the integer part of \( x > 0 \). The presence of extra quantum number is natural from the algebraic point of view. But it is rather surprising from the counting degree of freedom. We postpone the dynamics of associated \( K \) to next section where we discuss the problem with a simpler model.

Table \([\text{II}]\) shows some real roots of \( a_0^2 \)’s for each \( L \) with fixed \( N = 8 \); here, \( a_0^2 \) is the \( i \)-th root of \( a_0^2 \) with given \( N, L \). Similarly, Table \([\text{II}]\) shows real roots of \( a_0^2 \)’s for each \( L \) when \( N = 9 \).

For lower value of \( K \), we can find an approximate fitting function. For example for \( K = 0 \) and for odd \( N \), it is given by

\[
a_{0,N,L0}^2 \approx 1.22\tan^{-1}\left(\frac{(L+1)^{0.6} - 0.5}{0.55N^{0.7} + 0.5}\right) + 0.18. \quad (12)
\]

We calculated 338 different values of \( a_0^2 \)’s at various \((N,L)\) and the result is the dots in Fig. \([\text{I}]\). These data fits well by above formula. Notice also that for even \( N \), \( a_0 = 0 \) is always a solution for any \( L \).

By substituting eq.\([12]\) into eq.\([11]\), we can fit the experimental data of \( E \), which is the hadron mass.

\[
E_{N,L} \simeq \sqrt{2hc \cdot b^2 \cdot 2N + 2 + \sqrt{(2L + 1)^2 - a_{0,N,LK}^2}}, \quad (13)
\]

where \( a_0 = a/\hbar c \). What is surprising is the fact that the charge parameter \( a \) should be quantized as values approximately given in eq.\([12]\) if the charge is coming in the presence of the linear scalar potential which gives the confinement. Our treatment gives the analytic results in the presence of the both linear potential together with Coulomb potential. However, we must also comment that in the presence of the quark mass our method breaks down.

3. Quantum dot with Coulomb and harmonic potential

Here we consider Non-relativistic Schrödinger equation with Coulomb potential and external harmonic
The oscillator potential for a system of two electrons in a three dimensional Euclidean space \([14][17]\). The Schrödinger equation is given by
\[
\left[ -\frac{\hbar^2}{2m} \left( \frac{d^2}{dr^2} + \frac{2 \hbar^2}{r} \frac{d}{dr} \right) + V_{\text{eff}}(r) \right] \psi(r) = E \psi(r),
\]
(14)
with \(V_{\text{eff}}(r) = \omega^2 r^2 - \frac{a}{r} + \frac{\hbar^2}{2m} L(L+1) \frac{r^2}{r^2}\),
(15)
Introducing \(\rho = r \left( \frac{\hbar a}{2m} \right)^{1/4}\), above equation becomes
\[
\rho \frac{d^2 \psi}{d\rho^2} + 2 \frac{d\psi}{d\rho} + \left( \epsilon - \rho^2 + \frac{a0}{\rho} - \frac{L(L+1)}{\rho^2} \right) \psi = 0.
\]
(16)
where
\[
\epsilon = \frac{E}{\sqrt{\omega}} \sqrt{\frac{2m}{\hbar^2}} \quad a0 = a \sqrt{\omega} \left( \frac{\hbar^2}{2m} \right)^{3/4}.
\]
(17)
Factoring out the behavior near \(\rho = 0\) by \(\psi(\rho) = \rho^\beta f(\rho)\), it becomes
\[
\frac{d^2 f(\rho)}{d\rho^2} + \frac{2(L+1) df(\rho)}{d\rho} + \left( \epsilon - \rho^2 + \frac{a0}{\rho} \right) f(\rho) = 0.
\]
(18)
Factoring out near \(\infty\) behavior by \(f(\rho) = e^{-\rho^2/2} g(\rho)\), we get the standard form eq. (14) with
\[
\mu = -2, \epsilon = 0, \nu = 2L+1, \beta = a0, \Omega = \epsilon - (2L+3).
\]
Similarly, if we impose eq. (10), the series expansion becomes a polynomial of degree \(N\). the solution becomes a polynomial \(y_N(\rho) = \sum_{i=0}^{N} d_i \rho^i\). In general, \(d_{N+1} = 0\) will define a \((N+1)\)-th order polynomial \(P_{N+1}\) in \(a0\), so that Eq. (10) gives
\[
\epsilon_N = 2N + 2L + 3, \quad P_{N+1}(a0) = 0.
\]
(19)
where the first comes from \(B_{N+1} = 0\) which is the energy quantization condition. Below we will examine the meaning of the second equation. To do that we need explicit expressions of a few lower order polynomial \(P_{N+1}\):
\[
P_1(a0) = a0,
\]
\[
P_2(a0) = a_0^2 - 4(L+1),
\]
\[
P_3(a0) = a_0^3 - 4(4L+5)a0,
\]
\[
P_4(a0) = a_0^4 - 20(2L+3)a_0^2 + 144(L+1)(L+2),
\]
\[
P_5(a0) = a_0^5 - 20(4L+7)a_0^3 + 32(89 + 16L(2L+7))a0.
\]
(20)
In appendix, we gave a few low order polynomial \(y_N(\rho)\) with \(d0 = 1\).

We have seen that \(a\) and \(\omega\) are related by eq. (17) and \(P_{N+1}(a0) = 0\) does not contain any dimensional parameter. This means that \(a/\sqrt{\omega}\) should be a solution of a polynomial equation, which depends on \(N, L\). Such extra quantization is a consequence of the Heun’s equation. For the hypergeometric equations, the recurrence relation is reduced to two term after factoring out the asymptotic behavior. There, we do not have \(d_{N+1} = 0\). Hence to have a normalizable polynomial solution, we only need to fine tune just one parameter, the energy. For the Heun’s equation, we have to impose two constraints, which in turn request the charge quantization of the system. In short, its higher singularity requests higher regularity condition. This is the origin of the charge quantization.

Notice that a depends on the quantum numbers that parametrize quantum states. It means that when the electron make a transition from one state to another, the charge parameter must be changed to a new value. This raises the question, how dynamics of one particle can change the potential energy which is determined by the surrounding system. In fact, \(V\) is not the potential but the potential energy. The potential belongs to the surroundings while the potential energy contains both surrounding and particle information. Therefore \(a\) should be written as product of particle’s charge \(q\) times the charge \(Q\) which makes the potential \(\phi_Q\), so that \(V = q\phi_Q\). When one say charge is quantized, what we mean is the quantization of \(q\). In short, when the potential energy has higher singularity, the charge as well as the energy should depends on the state. At first, this concept was rather drastic, but this is consequence of requesting \(d_{N+1}\), whose necessity was confirmed by numerical investigation: without it, the shooting method did not work.

Notice that in this model, the energy \(\epsilon\) is linear in \(N, L\) and does not depend on a quantized value of \(a_0^2\). Table III shows all roots of \(a_0^2\) for each \(L\) when \(N = 4, 5\).

| \(N = 4\)          | \(N = 5\)          |
|-------------------|-------------------|
| \(\alpha_0 = \alpha_1 = \alpha_2\) | \(\alpha_0 = \alpha_1 = \alpha_2\) |
| \(L=0\) \(0, 24.701, 115.299\) | \(L=0\) \(0, 38.342, 61.813, 208.803\) |
| \(L=1\) \(41.654, 178.147\) | \(L=1\) \(10.9642, 102.963, 306.069\) |
| \(L=2\) \(65.414, 281.686\) | \(L=2\) \(179.2359, 140.155, 104.609\) |
| \(L=3\) \(74.148, 305.256\) | \(L=3\) \(19.3928, 176.899, 654.709\) |
| \(L=4\) \(90.9604, 369.04\) | \(L=4\) \(23.4559, 213.401, 663.101\) |
| \(L=5\) \(107.114, 332.886\) | \(L=5\) \(27.5688, 249.768, 702.664\) |

TABLE III. Roots of \(a_0^2\)

In three dimension, spinless Hydrogen atom has three quantum number: \(N, L, m\): \(N\) for radial and the other two for angular momentum. However, in the presence of the harmonic potential, the charge and energy
have discrete values depending on four quantum numbers \( N, L, m, K \), which shows apparent mismatch between the number of degrees of freedom and that of quantum numbers. However, as we have shown above, with \( K = 0 \), only half of the nodes of radial wave function are on positive region. This means that the radial solution for fixed \( K \), say \( K = 0 \), can not span arbitrary shape of radial function in the positive region. In fact, \( K \) counts the number of nodes which is moved from negative to positive region compared with \( K = 0 \) case. This means that \( N \) together with \( K \) counts full radial degrees of freedom, and without the extra quantum number \( K \), the solutions cannot be a basis of the radial wave functions.

We expect that the presence of extra quantum number to count correct radial degrees of freedom is a general feature of differential equation with higher singularity like the Heun’s equation.

4. Discussion: Caruso et.al [14] investigated non-relativistic 2-D radial Schrödinger equation which can be related to ours just by shifting \( L \) to \( L - 1/2 \) in [15]. They obtained part of result of section 3 of this paper but they interpreted the result as the quantization of \( \omega \), the coefficient of the harmonic potential. The quantization of \( \omega \) would imply that the single particle dynamics changes the potential’s parameter, which does not sound plausible. In our case, \( a \) is split into particle charge \( q \) and charge \( Q \) in the potential, so that Coulomb term can be written as \( V_{Coulomb} = q\phi Q(r) \). \( q \) is a property of the particle, therefore dependence of the particle charge on the state is natural although the concept is still not familiar so far. In field theory, charge depends on probe energy scale due to the renormalization. So the state dependence of the charge can be regarded as discrete renormalization of the charge induced by smoothing out process of the the singularity of the potential.

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Appendix A: $\mathcal{P}_N$ for $N = 0, 1, \ldots, 5$

\[
\begin{align*}
\mathcal{P}_1(a_0) &= a_0, \\
\mathcal{P}_2(a_0) &= a_0^2 \left( 4 + \sqrt{(2L + 1)^2 + a_0^2} \right) - 2 \left( 1 + \sqrt{(2L + 1)^2 + a_0^2} \right), \\
\mathcal{P}_3(a_0) &= a_0 \left( -a_0^4 \left( 6 + \sqrt{(2L + 1)^2 + a_0^2} \right) + 12 + 8 \sqrt{(2L + 1)^2 + a_0^2} \right), \\
\mathcal{P}_4(a_0) &= -a_0^6 + a_0^4 \left( 85 + 4L(L + 1) + 16 \sqrt{(2L + 1)^2 - a_0^2} \right) \\
&\quad - 8a_0^2 \left( 47 + 10L(L + 1) + 25 \sqrt{(2L + 1)^2 - a_0^2} \right) \\
&\quad + 144 \left( L^2 + L + 1 + \sqrt{(2L + 1)^2 - a_0^2} \right), \\
\mathcal{P}_5(a_0) &= a_0^5 \left( 384(L + 1)(L + 2) - 4(25 + 16L)a_0^2 + a_0^4 \right) + 4(2L + 5)(52 + 40L - a_0^2) a_0 \rho^2 \\
&\quad - 24(L + 2)(2L + 5)(16 + 16L - a_0^2) \rho^2 - 48(L + 2)(2L + 3)(2L + 5)a_0 \rho \\
&\quad + 60a_0(2L + 3)(2L + 5)(960(L + 1)(L + 2)(L + 3)(2L + 3)(2L + 5)} \\
\end{align*}
\]

Appendix B: $y_N(\rho)$ polynomials for $N = 0, 1, \ldots, 5$

We lists expressions of a few lower order polynomial $y_N(\rho)$:

\[
\begin{align*}
y_0(\rho) &= 1, \\
y_1(\rho) &= 1 - \frac{a_0 \rho}{2(1 + L)}, \\
y_2(\rho) &= 1 + \frac{(a_0^2 - 8(L + 1))\rho^2}{4(L + 1)(2L + 3)} - 2a_0(2L + 3) \rho, \\
y_3(\rho) &= 1 + \frac{a_0(36 + 28L - a_0^2)\rho^3 + 6(L + 2)(a_0^2 - 12(L + 1))\rho^2 - 12(L + 2)(2L + 3)a_0 \rho}{24(L + 1)(L + 2)(2L + 3)} \\
&\quad + \frac{a_0^4 \rho^3}{384(L + 1)(L + 2) - 4(25 + 16L)a_0^2 + a_0^4} + 4(2L + 5)(52 + 40L - a_0^2) a_0 \rho^2 \\
&\quad - 24(L + 2)(2L + 5)(16 + 16L - a_0^2) \rho^2 - 48(L + 2)(2L + 3)(2L + 5)a_0 \rho \biggr) \\
y_4(\rho) &= 1 + \frac{1}{960(L + 1)(L + 2)(L + 3)(2L + 3)(2L + 5)} \biggr) \biggr) \\
&\quad - a_0(6880 + 2384L^2 + 24L(354 - 5a_0^2) + a_0^2)(a_0^2 - 220)) \rho^5 \\
&\quad + 10(L + 3)(720(L + 1)(L + 2) - 4(35 + 22L)a_0^2 + a_0^4) \rho^4 \\
&\quad + 40a_0(2L + 3)(2L + 5)(68 + 52L - a_0^2) \rho^3 - 240(L + 2)(L + 3)(2L + 5)(20 + 20L - a_0^2) \rho^2 \\
&\quad - 480a_0(2L + 3)(2L + 3)(2L + 5)a_0 \biggr) \\
\end{align*}
\]

In eq. $\text{(A1)}$ the roots $\mathcal{P}_{N+1}(a_0) = 0$ are simple and there is the orthogonality relation $\text{(A2)}$:

\[
\int_0^\infty d\rho \rho^{2L^2+1} e^{-\rho^2} y_{N,K}(\rho) y_{N',K'}(\rho) = \mathcal{M}(N,K) \delta_{NN'} \delta_{KK'}.
\]

here, $a_0 \in \{a_{0,0}, a_{0,1}, a_{0,2}, \ldots, a_{0,K}\}$ for $0 \leq K \leq [N/2 + 1]$ for normalization constnat.