Near-the-origin divergence of Klein-Gordon wave functions for hydrogen-like atoms and operator product expansion

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Abstract

There have been some long-standing puzzles related to the Coulomb solutions of the Klein-Gordon and Dirac equations, namely how to understand the physics underlying the weakly divergent near-the-origin behavior of the $S$-wave wave functions for the hydrogen-like atoms. Taking the Klein-Gordon wave function as a simpler example, in this work we demonstrate that, with the aid of the renormalization group equation, this universal short-distance behavior can be successfully taken into account by the operator product expansion (OPE) formulated in the nonrelativistic effective field theory (EFT), which is tailored for Coulombic atoms. The key is to include the relativistic kinetic correction in the EFT. Somewhat counterintuitively, these universal near-the-origin logarithmic divergences can not be addressed by the OPE set up in the relativistic scalar QED. We conclude that the Klein-Gordon wave function at a length scale shorter than the electron Compton wavelength may cease to make physical significance.

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I. INTRODUCTION

Back to the late 1920s, the Klein-Gordon (KG) and Dirac equations in an external electrostatic Coulomb field, has played a vital role in accounting for the by-then measured hydrogen spectroscopy, and more importantly, establishing quantum mechanics as the true science [1]. As everyone knows, KG equation quickly lost its battle with the Dirac equation in predicting the fine structure of the hydrogen atom, since the former only describes the relativistic wave equation for a fictitious spinless electron. Later, KG equation has resurrected as a viable field equation in the relativistic quantum field theory.

Since the birth of relativistic quantum mechanics, it was known that both KG and Dirac wave functions for the $S$-wave hydrogen-like atoms are divergent near the origin, albeit very weakly, when the electron coincides with the nucleus [1, 2]. For the long time, this symptom has been thought of only academic interest. The logarithmic singularity would bring pronounced effect only when the electron is extremely close to the origin. At practical level, the realistic nucleus has a finite size, and this distance scale is already many orders-of-magnitude smaller than the radius of the nucleus. Even for an idealized nucleus, i.e., an infinitely heavy positively-charged point particle, the divergence is so weak so the KG and Dirac wave functions are still square integrable near the origin, thereby does not ruin the canonic probabilistic interpretation of wave function.

However, we take a different attitude in this work. Our goal is to unravel the physical origin underlying the logarithmically divergent near-the-origin behavior for the relativistic hydrogen wave function. For simplicity, in this work we will focus on the Coulomb solution of the Klein-Gordon wave function, which seems considerably simpler than the Dirac equation, yet still captures some essential piece of physics. The analogous analysis for the Dirac wave functions for the $nS_{1/2}$ hydrogen atom will be presented elsewhere [3].

In Ref. [4], we have showed that, within the framework of the nonrelativistic Coulomb-Schrödinger effective field theory (EFT), the operator product expansion (OPE) [5] technique can be fruitfully applied to decipher the universal short-distance behavior of the atomic Schrödinger wave functions, which are always regular near the origin. In this work, we extend [4] by incorporating the relativistic kinetic correction into the Coulomb-Schrödinger EFT. We will illustrate that, by conducting the Wilson expansion of the product of the nonrelativistic electron field and the HQET-like nucleus field, we are able to interpret the universal logarithmic near-the-origin divergence of the KG wave functions as the Wilson coefficients. Moreover, with the help of the renormalization group equation (RGE), one can successfully reproduce the anomalous scaling behavior exhibited in the KG wave function at small $r$.

The motif of this work is also to clarify the nature of the Klein-Gordon wave function. The Klein-Gordon equation in an external Coulomb field is often viewed as the relativistic wave equation, and one is allowed to probe the arbitrarily small distance profile of the wave function. As we will see, our OPE analysis based on the relativistic scalar QED would falsify this misconception. In our opinion, the KG equation actually secretly describes the nonrelativistic rather than relativistic bound-state wave function. We believe that it does not make too much sense to talk about the near-the-origin behavior of the KG wave function when $r$ is much smaller than the electron Compton wavelength. On the contrary, when probing the short-range behavior of the KG wave function, the minimum value of $r$ should be frozen around the Compton length of the electron.

The rest of the paper is organized as follows. In section II, we revisit the Coulomb
solution of the KG equation, focus on the weak singularity associated with the S-wave KG wave functions near the origin. In section III, we perform a nonrelativistic reduction to KG equation, then apply quantum-mechanical perturbation theory to compute the first-order correction to the wave function at the origin. In section IV, we study the local composite operator renormalization and OPE within a relativistic field theory that contains the scalar QED and heavy nucleus effective theory. Unfortunately, this theory fail to reproduce the intended logarithmic divergence of the KG wave function near the origin.

In section V, we switch the gear and set up a proper nonrelativistic EFT to describe the atoms bounded by the slowly moving spin-0 electrons and a static nucleus through Coulomb interaction. We explicitly match the UV theory onto the nonrelativistic EFT through one-loop order, and verify no contact interaction can arise at least at order-$Z^2\alpha^2$. In section VI, we study the renormalization of the local composite S-wave operator composed of the electron and nucleus fields in this nonrelativistic EFT. It is found that this operator becomes logarithmic divergent at order $Z^2\alpha^2$, and a multiplicative renormalization is required to render it finite.

Section VII is the main part of the paper. We establish the Wilson expansion for the product of nonrelativistic electron field and nucleus field in both momentum and coordinate space, through order-$Z^2\alpha^2$. We use the renormalization group equation for the Wilson coefficient to resum the leading logarithms to all orders. Finally we summarize in VIII.

II. COULOMB SOLUTION OF KLEIN-GORDON EQUATION, S-WAVE RADIAL WAVE FUNCTIONS NEAR THE ORIGIN

For the sake of completeness, in this section we briefly recapitulate the celebrated Coulomb solution of the Klein-Gordon equation, with primary interest in the near-origin behavior of the KG radial wave function for hydrogen-like atoms. In particular, we will concentrate on the coalescence behavior of the S-wave wave functions. For a spinless electron orbiting around an infinitely heavy nucleus carrying electric charge $Ze$, the relativistic wave equation reads

$$\left( E + \frac{Ze^2}{4\pi r} \right)^2 + \hbar^2 c^2 \nabla^2 - m^2 c^4 \right] \Psi(r) = 0. \quad (1)$$

As usual, the KG wave function can be separated into the radial and angular part,

$$\Psi_{nlm}(r) = R_{nl}(r)Y_{lm}(\hat{r}), \quad (2)$$

where $Y_{lm}$ is the spherical harmonics, with $l$ and $m$ denoting the orbital angular momentum and the magnetic quantum number.

The radial wave function obeys the following differential equation [2]:

$$\left[ \frac{d^2}{dr^2} + \frac{Z^2\alpha^2 - l(l + 1)}{r^2} + \frac{2Z\alpha E}{\hbar cr} + \frac{E^2 - m^2 c^4}{\hbar^2 c^2} \right] rR_{nl}(r) = 0, \quad (3)$$

with the fine structure constant $\alpha = \frac{e^2}{4\pi\hbar c}$.

The bound-state solution is well-known, which yields the corresponding discrete eigen-
energy:

\[ E_{nl} = mc^2 \left\{ 1 + \frac{Z^2 \alpha^2}{n - l - \frac{1}{2} + \sqrt{(l + \frac{1}{2})^2 - Z^2 \alpha^2}} \right\}^{-\frac{1}{2}} \]

\[ = mc^2 \left\{ 1 - \frac{Z^2 \alpha^2}{2n^2} - \frac{Z^4 \alpha^4}{2n^4} \left( \frac{n}{l + \frac{1}{2}} - \frac{3}{4} \right) + \cdots \right\}, \quad (4) \]

where the principal quantum number \( n = 1, 2, \ldots \), and the orbital angular momentum \( l = 0, \ldots, n-1 \) are non-negative integers. In the second line of (4), we have expanded the exact energy level in power series of \( Z\alpha \).

The solution for radial wave function is [2]

\[ R_{nl}(r) = N_{nl} \rho^{\ell'} e^{-\frac{r}{\beta}} {_1F_1}(\ell' + 1 - \lambda, 2\ell' + 2; \rho), \quad (5) \]

where \( {_1F_1} \) stands for the confluent hypergeometric function, and

\[ \ell' \equiv -\frac{1}{2} + \sqrt{\left( l + \frac{1}{2} \right)^2 - Z^2 \alpha^2}, \quad \beta \equiv \frac{2}{\hbar c} \sqrt{m^2 c^4 - E_{nl}^2}, \quad \rho \equiv \beta r, \quad \lambda = \frac{2Z\alpha E_{nl}}{\hbar c \beta}. \quad (6) \]

In the \( Z\alpha \ll 1 \) limit, \( \beta \approx \frac{2mcZ\alpha}{\hbar n} = \frac{2}{(na_0)} \), proportional to the reciprocal of the Bohr radius \( a_0 \equiv \hbar/(mcZ\alpha) \), and \( \lambda \approx n \). The normalization constant \( N_{nl} \) can be determined by enforcing the spatial integral of the density of the conserved charged current in KG equation to be unity,

\[ \int dr \, r^2 R_{nl}^2(r) \left( \frac{E_{nl}}{mc^2} + \frac{Ze^2}{4\pi rmc^2} \right) = 1. \quad (7) \]

In the \( Z\alpha \ll 1 \) limit, this constraint is very close to the conventional normalization condition \( \int dr \, r^2 R^2(r) = 1 \) for \( Z\alpha \ll 1 \).

The power-law scaling of the wave function near the origin can be simply inferred from the \( r \to 0 \) behavior of (3):

\[ R_{nl}'' + \frac{2}{r} R_{nl}' + \frac{Z^2 \alpha^2 - l(l + 1)}{r^2} R_{nl} = 0. \quad (8) \]

Substituting the ansatz \( R_{nl}(r) \propto r^{\ell'} \), one can solve \( \ell' \) from the following quadratic equation:

\[ \ell' (\ell' + 1) = l(l + 1) - Z^2 \alpha^2, \quad (9) \]

and take the greater root as specified in (6). Note the scaling behavior is called “anomalous”, since it qualitatively differs from that affiliated with the Schrödinger radial wave functions \( R_{nl}^{\text{Sch}}(r) \propto r^{\ell} \).

\[ ^1 \text{It is historically well known that, the } Z^4 \alpha^4 \text{ term yields the wrong fine structure of hydrogen spectroscopy, thereby the KG equation, which governs the dynamics of a spin-0 electron, must be abandoned as being the realistic relativistic wave equation to describe the hydrogen atom [1].} \]
FIG. 1: The Klein-Gordon and Schrödinger radial wave functions for the 1S, 2S and 5S hydrogen-like atom. To clearly discern the difference between the KG and Schrödinger wave functions, we deliberately take $Z\alpha = \frac{1}{10}$ with $m = 1$.

In the $Z\alpha \ll 1$ limit, the difference between $l$ and $l'$ is tiny for high $l$. Nevertheless, for $S$-wave hydrogen-like atom, $l' \approx -Z^2\alpha^2$, is a very small negative number. Consequently, the corresponding KG radial wave function at the origin then becomes divergent, despite being a very weak singularity.

Near the origin, the KG wave function can be approximated as

$$ R_{n0}^{KG}(r) \approx R_{n0}^{Sch}(0)\rho\sqrt{1-\frac{Z^2\alpha^2}{4\rho}} \approx R_{n0}^{Sch}(0)\rho^{-Z^2\alpha^2} $$

$$ = R_{n0}^{Sch}(0)\left[1 - Z^2\alpha^2 \ln \frac{2r}{na_0} + O\left(Z^4\alpha^4 \ln^2 r\right)\right], \quad (10) $$

where the expansion is in power series of $Z\alpha$. Therefore, the wave function near the origin only develops a logarithmic divergence. It is very important to note that this divergence is universal, in the sense it applies to all the $S$-wave Coulombic state, irrespective of $n$ being a discrete or continuum quantum number.

The universal near-the-origin behavior of the Schrödinger wave function is also widely known [4, 6]. For example, for $S$-wave hydrogen-like atom, one has $R_{n0}^{Sch}(r) = R_{n0}^{Sch}(0)(1 - r/a_0)$. Carefully expanding the $S$-wave KG wave functions from (5), we find their near-the-origin behaviors to be

$$ R_{n0}^{KG}(r) \approx R_{n0}^{Sch}(0)(1 - mZ\alpha r)\rho^{-Z^2\alpha^2} \approx R_{n0}^{Sch}(0)(1 - Z^2\alpha^2 \ln r + \cdots) $$

$$ = R_{n0}^{Sch}(0)(1 - mZ\alpha r - Z^2\alpha^2 \ln r + mZ^3\alpha^3 r \ln r + \cdots), \quad (11) $$

where only the universal terms are exhibited. For the sake of clarity, in Fig. 1 we plot the various lowest-lying $S$-wave KG and Schrödinger radial wave functions normalized with respect to the corresponding Schrödinger radial wave functions at the origin, from which the universal coalescence behavior encoded in (11) can be seen.
The very goal of this work is to understand the physics underlying these universal short-range terms from the perspective of quantum effective field theory and renormalization program.

We summarize the key aspects observed for the $S$-wave KG wave functions near the origin, and raise some questions that will be answered in the following sections:

- As indicated in (10), the $S$-wave KG wave functions exhibit weak logarithmic singularity as $r \to 0$. This seems to be reminiscent of UV divergence and calls for renormalization.

- The logarithmic coalescence divergence is universal. That is, it does not depend on the principle quantum number $n$, regardlessly of being a discrete or continuum label. Since the wave functions may be regarded as the product of quantum fields sandwiched between the vacuum and the atom, it is conceivable that their short-range behaviors might be probed with the aid of OPE. The universal yet regular coalescence behavior observed for Schrödinger wave functions, $R_{n0}^{\text{Sch}}(r) = R_{n0}^{\text{Sch}}(0)(1 - r/a_0)$, has indeed been deciphered by invoking the OPE technique in the nonrelativistic Coulomb-Schrödinger EFT [4]. Is it possible to further interpret the universal logarithmic divergences as Wilson coefficients related to the OPE? A crucial difference is that in the Schrödinger case, the only nontrivial Wilson coefficients is of order $Z\alpha$, but in the KG case, the first nontrivial Wilson coefficient appears to begin at order $Z^2\alpha^2$.

- If the OPE turns out to be the viable arsenal to unravel this riddle, then what is the appropriate field theory to formulate the product of two fields? Is it appropriate to start from a relativistic quantum field theory such as the scalar QED, which is closely tied with the Klein-Gordon equation in an external electrostatic field?

- If the OPE is formulated properly, is it feasible to interpret all the universal terms in (11) as the Wilson coefficients? That is, can we treat both regular and divergent Wilson coefficients on an equal footing?

III. NONRELATIVISTIC REDUCTION OF KG EQUATION, FIRST-ORDER QUANTUM-MECHANICAL PERTURBATION THEORY

Before launching into the field-theoretical formalism, we would like to dig more physics out of the single-electron wave equation (1). Since the spinless electron in a KG hydrogen atom is nonrelativistic, $v/c \sim Z\alpha \ll 1$, it is useful to carry out a nonrelativistic reduction to the KG equation, to obtain an effective Schrödinger equation. This reduction procedure is explained in great details in many nice textbooks [7], and the resulting effective Schrödinger equation reads

$$H_{\text{eff}}\psi(r) = E\psi(r),$$

with the effective Hamiltonian

$$H_{\text{eff}} = H_0 + \Delta H = H_0 + H_{\text{kin}} + H_{\text{Darwin}},$$

(13a)

$$H_0 = -\frac{\nabla^2}{2m} - \frac{Ze^2}{4\pi r},$$

(13b)

$$H_{\text{kin}} = -\frac{\nabla^4}{8m^2c^2}, \quad H_{\text{Darwin}} = \frac{1}{32m^4c^4}\left[\nabla^2, \left[\frac{Ze^2}{4\pi r}, \nabla^2\right]\right].$$

(13c)
Eq. (13b) is the standard nonrelativistic Coulomb Hamiltonian. Eq. (13c) represents some perturbations due to relativistic effects. $H_{\text{kin}}$ stands for the leading relativistic correction to the kinetic energy, and $H_{\text{Darwin}}$ stands for the Darwin term, which is responsible for the zitterbewegung motion of the electron [7]. For simplicity, we have set $\hbar = 1$, but still keep $c$ manifest at this stage. It is seen that $H_{\text{kin}}$ makes a contribution of relative order $v^2/c^2$, much more important than the Darwin term, whose contribution is of relative order $v^4/c^4$.

The first-order corrections to the hydrogen energy level from $\Delta H$ can be found in virtually every textbook on advanced quantum mechanics (for example, see [7]),

$$\Delta E^{(1)}_{nl} \bigg|_{\text{kin}} = \langle nl | H_{\text{kin}} | nl \rangle = -mc^2Z^4\alpha^4 \frac{n}{l+\frac{1}{2}} - \frac{3}{4},$$

$$\Delta E^{(1)}_{nl} \bigg|_{\text{Darwin}} = \langle nl | H_{\text{Darwin}} | nl \rangle = 0,$$

which just reproduces the fine structure of hydrogen, derived from the exact solutions of the KG equation (4).

The structure revealed in (10) may suggests us to explore the effect of first-order correction brought by $\Delta H$ to the Schrödinger wave function at small $r$. For definiteness, let us investigate the perturbative correction to the Schrödinger wave function at the origin for the ground state of hydrogen atom, $\Delta R_{10}^{\text{Sch}}(0)$. In accordance with the standard first-order perturbation theory in quantum mechanics, we have

$$\Delta R_{10}^{(1)}(0) = \sum_{n=2}^{\infty} R_{n0}^{\text{Sch}}(0) \frac{\langle n0 | \Delta H | 10 \rangle}{E_{10} - E_{n0}} + \int_0^{\infty} dk \frac{2\pi}{2\pi} R_{k0}^{\text{Sch}}(0) \frac{\langle k0 | \Delta H | 10 \rangle}{E_{10} - E_{k0}},$$

where both discrete and continuum intermediate states are included. Since $\Delta H$ are rotation scalar, we only need retain those intermediates states with $l = 0$.

We are only interested in whether the correction to the wave function at the origin can lead to divergence or not. For this purpose, we ignore the sum over those discrete states, which renders finite results. We just focus on the the high-frequency part of the integration over the continuum $S$-wave states. The corresponding continuum Coulomb wave functions read [8]:

$$R_{k0}^{\text{Sch}}(r) = \sqrt{\frac{8\pi mZ\alpha k}{1 - e^{-2\pi mZ\alpha}}} \cdot e^{-ikr} F_1 \left(1 + \frac{imZ\alpha}{k}, 2; 2ikr \right), \quad E_{k0} = \frac{k^2}{2m},$$

$$\int dr \, r^2 R_{k0}^{\text{Sch}}(r) R_{k'0}^{\text{Sch}}(r) = 2\pi \delta(k - k'),$$

where the “$k/2\pi$-scale” convention is chosen for normalization [8]. For brevity, from now on we will adopt the natural unit $\hbar = c = 1$. 

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It is straightforward to compute the matrix elements encountered in (15):

\[
\langle k_0 | H_{\text{kin}} | 10 \rangle = -2Z^3 \alpha^3 \left( \frac{\pi k}{2 (1 - e^{-2 \pi mZ \alpha / k})} \right) \left[ 1 - \frac{2m^2 Z^2 \alpha^2 \cosh \left( \frac{\pi mZ \alpha}{k} \right)}{k^2 + m^2 Z^2 \alpha^2} \exp \left( \frac{2mZ \alpha}{k} \tan^{-1} \frac{mZ \alpha}{k} \right) \right]
\]

\[
\langle k_0 | H_{\text{kin}} | 10 \rangle \rightarrow -\sqrt{mZ \alpha} Z^3 \alpha^3 \left( \frac{k}{mZ \alpha} + \frac{\pi}{2} + \cdots \right),
\]

\[
\langle k_0 | H_{\text{Darwin}} | 10 \rangle = -\frac{Z^3 \alpha^3}{4} \left( \frac{\pi k}{2 (1 - e^{-2 \pi mZ \alpha / k})} \right) \left( \frac{k^2}{m^2} + Z^2 \alpha^2 \right)
\]

\[
\langle k_0 | H_{\text{Darwin}} | 10 \rangle \rightarrow -\sqrt{mZ \alpha} Z^3 \alpha^3 \left( \frac{k^3}{mZ \alpha} + \frac{\pi k^2}{2} + \frac{(24 + \pi^2)k(mZ \alpha)}{24} + \frac{\pi (\pi^2 - 24)(mZ \alpha)^2}{48} + \cdots \right),
\]

where we also presented the expanded expressions for these matrix elements in inverse powers of \( k \), up to the \( k^0 \) terms.\(^2\)

Simple power counting indicates that the integrations in (15) are severely UV divergent, which indicates that the corrections are dominated by contributions from the high-energy intermediate states. It is natural to imposing a momentum cutoff \( \Lambda < m \) in the integral in (15), to exclude those dangerous high-energy states that defy a trustworthy description by nonrelativistic quantum mechanics. Accordingly, both \( H_{\text{kin}} \) and \( H_{\text{Darwin}} \) bring the following divergent corrections to the 1S wave function:

\[
\Delta R_{10}^{(1)}(0) \bigg|_{\text{kin}} = R_{10}^{\text{Sch}}(0) \left( \frac{Z \alpha \Lambda}{\pi m} + Z^2 \alpha^2 \ln \Lambda + \text{finite} \right),
\]

\[
\Delta R_{10}^{(1)}(0) \bigg|_{\text{Darwin}} = R_{10}^{\text{Sch}}(0) \left( \frac{Z \alpha \Lambda^3}{24\pi m^3} + \frac{Z^2 \alpha^2 \Lambda^2}{16m^2} + \frac{Z^3 \alpha^3 \pi \Lambda}{24m} + \text{finite} \right).
\]

Setting \( \Lambda \sim mZ \alpha \), we indeed verify that the kinematic correction term renders a correction of relative order \( v^2 \sim Z^2 \alpha^2 \), and the Darwin term yields a correction \( \propto v^4 \), in conformity with the velocity counting rule in (13). Although both types of the corrections start from a leading power divergence, it is important to note that the former also develops a subleading logarithmic divergence, whereas the latter does not. Comparing (18a) with (10), we find that, provided that \( r \) is replaced with \( 1/\Lambda \), the coefficients of the logarithmic divergences in both expressions exactly coincide.\(^3\) This is an encouraging sign that the kinetic term \( H_{\text{kin}} \) might well be the agent governing the mild logarithmic divergence of the KG wave function near the origin.

The power divergences in (18) are clearly absent in the original KG wave function (10). It is suggestive to attribute these severe UV power divergences to our use of sharp momentum

\(^2\) Recall for large wavevector \( k \) in (15), \( R_{k0}(0) \propto k \), and the energy denominator yields a contribution \( \propto k^{-2} \). Thereby it suffice for us to truncate the power series in (17c) at the order \( k^0 \), which just generates a mild logarithmic divergence.

\(^3\) In the course of the integration over the intermediate states, if we were replacing the continuum Coulomb states by the free continuum spherical waves, we might anticipate that the coefficients of the UV divergences would not change. Unfortunately, this naive anticipation is true only for the leading UV divergence, but not for the subleading ones. For example, the coefficient of the logarithmic divergence in (18a) would be only half of the correct value.
cutoff as the UV regulator, which is known to break our cherished spacetime symmetries. Thus, these power UV divergences need not to be endowed with any physical significance. On the other hand, the logarithmic UV divergence in (18a) appears to capture some regulator-independent, realistic physical effect, in which we are most interested.

IV. RELATIVISTIC QFT FOR ATOMS AND OPE: AN UNSUCCESSFUL EXPLORATION

Intuitively, the field-theoretical counterpart of the KG equation in a static potential is just the complex scalar field theory coupled with an external electrostatic field. Similar to our preceding work to describe a Schrödinger atom, rather than introduce classical electromagnetic field, we employ the heavy nucleus effective theory (HNET) which is simply analogous to the famous heavy quark effective theory [9, 10], to take into account the quantum fluctuation around a static, positively-charged, and infinitely-heavy nucleus. The spin-zero electron coupled with electromagnetism is formulated by the scalar QED (sQED). The relativistic UV theory that governs all dynamical aspects of atoms is thus formulated by combining the sQED and HNET,

\[ \mathcal{L}_{UV} = (D_{\mu} \phi) \bar{\phi} D^{\mu}\phi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}, \]  

(19)

where the covariant derivatives acting on electron and nucleus are

\[ D_{\mu} = \partial_{\mu} + ieA_{\mu}, \quad D_{\mu} = \partial_{\mu} - iZeA_{\mu}, \]  

(20)

respectively. Equation (19) is obviously gauge invariant. To our purpose, we only need keep the leading-order term in HNET. Therefore, our formalism has not incorporated the effects of finite charge radius and magnetic dipole moment of the nucleus, which are suppressed by powers of \(1/M_N\).

Following [4], we may tentatively express the KG wave function of a hydrogen-like atom in term of the following vacuum-to-atom matrix element 4:

\[ \Psi_{nlm}(r) \equiv \langle 0|\phi(x)N(0)|nlm\rangle. \]  

(21)

Note both field operators are defined in an equal time \(t = 0\). Similar to the familiar Bethe-Salpeter wave function of a hadron in QCD, this spatially-nonlocal matrix element is certainly not gauge invariant.

The universal near-origin behavior of the KG wave function may be transparently understood from (21), once the Wilson expansion of the products \(\phi(x)N(0)\) is conducted. In the \(r \to 0\) limit, the anticipated OPE relation reads

\[ \phi_R(r)N_R(0) = C(r)[\phi N]_R(0) + \cdots, \]  

(22)

\[ ^4 \text{In Weinberg's influential text [1], he reinterpreted the Coulomb solution of the Dirac equation in a field-theoretical context, e.g., in which the corresponding Dirac wave function is regarded as the vacuum-to-hydrogen matrix element. He invokes the external field approximation, whose physical foundation very much resembles our HNET approach. Nevertheless, with a single electron Dirac field operator, it is not obvious to us how to formulate the OPE in the external field formalism.} \]
where the subscript “R” implies the renormalized operator, and \( r \equiv |\mathbf{r}| \). The ellipsis indicates all other higher-dimensional operators with less singular Wilson coefficients. For simplicity, we will only consider the leading S-wave operator throughout this work. It is instructive to also look at the momentum-space version of the OPE relation:

\[
\tilde{\phi}_R(\mathbf{q})N_R(0) \equiv \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}}\phi_R(\mathbf{r})N_R(0) = \tilde{C}(\mathbf{q})[\phi N]_R(0) + \cdots ,
\]

with \( q \equiv |\mathbf{q}| \). This OPE relation is understood to hold true in the \( q \to \infty \) limit.

Our goal in the rest of this section is to compute the Wilson coefficients \( C(r) \) and \( \tilde{C}(q) \) to the first nontrivial order in \( Z\alpha \). It is curious to examine whether the Wilson coefficient in (22) can reproduce the \( \ln r \) term encoded in (10), associated with expansion of the S-wave KG wave functions near the origin.

### A. Renormalization of local composite operator

Renormalization of local composite operator and OPE are two sides of one coin, are two concepts closely intertwined with each other. It is the OPE that endows the renormalized composite operator with a most unambiguous physical meaning [17]. Technically speaking, all the operators in the right-hand side of the OPE relation (22) must be the renormalized (finite) ones. So let us first investigate the renormalization of the composite operator \( \phi N \).

As usual, the renormalized operator is defined by

\[
[\phi N]_R(x) \equiv Z_{eN}\phi^{(0)}(x)N^{(0)}(x) = Z_{eN}\sqrt{Z_e Z_N}\phi_R(x)N_R(x),
\]

with

\[
Z_e = 1 + \delta_e, \quad Z_N = 1 + \delta_N, \quad Z_{eN} = 1 + \delta_{\phi N}.
\]

For later use, we further define a new renormalization constant \( Z_S \) through

\[
[\phi N]_R = Z_S \phi_R N_R,
\]

which is connected with \( Z_{eN} \) through

\[
Z_S = 1 + \delta_S = Z_{eN}\sqrt{Z_e Z_N}, \quad \delta_S = \delta_{\phi N} + \frac{\delta_e}{2} + \frac{\delta_N}{2}.
\]

The renormalization of \( \phi N \) is very similar to renormalization of the heavy-light quark current \( \bar{q}\Gamma h_v \) in HQET [11]. \( Z_{eN} \) is electromagnetic gauge invariant only if \( Z = 1 \), for \( \phi N \) being electrically neutral. All the other renormalization constants are gauge-dependent. In this section, we will choose the Feynman gauge and Coulomb gauge for quantized electromagnetic field. The photon propagator in Feynman gauge reads

\[
D_{\mu\nu}(k) = \frac{-ig_{\mu\nu}}{k^2 + i\epsilon},
\]

where \( \epsilon \) is a small positive number.
FIG. 2: The relevant one-loop diagrams for renormalization of the composite operator $\phi N$ in the relativistic QFT for atoms in (19). The solid line represents the electron field, the double line represents the HNET field, whereas the wavy line represents the full photon propagator, and the dashed line for the temporal component of the photon propagator.

\[ \begin{align*}
\delta_e & = \alpha \frac{Z^2}{\pi \epsilon} - \frac{Z \alpha}{2 \pi \epsilon} - \frac{Z \alpha}{2 \pi \epsilon} - \frac{\alpha}{2 \pi \epsilon}, \\
\delta_N & = 0 - \frac{Z \alpha}{\pi \epsilon} - \frac{Z \alpha}{\pi \epsilon} - \frac{\alpha}{2 \pi \epsilon}.
\end{align*} \]

TABLE I: Numerous counterterms in Feynman gauge and Coulomb gauge in the MS scheme.

while in Coulomb gauge, its nonvanishing components are

\[ D_{00}(k) = \frac{i}{k^2}, \quad D_{ij}(k) = \frac{i}{k^2 + i\epsilon} \left( \delta^{ij} - \frac{k^i k^j}{k^2} \right), \quad i, j = 1, 2, 3. \]  

(29)

Moreover, as indicated in (19), the electron and nucleus propagators are simply

\[ D_e(p) \equiv \frac{i}{p^2 - m^2 + i\epsilon}, \quad D_N(k) \equiv \frac{i}{k^0 + i\epsilon}. \]  

(30)

The corresponding one-loop diagrams for renormalization of $\phi N$ are shown in Fig. 2. The Feynman gauge results can be adapted from [11] with very little modification. For a gauge theory, it is practically most convenient to utilize the dimensional regularization (DR) as the UV regulator, which automatically preserves the Poincaré and gauge invariance. From now on, we will work in the $D = 4 - \epsilon$ spacetime dimensions to regularize the UV divergences. Furthermore, we will employ the minimal subtraction (MS) scheme as the renormalization prescription.

In Table I, we tabulate various renormalization constants in both gauges.\(^5\) One can readily verify $Z_{eN} = 1 - \frac{3\alpha}{2\pi\epsilon}$ is indeed gauge-independent if $Z = 1$.

To evaluate $Z_S$ defined in (26), one only needs consider the vertex correction diagram in Fig. 2, which turns out to be logarithmically UV divergent. The counterterm $\delta_S$ thus

\(^5\) Notice in Coulomb gauge, the nucleus self-energy diagram simply vanishes because the nucleus can only interact with the $A^0$ field, and the instantaneous Coulomb propagator does not contain the causal $i\epsilon$ factor, therefore the contour integral yields a vanishing result since the HNET propagator only contains a single pole in the complex $k^0$ plane.
does not vanish at one-loop order. As recorded in Table I, the specific value of \( \delta S \) is gauge-dependent, which equals
\[
Z_S \bigg|_{\text{Feyn}} = 1 - \frac{Z\alpha}{2\pi} \frac{1}{\epsilon}, \quad Z_S \bigg|_{\text{Coul}} = 1 - \frac{Z\alpha}{\pi} \frac{1}{\epsilon},
\]
in Feynman and Coulomb gauge, respectively. Therefore, the Wilson coefficient \( C(r) \) in (22) is anticipated to begin with \( Z\alpha \ln r \), in conflict with the factor \( Z^2 \alpha^2 \ln r \) in (11) for the \( S \)-wave KG wave function. This is a warning sign that we are on the wrong track.

B. Wilson expansion of the product of \( \phi \) and \( N \)

The remarkable merit of operator product expansion is that it holds at the operator level. It does not really matter which specific form of Green function or matrix element should be taken in order to formulate the Wilson expansion. For simplicity, we will consider the following four-point Green functions:
\[
\Gamma(r; p, k) \equiv \int d^4 y \, d^4 z \, e^{-ip \cdot y - ik \cdot z} \langle 0 | \{ \phi(r)N(0)\phi^\dagger(y)N^\dagger(z) \} | 0 \rangle_{\text{amp}},
\]
\[
\tilde{\Gamma}(q; p, k) \equiv \int d^4 y \, d^4 z \, e^{-ip \cdot y - ik \cdot z} \langle 0 | \{ \tilde{\phi}(q)N(0)\phi^\dagger(y)N^\dagger(z) \} | 0 \rangle_{\text{amp}},
\]
in the coordinate space and momentum space, respectively. Here \( p, k \) can be arbitrary (off-shell) “soft” momenta ⁶. For definiteness, one may simply assume \( p, k \sim m \). The subscript “amp” in (32) implies that the external propagators carrying soft momenta \( p \) and \( k \) get amputated. Two Green functions in (32) are related to each other through Fourier transform:
\[
\tilde{\Gamma}(q; p, k) = \int d^3 r \, e^{-iq \cdot r} \Gamma(r; p, k), \quad \Gamma(r; p, k) = \int \frac{d^3 q}{(2\pi)^3} e^{iqr} \tilde{\Gamma}(q; p, k).
\]

For convenience, we also define the three-point Green function with the renormalized local operator \( [\phi N]_R \) inserted:
\[
G(p, k) \equiv \int d^4 y \, d^4 z \, e^{-ip \cdot y - ik \cdot z} \langle 0 | \{ [\phi N]_R(0)\phi^\dagger(y)N^\dagger(z) \} | 0 \rangle_{\text{amp}},
\]

The OPE can be verified by ensuring the four-point Green functions do bear the following factorized form, order by order in \( Z\alpha \):
\[
\Gamma(r; p, k) \xrightarrow{q \gg m} C(r)G(p, k) + \cdots, \quad \tilde{\Gamma}(q; p, k) \xrightarrow{q \gg m} \tilde{C}(q)G(p, k) + \cdots.
\]

⁶ Some quantification on the term “soft” in the context of HNET may be necessary. In HQET, heavy quarks can only interact with the soft degrees of freedom, those with momentum \( k^\mu \sim \Lambda_{\text{QCD}} \ll m_Q \), where \( \Lambda_{\text{QCD}} \) signifies the intrinsic nonperturbative hadronic scale, and \( m_Q \) implies the heavy quark mass. There is no counterpart of \( \Lambda_{\text{QCD}} \) in QED. Thus one may regard any momentum scale, \( e.g. \), the electron mass, to be “soft”, provided that it is much smaller than the nucleus mass \( M_N \). In this work, we are considering the infinite-nucleus-mass limit, thereby any finite momentum scale can be treated as “soft” in this sense.
FIG. 3: The leading term in the expansion for the product of $\varphi$ and $N$ fields in the free theory.

\[ \phi_N = (\ldots + \text{UVCT}) + (\ldots - \text{UVCT}) \]

a) \hspace{2cm} b)

FIG. 4: The next-to-leading term in the expansion for the product of $\varphi$ and $N$ fields in the coordinate space. The original four-point Green function is reexpressed as the sum of two terms, by subtracting and adding back the renormalized Green function inserted with a local $\phi N$ operator.

As indicated in Fig. 3, the lowest-order prediction of the four-point Green function in the coordinate space comes from the free theory:

\[ \Gamma^{(0)}(0; \mathbf{r}, \mathbf{p}, \mathbf{k}) = e^{i \mathbf{p} \cdot \mathbf{r}} = 1 + O(pr), \quad (36) \]

just arising from the naive Taylor expansion. Since $G^{(0)}(\mathbf{p}, \mathbf{k}) = 1$, we can read off the leading Wilson coefficient to be $C(\mathbf{r}) = 1 + O(Z\alpha)$. It corresponds to $\tilde{\Gamma}^{(0)}(\mathbf{q}; \mathbf{p}, \mathbf{k}) = (2\pi)^3 \delta^3(\mathbf{q})$, therefore $\tilde{C}(\mathbf{q}) = (2\pi)^3 \delta^3(\mathbf{q}) + O(Z\alpha)$.

Next we consider the correction to the Wilson coefficients after inclusion of the interaction. We may express these coefficients as

\[ C(\mathbf{r}) = 1 + c_1(\mathbf{r}) + \ldots, \quad \tilde{C}(\mathbf{q}) = (2\pi)^3 \delta^3(\mathbf{q}) + \tilde{c}_1(\mathbf{q}) + \ldots, \quad (37) \]

where $c_1(\mathbf{r})$ and $\tilde{c}_1(\mathbf{q})$ are the Wilson coefficients at the order $Z\alpha$.

Let us first analyze the large-$\mathbf{q}$ behavior of the four-point Green function in momentum space in (32b), as depicted by the leftmost diagram in Fig. 4. A short calculation in Feynman gauge leads to

\[ \tilde{\Gamma}^{(1)}(\mathbf{q}; \mathbf{p}, \mathbf{k}) \bigg|_{\text{Feyn}} = Z e^2 \int \frac{dq^0}{2\pi} (q^0 + p^0) D_c(q) D_{\phi 0}(q - p) D_N(k + p - q) \]

\[ = -Z e^2 \left[ \frac{\sqrt{q^2 + m^2 + p^0}}{\sqrt{q^2 + m^2}(\sqrt{q^2 + m^2} - k^0 - p^0)} \left( (\sqrt{q^2 + m^2} - p^0)^2 - (q - p)^2 \right) \right. \]

\[ + \frac{2p^0 + |q - p|}{(|q - p| - k^0)|q - p|((p^0 + |q - p|)^2 - q^2 - m^2)} \bigg], \quad (38) \]

where the standard contour method is utilized. Expanding (38) around the $q \to \infty$ separately, one finds that the leading $1/|\mathbf{q}|$ term cancels upon summing the two terms inside the
bracket, and the net limiting behavior turns out to scale as only $1/|q|^3$:

$$\tilde{\Gamma}^{(1)}(q; p, k) \left|_{\text{Feyn}} \right. \xrightarrow{q \gg m} \frac{\pi Z \alpha}{|q|^3} + \ldots.$$  \hfill (39)

Using $G^{(0)}(p, k) = 1$, we thus verify that $\tilde{\Gamma}$ does possess the desired OPE texture, and obtain

$$\tilde{c}_1(q) \left|_{\text{Feyn}} \right. = \frac{\pi Z \alpha}{|q|^3}. \hfill (40)$$

The same analysis can be repeated in Coulomb gauge, resulting in simpler form. The corresponding momentum-space Green function is

$$\tilde{\Gamma}^{(1)}(q; p, k) \left|_{\text{Coul}} \right. = -\frac{Ze^2}{2} \frac{p^0 + \sqrt{q^2 + m^2}}{\sqrt{q^2 + m^2(k^0 + p^0 - \sqrt{q^2 + m^2})(q - p)^2}} \xrightarrow{q \gg m} \frac{2\pi Z \alpha}{|q|^3} + \ldots. \hfill (41)$$

Thus we have

$$\tilde{c}_1(q) \left|_{\text{Coul}} \right. = \frac{2\pi Z \alpha}{|q|^3}. \hfill (42)$$

When Fourier-transforming $\tilde{\Gamma}^{(1)}$ into $\Gamma^{(1)}$ in accord with (33), the integration variable $q$ can range from soft to hard. If $|q| \sim p, k, m$, the characteristic soft regime, it is legitimate to approximate the exponential $e^{i\mathbf{q} \cdot \mathbf{r}}$ by 1. Supplemented with the UV counterterm, this piece of contribution is captured by the renormalized Green function, as represented by Fig. 4a). On the contrary, when $q$ is in the hard regime, i.e., $|q| \gg m \sim 1/r$, one can no longer expand the Fourier exponential $e^{i\mathbf{q} \cdot \mathbf{r}}$. But the integration over the hard region should be encapsulated in the Wilson coefficient. Precisely speaking, the Wilson coefficient can then be identified with the original coordinate-space Green function $\Gamma^{(1)}(\mathbf{r})$ subtracting off the Green function containing the renormalized $\phi N$ operator:

$$c_1(\mathbf{r}) = \lim_{r \to 0} \Gamma^{(1)}(\mathbf{r}; p, k) - G_R^{(1)}(p, k). \hfill (43)$$

This add-and-subtract procedure has been pictured in Fig. 4, which can also be derived from (35).

As represented in Fig. 4a), the NLO renormalized Green function with the $\phi N$ insertion, $G_R^{(1)}$, is defined by

$$G_R^{(1)}(p, k; \mu) = \mu^\varepsilon \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \tilde{\Gamma}^{(1)}(\mathbf{q}; p, k) + \delta_S, \hfill (44)$$

where the UV counterterm $\delta_S$ for both gauges are given in Table 2 as well as (31). The MS scheme has been utilized to renormalize the Green function $G^{(1)}$.

In accordance with Fig. 4b), making use of (33) and (44), we reexpress $c_1(\mathbf{r})$ in (43) as

$$c_1(\mathbf{r}) \approx \mu^\varepsilon \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \tilde{\Gamma}^{(1)}(\mathbf{q}; p, k) (e^{i\mathbf{q} \cdot \mathbf{r}} - 1) - \delta_S$$

$$\approx \mu^\varepsilon \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \tilde{c}_1(q) (e^{i\mathbf{q} \cdot \mathbf{r}} - 1) - \delta_S. \hfill (45)$$
In the second line, we have only kept the leading asymptotic form of \( \tilde{\Gamma}^{(1)} \) in the \( q \to \infty \) limit. Note the subtraction form automatically guarantees that, upon dropping all the occurrence of the \( p, k \) and \( m \), the infrared divergence that may potentially arise in the \( q \to 0 \) limit does not actually arise! By construction, \( c_1(r) \) in (45) is both UV and IR finite, as it must be.

Substituting (40) and (42) into (45), it is straightforward to obtain the intended order-\( Z\alpha \) coordinate-space Wilson coefficients in both gauges:

\[
\begin{align*}
c_1(r)_{\text{Feyn}} &= -\frac{Z\alpha}{2\pi} \left( \ln \mu r + \frac{\gamma_E}{2} + \ln \pi \right), \\
c_1(r)_{\text{Coul}} &= -\frac{Z\alpha}{\pi} \left( \ln \mu r + \frac{\gamma_E}{2} + \ln \pi \right),
\end{align*}
\]

where \( \gamma_E = 0.5772 \cdots \) is the Euler gamma constant. As expected, the coefficients of the \( \ln r \) term in two gauges are identical to the coefficient of the single pole in \( \delta_S \) in (31).

Albeit being gauge-dependent, the Wilson coefficient \( C(r) \) in (22) indeed contains the \( \ln r \) term, which however arises already at order \( Z\alpha \). This is in sharp contrast with the weak logarithmic singularity of the \( S \)-wave KG wave functions near the origin encapsulated in (10), in which the \( \ln r \) term is accompanied with a coefficient \( \propto Z^2 \alpha^2 \).

Therefore, we must admit that the Wilson expansion based on relativistic scalar QED fails to account for the divergence symptom of KG wave function near the origin. It may cast some doubt on the legitimateness of interpreting the matrix element (21) as the KG wave function, which somewhat contradicts the underlying assumption in Weinberg’s text on Dirac equation in Coulomb potential \[1\]. In particular, the short-distance \( (r \ll 1/m) \) behavior of KG wave function cannot be correctly accounted by the OPE formalism described in this section. As a superficially relativistic wave equation, incorporation of the instantaneous Coulomb potential forces us to choose a special reference frame for the KG equation, namely the rest frame of the nucleus. Since the simultaneous production of the electron-positron pair becomes inevitable once the distance is probed in a distance shorter than Compton wavelength, the single-particle probabilistic interpretation of relativistic wave equation must breakdown. The lesson seems to be that one should not attempt to discuss the very short-distance behavior of the KG equation, which might not bear enough physical significance.

V. A PROPER NONRELATIVISTIC EFFECTIVE FIELD THEORY FOR_ATOM

In the preceding section, having started with a relativistic QFT to describe the atom, which is based on the sQED plus HNET, we have gone through a long way to prove the OPE along this direction actually leads to a dead end. Nevertheless, we recall that in section III, upon a nonrelativistic reduction of KG equation into an effective Schrödinger equation, one is able to embed the relativistic effects into a few corrections to the Coulomb Hamiltonian. The kinetic correction term appears to capture the correct structure of the short-range logarithm by employing the quantum-mechanical perturbation theory to analyze the first-order correction to the Schrödinger wave function at the origin. This is a very encouraging result, which insinuates the correct way is to formalize the OPE in the framework of a non-relativistic effective field theory framework, rather than the relativistic QFT considered in section IV.

The original KG equation in (1) only involves the Coulomb interaction between the electron and nucleus, since that equation is specified in the rest frame of the nucleus. To caputure this feature, we drop all the occurrences of the vector potential \( A \) in (19). The
simplified UV field theory for atom now reads

$$\mathcal{L}_{UV} = (D_0\phi)\dagger D^0\phi - \nabla\phi\dagger \cdot \nabla\phi - m^2\phi\dagger \phi + N\dagger iD_0 N + \frac{1}{2}(\nabla A_0)^2. \quad (47)$$

Eq. (47) is certainly no longer gauge invariant. However, this does not necessarily imply a nuisance. Coulomb gauge $\nabla \cdot A = 0$ is a particularly convenient choice for tackling nonrelativistic bound state problem, where the effect of $A$ and $A^0$ can be cleanly separated. The former encodes the dynamics of the transversely polarized photon, whose effect is absent in this work; the latter is the very agent for mediating the instantaneous Coulomb interaction, which provides the crucial binding mechanism for all atoms. From now on, we will stay exclusively with the Coulomb gauge in the rest of the work.\(^7\)

A. NREFT from field redefinition

Analogous to deriving the effective Hamiltonian in (13) from the single-particle relativistic KG equation, our goal is to present a quick construction of the nonrelativistic EFT, starting from the scalar QED sector of (47),

$$\mathcal{L}_{sQED} = (D_0\phi)\dagger D^0\phi - c^2(\nabla\phi)\dagger \cdot \nabla\phi - m^2c^4\phi\dagger \phi, \quad (48)$$

with the corresponding Euler-Lagrange equation reading

$$\left(D_0^2 - c^2\nabla^2 + m^2c^4\right)\phi = 0. \quad (49)$$

To separate the electron and positron degrees of freedom, we first rewrite $\phi$ as\(^8\)

$$\phi = \frac{1}{\sqrt{2mc^2}}e^{-imc^2t}(\varphi + \tilde{\varphi}), \quad (50)$$

with

$$\varphi = e^{imc^2t}\frac{1}{\sqrt{2mc^2}}(iD_0 + mc^2)\phi, \quad \tilde{\varphi} = e^{imc^2t}\frac{1}{\sqrt{2mc^2}}(-iD_0 + mc^2)\phi, \quad (51)$$

where $\varphi$ ($\tilde{\varphi}$) may be referred to as the large (small) component. Substituting (50) into (48), we then obtain

$$\mathcal{L}_{sQED} = (\varphi + \tilde{\varphi}^\dagger) \left(iD_0 + \frac{\nabla^2}{2m} - \frac{D_0^2}{2mc^2}\right)(\varphi + \tilde{\varphi}), \quad (52)$$

where integration by part is used to make all differential operators act to the right.

Acting the covariant derivative $-iD^0$ on $\varphi + \tilde{\varphi}$, with the aid of (50) and (51), we can find the relation

$$\tilde{\varphi} = -\frac{1}{2mc^2}iD_0 (\varphi + \tilde{\varphi}). \quad (53)$$

---

\(^7\) A common representation of (47) it to get rid of $A^0$ and in favor of explicit introducing the instantaneous Coulomb potential. Nevertheless, we stress that (47) is still a local field theory. Note locality plays an essential role in corroborating OPE, in accord with Weinberg’s proof of OPE using path integral [12].

\(^8\) The field redefinition (50) is employed to derive the heavy scalar effective theory (HSET) lagrangian to sub-leading order in $1/m$ expansion [13]. Here we use this technique to derive the nonrelativistic sQED (NRsQED) lagrangian to order $v^4/c^4$. 
Assuming \( iD_0 \sim mv^2 \), one infers from (53) that \( \tilde{\varphi} \approx -\frac{1}{2mc^2}iD_0\varphi, \) thus justifying the nomenclature “small” component for \( \tilde{\varphi} \).

Substituting (50) into (49), or directly starting from the lagrangian (52), we obtain the following equation of motion for \( \varphi \) and \( \tilde{\varphi} \):

\[
\left[ iD_0 + \frac{\nabla^2}{2m} - \frac{D_0^2}{2mc^2} \right] (\varphi + \tilde{\varphi}) = 0. \tag{54}
\]

Utilizing (53) to get rid of \( iD_0(\varphi + \tilde{\varphi}) \) in (54), after some straightforward algebra, one finds

\[
iD_0\varphi = \frac{1}{2m}\nabla^2(\varphi + \tilde{\varphi}). \tag{55}
\]

Now we are ready to derive the nonrelativistic scalar QED lagrangian. First we retain the \( \varphi^\dagger(iD_0 + \frac{\nabla^2}{2m})\varphi \) term in (52) as the minimal NRsQED lagrangian. We the apply equations (53) and (55) iteratively, to get rid of the occurrence of \( \tilde{\varphi} \) consecutively order by order in \( v \) expansion. To be explicit, let us take the \( \mathcal{O}(v^4/c^4) \) term \( \tilde{\varphi}^\dagger(iD_0)\tilde{\varphi} \) as an explicit example to illustrate our procedure:

\[
\tilde{\varphi}^\dagger iD_0 \tilde{\varphi} \approx \left( -\frac{1}{2mc^2}iD_0\varphi \right)^\dagger iD_0 \left( -\frac{1}{2mc^2}iD_0\varphi \right) \approx \frac{1}{16m^4c^4}(\nabla^2 \varphi)^\dagger iD_0 \nabla^2 \varphi
\]

\[
= \frac{1}{16m^4c^4}(\nabla^2 \varphi)^\dagger \left( \nabla^2 iD_0 + [iD_0, \nabla^2] \right) \varphi
\]

\[
\approx -\frac{1}{32m^4c^4}\varphi^\dagger \nabla^6 \varphi - \frac{1}{16m^4c^4}\varphi^\dagger \nabla^2[e\varphi^\dagger, eA_0]. \tag{56}
\]

In deriving this, we have used (53), (55) and the integration by part in the last step.

After some straightforward yet tedious iterative derivations, we arrive at the NRsQED lagrangian accurate to relative order \( v^4/c^4 \),

\[
\mathcal{L}_{\text{NRsQED}} = \varphi^\dagger(iD_0 + \frac{\nabla^2}{2m} + \frac{\nabla^4}{8mc^2} + \frac{\nabla^6}{16m^3c^4} + \frac{1}{16m^4c^4}\nabla^2[e\varphi^\dagger, eA_0])\varphi. \tag{57}
\]

The last term is not in the right form of the Darwin term as given in (13c). One may supplement the effective lagrangian (57) with the following total time derivative term:

\[
\frac{1}{32m^4c^4}i\partial_0(\varphi^\dagger \nabla^4 \varphi) = -\frac{1}{64m^5c^4}\varphi \cdot \left[ (\nabla \varphi)^\dagger \nabla^4 \varphi - \varphi^\dagger \nabla^4 (\nabla \varphi) \right] \tag{58}
\]

\[
+ \frac{1}{32m^4c^4}\varphi^\dagger \left[ \nabla^4 eA_0 - eA_0 \nabla^4 \right] \varphi,
\]

where (55) is used.

Now the nonrelativistic sQED is put in the canonic form. Together with the HNET and the reduced Maxwell lagrangian, we finally write down our nonrelativistic EFT for atoms:

\[
\mathcal{L}_{\text{NREFT}} = \varphi^\dagger \left( iD_0 + \frac{\nabla^2}{2m} \right) \varphi + \varphi^\dagger \frac{\nabla^4}{8mc^2} \varphi + \frac{\nabla^6}{16m^3c^4} \varphi + \frac{1}{32m^4c^4} \varphi^\dagger \nabla^2[eA_0, \nabla^2] \varphi
\]

\[
+ N^\dagger iD_0^0 N + \frac{1}{2}(\nabla A_0)^2 + \frac{eA_0}{m^2c^2} \varphi^\dagger \varphi N^\dagger N + \cdots, \tag{59}
\]
where we have recovered natural unit. In the NRsQED sector, we retain all the allowed terms through the relative order $v^4$. Apart from rotational invariance, this NREFT also obeys a global $U(1) \times U(1)$ phase symmetry, which reflects the separate number conservation law for electrons and nucleus, respectively. Rotation and phase invariance also allows us to add a contact interaction $\phi \phi^\dagger N N^\dagger$ to (59). The corresponding dimensionless coefficient $c_4$ encodes some possible short-distance dynamics.

We emphasize that, as a nonrelativistic effective theory, (59) is only valid when the probed momentum is smaller than its intrinsic UV cutoff, which is of order electron mass $m$.

### B. Tree-Level Matching

Let us use the more standard perturbative matching method to verify our NREFT lagrangian in (59). The strategy is familiar, to demand both UV theory (47) and EFT (59) yield equal $S$-matrix for the elastic scattering $e(p)N \rightarrow e(p')N$ in the low-energy limit, order by order in loop and velocity expansion.

We first consider matching the tree-level amplitude, which is illustrated in Fig. 5. The UV theory generates the amplitude:

$$i M^\text{tree}_{\text{UV}} = \frac{i Z e^2}{\sqrt{2} p^0 \sqrt{2} p'^0} \left( \frac{p^0 + p'^0}{(p - p')^2} + \frac{i Z e^2 (p^4 - 2 p^2 p'^2 + p'^4)}{32 m^4 (p - p')^2} + O(v^5) \right).$$

(60)

We have adopted the nonrelativistic normalization convention for states, which is reflected in the prefactor $\frac{1}{\sqrt{2} p^0 \sqrt{2} p'^0}$. In deriving the final expression in (60), we have expanded the energies of the incoming and outgoing electron according to

$$p^0 = \sqrt{p^2 + m^2} = m \left( 1 + \frac{p^2}{2m^2} - \frac{p^4}{8m^4} + \cdots \right).$$

(61)

As instructed by Fig. 5, if one includes the Coulomb interaction together with the Darwin term in the EFT side, it is then straightforward to verify that the resulting tree-level NREFT amplitude exactly coincides with (60).

### C. One-loop Matching and absence of contact interaction

We continue to match the low-energy scattering amplitude for $eN \rightarrow eN$ from the UV theory onto NREFT at order $Z^2 \alpha^2 v^0$, with the corresponding diagrams shown in Fig. 6.
The goal is to determine the Wilson coefficient $c_4$ for the contact interaction, which may encapsulate some effects related to the short-lived electron-positron intermediate state.

On the UV theory side, the seagull diagram does not contribute, since only a single pole is present in the integrand that originates from the HNET propagator, thereby simply generating vanishing result upon contour integral. Therefore we only need consider the box and crossed box diagrams,

$$i\mathcal{M}_{\text{UV}}^{\text{one-loop}} = \frac{Z^2 e^4 \mu^2}{\sqrt{2} p^0 \sqrt{2} p'^0} \int \frac{d^{D-1}l}{(2\pi)^{D-1}} D_e(l) D_{00}(p-l) D_{00}(l-p')$$

$$\times [D_N(p-l) + D_N(l-p')] (p^0 + l^0) (l^0 + p'^0)$$

$$= \frac{i Z^2 e^4 \mu^2}{\sqrt{2} p^0 \sqrt{2} p'^0} \int \frac{d^{D-1}l}{(2\pi)^{D-1}} \frac{1}{(p-1)^2(p'-1)^2 2\sqrt{p^2 + m^2}} \left( \frac{p^0 + \sqrt{p^2 + m^2}}{\sqrt{p^2 + m^2} - p^0} + \frac{p^0 - \sqrt{p^2 + m^2}}{\sqrt{p^2 + m^2} + p^0} \right)$$

$$= \frac{i Z^2 e^4 \mu^2}{\sqrt{2} p^0 \sqrt{2} p'^0} \int \frac{d^{D-1}l}{(2\pi)^{D-1}} \frac{4m^2 + 3p^2 + l^2}{(1-p)^2(1-p')^2(l^2 - p^2)}.$$

where the on-shell condition $p^0 = p'^0 = \sqrt{p^2 + m^2}$ has been used.

Next we turn to the calculation on the EFT side. Note the electron propagator in NREFT obeys the nonrelativistic dispersion relation,

$$\mathcal{D}_e(k) \equiv \frac{i}{k^0 - \frac{k^2}{2m} + i\epsilon}.$$  \hspace{1cm} (63)

Accordingly, the order-$Z^2 \alpha^2$ NREFT amplitude for $eN \rightarrow eN$ becomes

$$i\mathcal{M}_{\text{NREFT}}^{\text{one-loop}} = \frac{Z^2 e^4 \mu^2}{(2\pi)^D} \mathcal{D}_e(l) D_{00}(p-l) D_{00}(l-p') \left[ 1 + \mathcal{D}_e(l) \frac{i l_4}{8m^3} \right] + \frac{c_4}{m^2},$$

$$= \frac{i Z^2 e^4 \mu^2}{(2\pi)^D} \int \frac{d^{D-1}l}{(2\pi)^{D-1}} \frac{1}{(1-p)^2(1-p')^2 \left( \frac{p^2}{2m} - \frac{l^2}{2m} \right)} \left( -1 + \frac{l_4}{8m^3 \left( \frac{p^2}{2m} - \frac{l^2}{2m} \right)} \right) + \frac{c_4}{m^2}.$$ \hspace{1cm} (64)

where we have also included the diagram with one $p^4$ kinetic term inserted on the electron propagator.

In passing, we emphasize some remarkable calculational simplifications in NREFT compared with the relativistic UV theory. Due to the peculiar causal structure of the nonrelativistic propagators, and the non-propagating nature of the instantaneous Coulomb interaction, all diagrams of the crossed-ladder topology, or of the structure with the emission...
and absorption of a Coulomb photon by the same nonrelativistic line, will all yield vanishing results upon the contour integration over the 0-th component of the loop momentum. Therefore, in the rest of the paper, we need retain those diagrams only exchanging the instantaneous Coulomb ladders.

By construction, (62) and (64) must share the same IR/nonanalytic behavior. They can only differ in the ultraviolet regime of the loop integral as \( l \sim m \). This difference may be compensated by inclusion of the contact interaction in the NREFT. For the sake of deducing \( c_4 \), it is legitimate to expand the integrands in (62) and (64) in power series of \( p/l, p'/l \), since the Wilson coefficient receives the contribution entirely from the hard loop momentum regime.

Since the contact term corresponds to \( S \)-wave operator, it is feasible to set \( p = p' = 0 \) in (62) and (64). We then obtain

\[
\begin{align*}
\mathcal{M}_{\text{Full}}^{\text{one-loop}} &= iZ^2 e^4 \mu^2 \epsilon \int \frac{d^{D-1}l}{(2\pi)^{D-1}} \left( \frac{2m}{l^6} + \frac{1}{2ml^4} \right) + \cdots, \\
\mathcal{M}_{\text{NREFT}}^{\text{one-loop}} &= iZ^2 e^4 \mu^2 \epsilon \int \frac{d^{D-1}l}{(2\pi)^{D-1}} \left( \frac{2m}{l^6} + \frac{1}{2ml^4} \right) + \frac{c_4}{m^2} + \cdots,
\end{align*}
\]

(65a)

(65b)

where the ellipsis indicates terms proportional to powers of \( p \) and \( p' \). Both integrals in (65) are scaleless, thus vanish in DR. A close look indicate that each of the integrals is severely IR divergent. However, as warranted by the guiding principle of EFT, they must share the identical IR divergence. Moreover, since these two expanded integrals turn out to be exactly identical at order \( Z^2\alpha^2 \), there is no room for \( c_4 \) to contribute at this order. Thus we have

\[ c_4 = 0 + \mathcal{O}(Z^3\alpha^3). \] (66)

One may wonder that the vanishing of \( c_4 \) may persist to even higher order [1]. Nevertheless we will not dwell on this issue further in this work.\(^9\)

VI. RENORMALIZATION OF LOCAL COMPOSITE OPERATOR \( \varphi N \)

In our preceding work on the nonrelativistic Coulomb-Schrödinger EFT, the local composite operator made of the electron and nucleus fields is free from UV divergences [4]. Nevertheless, in the enlarged NREFT defined in (59), when a certain class of relativistic corrections are included, it is conceivable that the composite operator \( \varphi N \) becomes UV divergent, and calls for renormalization.

The major goal of this section is pursue that, to which order in \( Z\alpha \), the logarithmic UV divergence would arise to necessitate the renormalization of the the \( S \)-wave composite operator \( \varphi N \). In some sense, this section is analogous to section IV A, yet with the relativistic QFT of (19) replaced with the NREFT of (59).

As inspired by the analysis based on the quantum-mechanical perturbation theory in section III, we see that the \( p^4 \) kinetic correction does bring the logarithmic UV divergence,

\(^9\) Recall that the famous \( \delta^{(3)}(r) \)-type Uehling potential, which arises from the vacuum polarization correction to the photon propagator, may mimic the \( c_4 \) contact interaction. Nevertheless, the vacuum polarization is a genuinely QED effect, which is not contained in the Klein-Gordon equation (1) at all. Therefore we discard this complication.
FIG. 7: Some representative higher-order NREFT diagrams for $G(p, E)$ defined in (68). Except for the last two diagrams that contain a contact interaction vertex, all other diagrams arise at most at $\mathcal{O}(Z^2\alpha^2)$, as well as contain at most a single insertion of the $p^4$ kinematic term.

while the Darwin term does not. Therefore, in our explicit calculation, we will not include $p^6$ kinetic correction and the Darwin term.

Similar to (24), we adopt a multiplicative renormalization procedure for the local operator $\varphi_N$:

$$[\varphi_N]_R = Z_S \varphi_R \varphi = Z_{\varphi_N} \varphi(0) N(0),$$  
(67)

where $Z_S$ and $Z_{\varphi_N}$ are divergent renormalization constants. Due to the single-pole structure of the nonrelativistic propagators and the instantaneous Coulomb interaction, self-energy diagrams for the $\varphi$ and $N$ fields simply vanish in arbitrarily high order. As a consequence, we do not bother to distinguish the bare and renormalized fields for $e$ and $N$, therefore, $Z_S = Z_{\varphi_N}$ in (67).

In analogue with (34), for future use we also introduce the three-point Green function inserted with the renormalized local operator $[\varphi N]_R$:

$$G(p, E \equiv p^0 + k^0) \equiv \int d^4y d^4z \ e^{-ip \cdot y - ik \cdot z} \langle 0 | T \{[\varphi N]_R(0) \varphi(y) N(z) \} | 0 \rangle_{\text{amp}}. \quad (68)$$

The subscript “amp” again implies that the external electron and nucleus legs get amputated. Some higher-order corrections to this Green function through $\mathcal{O}(Z^2\alpha^2)$ are portrayed in Fig. 7. We assume the external momenta $p$ and $k$ to be soft, in the sense that they are of order $mZ\alpha \ll m$. For simplicity, we further assume $E \equiv p^0 + k^0 < 0$, and define $\kappa = \sqrt{-2mE} > 0$.

The NLO correction depicted in Fig. 7a) is finite,

$$G^{(1)}_{7a}(p, E) = Ze^2 \mu \int \frac{d^Dl}{(2\pi)^D} D_e(l) D_{00}(p - l) D_N(k - p - l)$$
$$= 2mZe^2 \int \frac{d^3l}{(2\pi)^3} \frac{1}{(l^2 + \kappa^2)(1 - |p|)} = \frac{2mZ\alpha}{|p|} \tan^{-1} \frac{|p|}{\kappa},$$
(69)

hereafter we use the superscript $(n)$ to denote the order of $Z\alpha$ for the corresponding diagram.

With one insertion of the kinetic correction onto the electron propagator, Fig. 7b) turns to be linearly UV divergent. Nevertheless, it gives finite result within DR,

$$G^{(1)}_{7b}(p, E) = i\mu \frac{e^2}{2m} \int \frac{d^Dl}{(2\pi)^D} D_e^2(l) D_{00}(p - l) D_N(k + p - l) \frac{l^4}{8m^2}$$
$$= -Ze^2 \mu \int \frac{d^3l}{(2\pi)^3} \frac{l^4}{(l^2 + \kappa^2)^2(1 - |p|)} = \frac{2EZ\alpha}{|p|} \left( \tan^{-1} \frac{|p|}{\kappa} - \frac{\kappa|p|}{4(|p|^2 + \kappa^2)} \right),$$
(70)

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which is order-$v^2$ suppressed relative to (69). Furthermore, one can prove that, the one-loop vertex diagram with arbitrary number of insertion of the kinetic corrections would never bring logarithmic divergence in DR. The technical reason is because the argument of the Gamma function is always half of an odd integer when $D \to 4$.

At next-to-next-to-leading order (NNLO), the two-loop diagram without insertion of relativistic correction, as depicted in Fig. 7c, is still UV finite. Depending on which electron propagator is inserted with the kinetic term, we are left with two distinct diagrams, Fig. 7d and Fig. 7e, respectively.

We first consider the relativistic correction is inserted in the upper loop, as indicated in Fig. 7d. Some straightforward calculation leads to

$$ G_{te}^{(2)}(p, E) = iZ^2 e^4 \mu^{2\epsilon} \int \frac{d^{D-1}l}{(2\pi)^D} \int \frac{d^Dq}{(2\pi)^D} D_e(l) D_{00}(p - l) D_N(k + p - l) $$

$$ \times D_c(q) D_{00}(l - q) D_N(k + p - q) \frac{q^4}{8m^3} \quad (71) $$

$$ = Z^2 e^4 \mu^{2\epsilon} \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \frac{1}{(1 - p)^2 (1 - q)^2 + \kappa^2} \frac{1}{(q^2 + \kappa^2)^2} $$

$$ \times Z^2 e^4 \mu^{2\epsilon} \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \frac{1}{(1 - q)^2 + \kappa^2} \left[ 1 - \frac{2\kappa^2}{q^2 + \kappa^2} + \frac{\kappa^4}{(q^2 + \kappa^2)^2} \right]. $$

Simple counting of the superficial degrees of divergence implies that, in order to nail down the potential UV divergence, it is sufficient to retain only the first term in the bracket. For the integral over $q$, one may simply shift the variable and obtain

$$ \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \frac{1}{q^2} = 0, \quad DR \quad (72) $$

since scaleless integrals are set to zero in dimensional regularization. Obviously, this integral actually corresponds to a linear UV divergence provided the momentum hard cutoff is imposed. It is reminiscent of the leading linear divergence encountered in (18a), the first-order correction to the Schrödinger wave function at the origin from the $p^4$ kinetic perturbation.

So far, the diagrams we encountered are either UV finite or power divergent. In fact, Fig. 7e), the NNLO diagram with the kinetic term inserted on the electron propagator in the lower loop, is the most interesting one, because it gives the desired logarithmic singularity $^{10}$:

$$ G_{te}^{(2)}(p, E) = iZ^2 e^4 \mu^{2\epsilon} \int \frac{d^{D-1}l}{(2\pi)^D} \int \frac{d^Dq}{(2\pi)^D} D_e(l) D_{00}(p - l) D_N(k + p - l) $$

$$ \times D_c(q) D_{00}(l - q) D_N(k + p - q) \frac{1}{8m^3} $$

$$ \approx Z^2 e^4 \mu^{2\epsilon} \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \frac{1}{q^2(1 - q)^2 + \kappa^2} \left| q, \text{hard} \right| $$

$$ = Z^2 \alpha^2 \left( \frac{1}{2\epsilon} + \ln \mu \right) + \text{finite terms.} \quad (73) $$

$^{10}$ Note this kind of logarithmic UV singularity at two loop was first discovered when matching vector current from QCD onto NRQCD [18, 19]. For a calculation directly from the nonrelativistic EFT, see also [20].
Note that the UV divergence comes from the region when both loop momenta $q$ and $l$ become hard ($\sim m$). Simple power counting indicates the above two-loop integration does result in a logarithmic UV singularity.

Last but not the least, in principle one should also consider the one-loop diagram involving a contact interaction vertex, as depicted in Fig. 7f. This diagram turns out to be linearly UV divergent, yet without subleading logarithmic UV divergence. On the contrary, the two-loop diagram involving the contact interaction, Fig. 7g), does yield a leading logarithmic UV divergence. In accordance with (66), $c_4$ is at least of order $Z^3\alpha^3$, therefore Fig. 7g) would contribute a logarithmic divergence at least at order-$Z^4\alpha^4$, which is beyond the targeted accuracy of $Z^2\alpha^2$.

To summarize, among all the higher-order NREFT diagrams for $G(p, E)$ through the order-$Z^2\alpha^2$, only Fig. 7e) contributes an intended logarithmic UV divergence. The operator renormalization constant $Z_S$ can thus be determined:

$$Z_S = 1 - \frac{Z^2\alpha^2}{2e} + \cdots,$$  \hspace{1cm} (74)

in the MS scheme. The corresponding anomalous dimension of the composite operator $\varphi N$ is thus

$$\gamma_S \equiv \frac{d \log Z_S}{d \log \mu} = Z^2\alpha^2.$$  \hspace{1cm} (75)

VII. OPERATOR PRODUCT EXPANSION IN NREFT

In section IV, we have considered the Wilson expansion of the electron field in scalar QED and the nucleus field in HNET. The Wilson coefficient associated with the leading $S$-wave operator begins with $\ln r$ at first order in $Z\alpha$. This incorrect coefficient of $Z\alpha$ contradicts that in the KG wave function near the origin, thus we have to give up the OPE in the relativistic scalar QED. Numerous evidences have accumulated from section III and VI, which encouragingly suggest that the correct route is to formulate the OPE in the context of nonrelativistic EFT, by taking a certain class of relativistic corrections into account. In this section, we will pursue this trail comprehensively.

We will consider the product of $\varphi$ and $N$ at equal time, in the framework of the NREFT specified in (59). In the $r \to \frac{1}{m}$ limit $^{11}$, the Wilson expansion is anticipated to read $^{12}$

$$\varphi(r)N(0) = C(r)[\varphi N]_R(0) + \cdots,$$  \hspace{1cm} (76a)

$$C(r) = 1 + c^{(1)}(r) + c^{(2)}(r) + \cdots,$$  \hspace{1cm} (76b)

with $r \equiv |r|$. Hereafter the superscript $(n)$ again indicates the power of $Z\alpha$.

$^{11}$ In a renormalizable QFT, such as the sQED considered in section VI, the Wilson expansion can be conducted literally in the $r \to 0$ limit. However, as a low-energy effective theory, our NREFT remains only valid when the probed distance is greater than the electron’s Compton wavelength. Therefore, all the OPE relations in this section should be understood to work only in the limit $r \to \frac{1}{m}$.

$^{12}$ Note for the electron field appearing in OPE, we choose the nonrelativistic NRQED field in the spirit of [14, 15], rather than the lower energy EFT such as the potential NRQED [16], since we need to work with a local EFT.
It is also useful to express the OPE in momentum space:
\[
\tilde{\varphi}(q)N(0) \equiv \int d^3 r \ e^{-i q \cdot r} \varphi(r)N(0) = \tilde{C}(q)[\varphi N]_R(0) + \cdots ,
\]
with \(q \equiv |q| \rightarrow m\).

Very recently we have determined \(c^{(1)}(r) = -mZ\alpha\) and \(\tilde{c}^{(1)}(q) = \frac{8\pi mZ\alpha}{q^4}\) in the nonrelativistic EFT [4]. In the rest of the section, we will add the \(p^4\) kinetic correction into the Coulomb-Schrödinger EFT, and verify the OPE relations (76) and (77) through the order \(Z^2\alpha^2\), in both momentum space and coordinate space. The direct outcome is to ascertain the Wilson coefficients \(c^{(2)}(r)\) and \(\tilde{c}^{(2)}(q)\). We will verify that \(c^{(2)}(r)\) captures the desired \(Z^2\alpha^2 \ln r\) behavior, in perfect agreement with the near-the-origin behavior of the \(S\)-wave KG wave function. In the end we will employ the renormalization group equation (RGE) to resum large logarithms of \(r/a_0\) to all orders.

A. OPE in Momentum Space

We begin with examining the OPE relation (77) in the momentum space. To facilitate the study, in analogue with (32b), we introduce the following amputated four-point Green function:
\[
\tilde{\Gamma}(q; p, k) \equiv \int d^4 y d^4 z \ e^{-i p \cdot y - i k \cdot z} \langle 0| T \{ \tilde{\varphi}(q)N(0)\varphi(y)N^\dagger(z) \} |0\rangle_{\text{amp}}.
\]
As before, the momentum \(q\) is hard (\(\sim m\)), which flows into the upper-left electron line and exits from the upper-right nucleus line, while the momenta \(p\) and \(k\) signify the soft momenta carried by the amputated electron and nucleus, with \(p, k \ll m\). The key is to verify that \(\tilde{\Gamma}\) does possess the following factorized form, order by order in \(Z\alpha\):
\[
\tilde{\Gamma}(q; p, k) \xrightarrow{q \rightarrow m} \tilde{C}(q) \mathcal{G}(p, E) + \cdots ,
\]
where the three-point Green function with a \(\varphi N\) insertion has been defined in (68).

To examine (79) in perturbation theory, we write \(\tilde{\Gamma} = \sum_{n=1}^{\infty} \tilde{\Gamma}^{(n)}\), where the superscript \(n\) denotes the order in \(Z\alpha\). Thus at a given order \(n\), (79) becomes
\[
\tilde{\Gamma}^{(n)}(q; p, E) \xrightarrow{q \rightarrow m} \sum_{i=1}^{n} \tilde{c}^{(i)}(q) \mathcal{G}^{(n-i)}(p, E) + \cdots .
\]
It is worth mentioning that, whereas \(\tilde{c}^{(n)}(q)\) has to begin from \(n = 1\), \(\mathcal{G}^{(n)}\) actually starts from \(n = 0\).

1. \(q\)-scaling of \(\tilde{\Gamma}\) and our selecting recipe

Before moving into the detailed calculation, it is instructive to outline the leading scaling behavior with respect to the hard momentum \(q\) for a general four-point diagram. Recall that in [4], we proved that all the diagrams in Coulomb-Schrödinger theory exhibit a universal
FIG. 8: Leading $q$-scaling behavior of numerous higher-order diagrams for the momentum-space Green function $\tilde{\Gamma}$. The thick lines are meant to carry the hard momentum of order $q$, in order to contribute to the specified leading region. The cross, heavy dot, solid square refer to the $p^4$ kinetic term, Darwin term and contact interaction, respectively.

leading scaling behavior $\propto q^{-4}$. Nevertheless, with the relativistic correction included in the NREFT, it seems that we have opened Pandora’s box — in the sense that arbitrary scaling $\propto q^n$ with $n$ an integer greater than $-4$ might arise. In Fig. 8, we have shown some characteristic tree and one-loop diagrams, whose leading asymptotic behaviors may range from $q^{-4}$ to $q^0$.

Were $\tilde{c}(q)$ legally containing $q^{-2}$ (Fig. 8b, d, i), $|q|^{-1}$ (Fig. 8f, h) and $q^0$ (Fig. 8g), the corresponding Wilson coefficient in coordinate space would be proportional to $1/r^2$, $1/r$ and $\delta^{(3)}(r)$, respectively. These near-the-origin singular behaviors are much more severe than the logarithmic singularity exhibited by the actual KG wave function, and are not even square integrable.

It may seem natural to speculate whether there is any objective criterion to determine which types of diagrams we should keep or not? We first note that, when pinching the external electron and nucleus lines from the top of the diagrams in Fig. 8, one then obtains the three-point Green function $G$ defined in (68), some of which have been portrayed in Fig. 7. It is easy to see that those $q^n (n > -4)$ leading scaling of the four-point diagrams would correspond to the $\Lambda^{n+3}$ UV power divergences in $G$.

In section III about quantum mechanic perturbation theory, we have seen the emergence of various UV power divergences in (18), which are nevertheless absent in the original KG wave function (10). There we argued that since the hard momentum cutoff $\Lambda$ violates the spacetime symmetry, it may lead to some artificial and unphysical effects. Dimensional regularization turns out to be much more advantageous, not merely convenient. It is well-known that DR can only access the logarithmic rather than power divergences. Therefore we have agreed in section VI to exclusively use DR as the UV regulator. Since the Wilson coefficient in OPE is intimately connected with the renormalization of local composite operator, it may sound reasonable that in our case, we can throw away all the contributions to the Green function $\tilde{\Gamma}$ with a scaling behavior $\propto |q|^n$ with $n > -3$.

Another reason is from practical consideration. As indicated in (10), the worst near-the-origin behavior of the KG wave function for $S$-wave hydrogen-like atom can only be logarithmic. To be capable for accounting for this universal short-range behavior, we should
establish some organizing principles, which justify abandoning all the contributions to \( \tilde{\Gamma} \) that has a scaling behavior \( \propto |q|^n \) with \( n \geq -2 \).

Therefore, let us state explicitly our recipe of analyzing the asymptotic behavior of momentum-space four-point function \( \tilde{\Gamma} \). In the \( mZ\alpha \ll q \sim m \) limit, to ascertain the Wilson coefficients affiliated with the local composite operator \([\varphi N]_R\), we only need single out those contributions to the Green function \( \tilde{\Gamma} \) with the \( 1/|q|^3 \) and \( 1/q^4 \) scaling:

\[
\tilde{\Gamma}(q; \ p, E) \xrightarrow{q \to m} \frac{1}{q^4} \quad \text{and} \quad \frac{1}{|q|^3},
\]

with the accompanying factors can only involve \( m \) and \( Z\alpha \), instead of \( p \) and \( \kappa \). As will be made clear later, this specific selecting recipe would lead to the so-called “double-layer form of the OPE”.

A quantification for (81) is in order. By retaining only the \( q^{-4} \) or \( |q|^{-3} \) terms, we do not mean that we should neglect those diagrams with the leading scaling behavior \( \propto |q|^n \) (\( n \geq -2 \) as a whole, such as Fig. 8b, d)). Upon the expansion in \( 1/|q| \), as long as these diagrams would contain the \( q^{-4} \) or \( |q|^{-3} \) terms in the subleading order, there would be no reason to reject such contributions in our analysis.

It is not straightforward to present an all-order proof for the OPE identity in momentum space (79). Nevertheless, we will be satisfied if the OPE pattern can be nontrivially uncovered in the first few orders in \( Z\alpha \), in the spirit of (80). Concretely speaking, in the remaining subsections, we will investigate the asymptotic behavior of the diagrams in Fig. 8, verify the OPE indeed holds through order \( Z^2\alpha^2 \), and also determine the corresponding Wilson coefficients.

In Fig. 9, we present a closer examination on the asymptotic scaling of those most relevant diagrams in Fig. 8, by explicitly exhibiting their factorized structures in the large-\( q \) limit.
2. Determining $\tilde{c}^{(1)}(q)$

Let us first consider Fig. 9a, the simplest tree diagram at order $Z\alpha$, which was already analyzed in [4]:

$$\tilde{\Gamma}_{9a}^{(1)}(q; p, E) = Z e^2 \int \frac{dq}{2\pi} D_e(q) D_{00}(p-q) D_N(k+p-q)$$

$$= -Ze^2(2m) \frac{i}{q^2 - 2mE(q-p)^2}$$

$$\xrightarrow{q \to m} \frac{8\pi m Z\alpha}{q^4} + \cdots . \quad (82)$$

In the last line, we have used the fact $|q| \gg |p|, E$. In light of (81), we need only keep the leading term in the expansion.

As indicated by the in Fig. 9a, the leading $q^{-4}$ scaling comes from the subdiagram where the hard momentum of order $|q|$ flows into the upper-left electron line, passes through the Coulomb ladder, then exits from the upper-right nucleus line. For clarity, we have represented the lines carrying hard momentum by the thick lines. The factorization of Fig. 9a into the product of the hard factor and soft factor becomes manifest. In accordance with (80), one readily reads off the Wilson coefficient from (82):

$$\tilde{c}^{(1)}(q) = \frac{8\pi m Z\alpha}{q^4}, \quad (83)$$

where $G^{(0)} = 1$ has been used.

Next let us turn to Fig. 9b, the tree-level diagram with one insertion of the $p^4$ kinetic term onto the inflowing electron propagator:

$$\tilde{\Gamma}_{9b}^{(1)}(q; p, E) = Ze^2 \int \frac{dq}{2\pi} D_e(q) \frac{i q^4}{8m^3} D_{00}(p-q) D_N(k+p-q)$$

$$= \frac{Ze^2}{2m} \frac{q^4}{(q^2 + \kappa^2)(q-p)^2}$$

$$\xrightarrow{q \to m} \frac{2\pi Z\alpha}{mq^2} + \cdots . \quad (84)$$

According to (81), the leading $1/q^2$ term should be dismissed. The next term in the series expansion of (84) is of the order $1/q^4$, but is accompanied with the prefactor involving $p$ or $\kappa$. Therefore, these power-suppressed terms correspond to some operators other than $\varphi N$, which can be safely neglected for our purpose.

By the similar analysis, adding more $p^4$ kinematic corrections to the inflowing electron line, or including higher-order relativistic corrections, would not induce new contribution to the Wilson coefficient $\tilde{c}^{(1)}(q)$ as determined in (83).

3. Determining $\tilde{c}^{(2)}(q)$

At order $Z^2\alpha^2$, one encounters the one-loop box diagrams as exemplified in Fig. 8c) – h). The last three diagrams, e.g. Fig. 8f) – h), which contain the relativistic correction of $v^4/c^4$,
exhibit the leading scaling behaviors of $|q|^0$ or $|q|^{-1}$. One can verify that the sub-leading contributions to these diagrams neither bear the desired $|q|^{-3}$ or $|q|^{-4}$ scaling, nor generate new corrections to (83) for $\tilde{c}^{(1)}(q)$. We thereby neglect these diagrams, and instead focus on Fig. 8c) $- e)$, or equivalently, Fig. 9c) $- e)$.

It is possible to analytically work out these one-loop box integrals, but the resulting expressions are rather cumbersome. Fortunately, to deduce the asymptotic results in large $q$ limit, it is more effective to take a shortcut, by first expanding the integrand prior to conducting the loop integration. The loop momentum $l$ can be classified into two categories: hard ($l \sim q$) and soft ($l \sim p, \kappa \ll q$). This expansion-in-region technique leads to readily manageable integrals, which result in compact expressions.

Let us first examine the box diagram without relativistic insertion, Fig. 9c). We can work out the integral as follows:

$$\bar{\Gamma}^{(2)}_{9c}(q; p, E) = Z^2 e^4 \mu^2 e \int \frac{dq^0}{2\pi} D_e(q) D_N(k + p - q)$$

$$\times \int \frac{d^D q}{(2\pi)^D} D_e(l) D_{00}(p - l) D_N(k + p - l) D_{00}(l - q)$$

$$= \frac{4m^2 Z^2 e^4}{q^2 + \kappa^2 \mu^2 e} \int \frac{dD-1 l}{(2\pi)^{D-1}} \frac{1}{(1 - q^2)(1 - p^2)(l^2 + \kappa^2)}$$

$$\approx \frac{4m^2 Z^2 e^4}{q^2} \left[ \frac{1}{q^2 \mu^2 e} \int \frac{dD-1 l}{S (2\pi)^{D-1}} \frac{1}{(1 - p^2)(l^2 + \kappa^2)} + \mu^2 \int \frac{dD-1 l}{H (2\pi)^{D-1}} \frac{1}{(1 - q^2)^2 l^1} \right]$$

$$= \tilde{c}^{(1)}(q) G^{(1)}_{ta}(p, E) + O(1/|q|^5),$$

where $\tilde{c}^{(1)}(q)$ is given in (83), the one-loop Green function $G^{(1)}_{ta}$ is given in (69). In the middle of derivation, we have explicitly decomposed the loop integral into the soft and hard parts, which are labelled by the subscripts $S$ and $H$. The contribution from hard loop region yields a subleading contribution of order $1/|q|^5$, thus has been neglected. As can be visualized from the factorization structure in Fig. 9c), this box diagram does not bring any new correction to $C(q)$ at order $Z\alpha$ [4].

We then turn to Fig. 9d), with a $p^4$ kinetic term inserted onto the inflowing electron line outside the box. We have argued after (84) that the analogous tree diagram in Fig. 9d) needs not be considered. Here let us examine this more complicated example, again employing the expansion-by-region technique:

$$\bar{\Gamma}^{(2)}_{9d}(q; p, E) = Z^2 e^4 \mu^2 e \int \frac{dq^0}{2\pi} D_e(q) \frac{iq^4}{8m^4} D_N(k + p - q)$$

$$\times \int \frac{d^D l}{(2\pi)^D} D_e(l) D_{00}(l - q) D_N(k + p - l) D_{00}(p - l)$$

$$= \frac{Z^2 e^4 q^4}{(q^2 + \kappa^2 \mu^2 e} \int \frac{dD-1 l}{(2\pi)^{D-1}} \frac{1}{(1 - q^2)(1 - p^2)(l^2 + \kappa^2)}$$

$$\approx Z^2 e^4 \left[ \frac{1}{q^2 \mu^2 e} \int \frac{dD-1 l}{S (2\pi)^{D-1}} \frac{1}{(1 - p^2)(l^2 + \kappa^2)} + \mu^2 \int \frac{dD-1 l}{H (2\pi)^{D-1}} \frac{1}{(1 - q^2)^2 l^1} \right]$$

$$= \frac{2\pi Z\alpha}{m q^2} G^{(1)}_{ta}(p, E) + \frac{2\pi^2 Z^2 \alpha^2 e}{|q|^3} G^{(0)}(p, E),$$

where we have kept both contributions from the soft and hard regions, with the factorization form illustrated in Fig. 9d). It is observed that the short-distance coefficient $\propto Z\alpha/m q^2$,
which stems from the soft region, is identical to (84) in Fig. 9b. There we have argued such term should be dismissed. On the contrary, the contribution from the hard region appears to bear a factorized structure. Nevertheless, the would-be Wilson coefficient \( Z^2 \alpha^2/|q|^3 \) has a prefactor \( D - 4 \), thus cannot contribute to the desired \( Z^2 \alpha^2 \ln r \) term upon Fourier transform\(^\text{13}\). Therefore, we can discard the contribution of Fig. 9d as a whole.

Our final stake is then in Fig. 9e), which hopefully serves the key to account for the \( Z^2 \alpha^2 \ln r \) term in the KG wave function near the origin. In fact, this expectation is well-grounded. As indicated in (73), the \( \mathcal{O}(Z^2 \alpha^2) \) vertex diagram with a \( p^4 \) insertion in the lower loop, Fig. 7e), is indeed logarithmically UV divergent. Actually, we have already remarked that Fig. 8e) has a leading \( 1/|q|^3 \) scaling behavior when all the internal lines inside the loop become hard. When sewing up two upper external lines in Fig. 8e), one can recover the logarithmic UV divergence in Fig. 7e). As implied in Fig. 9e), we can separate the contributions from the soft and hard loop regions:

\[
\tilde{\Gamma}^{(2)}_{9e}(q; p, E) = Z^2 e^4 \mu^{2e} \int \frac{d^d q}{2\pi} D_0(q) D_N(k + p - q)
\]

\[
\times \int \left( \frac{d^D l}{(2\pi)^D} \right) D(l) D_{00}(l - p) D_N(k + p - l) D_{00}(l - q) \frac{d^4 l}{8m^3}
\]

\[
= \frac{Z^2 e^4 \mu^{2e}}{q^2 + \kappa^2} \int \left( \frac{d^{D-1} l}{(2\pi)^{D-1}} \right) \frac{1}{(l - p)^2(l - q)^2(l^2 + \kappa^2)^2}
\]

\[
\approx \frac{Z^2 e^4}{q^2} \left[ \frac{1}{q^2 \mu^{2e}} \int \left( \frac{d^{D-1} l}{(2\pi)^{D-1}} \right) \frac{1}{(l - p)^2(l^2 + \kappa^2)^2} \right] + \mu^{2e} \int \frac{d^{D-1} l}{(2\pi)^{D-1}} \frac{1}{(l - q)^2 l^2} \right]
\]

\[
= c^{(1)}(q) \mathcal{G}^{(1)}_{7b}(p, E) + c^{(2)}(q) \mathcal{G}^{(0)}(p, E),
\]

where the first term encapsulates the soft loop contribution, and the second term encodes the hard loop contribution. Note the former is entirely absorbed in the correction to the three-point Green function, \( \mathcal{G}^{(1)}_{7b} \) as given in (70). In contrast, the latter brings a new correction for the Wilson coefficient at order\(-Z^2 \alpha^2\):

\[
c^{(2)}(q) = -16\pi^2 \mu^{2e} Z^2 \alpha^2 \frac{2^{5-2D} \pi^2 - \frac{D}{2}}{\Gamma \left( \frac{D-2}{2} \right) \sin \frac{\pi(D-1)}{2}} \frac{1}{|q|^{7-D}} D \rightarrow 1 \frac{2^{5} Z^2 \alpha^2}{|q|^3}.
\]

This \( |q|^{D-7} \) scaling is just responsible for the logarithmic UV divergence observed in (73), which represents the two-loop vertex correction of Fig. 7e).

As was stated earlier, at order \( Z^2 \alpha^2 \), there is no need to consider diagrams implementing \( v^4/c^4 \) or higher-order relativistic corrections, \( e.g. \) Fig. 8f) – h), with two or more insertions of \( p^4 \) term or a Darwin term. This omission follows from the hypothesized working principle of double-layer OPE in (81), because these diagrams do not admit the intended \( 1/|q|^3 \) or \( 1/|q|^4 \) scaling behaviors.

4. Final expression of the OPE in momentum space

Following the iterative pattern (80), we have determined the Wilson coefficients up to the order \( Z^2 \alpha^2 \). Plugging (83) and (88) into (77), we find that the OPE in momentum space

\(^{13}\) This is compatible with the fact that the two-loop vertex diagram with a \( p^4 \) insertion in the upper loop, Fig. 7d), does not contain a logarithmic UV divergence, as analysed in (71).
explicitly reads

\[ \bar{\varphi}(\mathbf{q})N(0) = \left( \frac{8\pi m Z\alpha}{|\mathbf{q}|^4} + \frac{2\pi^2 Z^2 \alpha^2}{|\mathbf{q}|^3} + \cdots \right) [\varphi N]_R(0) + \cdots. \]  

(89)

The ellipsis inside the parenthesis indicates those uncalculated higher-order Wilson coefficients such as \( Z^3 \alpha^3 \ln|\mathbf{q}|/|\mathbf{q}|^4 \) and \( Z^4 \alpha^4 \ln|\mathbf{q}|/|\mathbf{q}|^3 \). Upon Fourier transform, these may correspond to the coordinate-space Wilson coefficients of the form \( Z^3 \alpha^3 r \ln r \) and \( Z^4 \alpha^4 \ln^2 r \), which are truly present in the near-the-origin behavior of the KG wave function in (11).

### B. OPE in coordinate space

We now supplement Section VII A with the corresponding OPE relation in the coordinate space, (76). This will provide the key element to explain the weakly divergent near-the-origin behavior of the \( S \)-wave KG wave function. Analogous to (32a), for convenience here we introduce the following four-point Green function in the coordinate space:

\[ \Gamma(\mathbf{r}; \mathbf{p}, E) \equiv \int d^4 y d^4 z e^{-i \mathbf{p} \cdot \mathbf{y}} e^{-i \mathbf{k} \cdot \mathbf{z}} \langle 0 | T \{ \varphi(\mathbf{r}) N(0) \varphi(\mathbf{y}) N(\mathbf{z}) \} | 0 \rangle_{\text{amp}}, \]

which can be reached from (78) by

\[ \Gamma(\mathbf{r}; \mathbf{p}, E) = \int \frac{d^3 \mathbf{q}}{(2\pi)^3} e^{i \mathbf{q} \cdot \mathbf{r}} \tilde{\Gamma}(\mathbf{q}; \mathbf{p}, E). \]

(91)

As before, the Green function is amputated with the lower lines carrying soft momenta \( p \) and \( k \).

Our goal is to establish that, in the small \( r \) (\( |r| \to \frac{1}{m} \)) limit, \( \Gamma \) exhibits the following factorized form order by order in \( Z\alpha \):

\[ \Gamma(\mathbf{r}; \mathbf{p}, E) \xrightarrow{|r| \to \frac{1}{m}} C(r) \mathcal{G}(\mathbf{p}, E) + \cdots, \]

(92)

where \( \mathcal{G} \) was first introduced in (68), signifying the amputated three-point Green function inserted with the composite operator \([\varphi N]_R\).

Following (76), we can decompose the Wilson coefficient in power series of \( Z\alpha \):

\[ C(r) = c^{(0)}(r) + c^{(1)}(r) + c^{(2)}(r) + \cdots. \]

(93)

The lowest-order Wilson coefficient can be readily deduced in free theory. Analogous to what is portrayed in Fig. 3, the Green function \( \Gamma \) possesses a disconnected topology, yields the very simple answer:

\[ \Gamma^{(0)}(\mathbf{r}; \mathbf{p}, E) = e^{i \mathbf{p} \cdot \mathbf{r}} = 1 + \mathcal{O}(pr). \]

(94)

Since \( \mathcal{G}^{(0)} = 1 \), it is straightforward to read off \( c^{(0)} = 1 \).

Eq. (92) can be recast into a iterative form, which is amenable to perturbation theory,

\[ \Gamma^{(n)}(\mathbf{r}; \mathbf{p}, E) \xrightarrow{|r| \to \frac{1}{m}} \sum_{i=0}^{n} c^{(i)}(r) \mathcal{G}^{(n-i)}(\mathbf{p}, E) \]

(95)
\[ r_0 k = \left( r_0 - r_0 \right) + \cdots \]

\[ r_0 = \left( r_0 - r_0 \right) + \cdots \]

\[ (r_0 + \text{UVCT}) + \left( r_0 - r_0 \right) + \left( r_0 - r_0 - \text{UVCT} \right) + \cdots \]

FIG. 10: Manifestation of the OPE structure in the coordinate-space Green function through order \( Z^2 \alpha^2 \). The Wilson coefficient \( \sim Z^2 \alpha^2 \ln r \) is stemming from the parenthesis in the last line.

In contrast with its counterpart in the momentum space (80), here both \( c^{(i)}(q) \) and \( G^{(i)} \) start from \( i = 0 \).

In (81), we put forward the hypothesized principle of “double-layer form of the OPE” in the momentum space version of OPE. Translated into the coordinate space, this principle indicates that we only need sort out those contributions to \( \Gamma \) with the following scalings:

\[
\Gamma(r; p, E) \xrightarrow{r \to 1} \ln^n r \quad \text{and} \quad r \ln^n r. \quad (n \geq 0)
\]

(96)

It is understood that the accompanying factors can only be composed of \( m \) and \( Z\alpha \).

In the rest of this subsection, we will compute the higher-order Wilson coefficients through \( \mathcal{O}(Z^2 \alpha^2) \).

1. Determining \( c^{(1)}(r) \)

Directly Fourier transforming \( \tilde{c}_1(q) \) in (83) to deduce \( c^{(1)}(r) \) in the the coordinate space turns out to be plagued with IR divergence associated with \( q \to 0 \), which is clearly unacceptable. As illustrated in Fig. 10a), the correct way to proceed is by expanding (95) through order \( Z\alpha \):

\[
\Gamma_{10a}^{(1)} (r; p, E) \xrightarrow{r \to 1} c^{(0)}(r)G_{7a}^{(0)}(p, E) + c^{(1)}(r)G_{7a}^{(0)}(p, E), \quad (97)
\]

where the one-loop correction to the three-point Green function, \( G_{7a} \), is given in (69). Therefore, \( c^{(1)}(r) \) can be obtained from the \( \Gamma^{(1)}(r) \) by subtracting off the local Green function \( G_{7a}^{(1)} \):

\[
c^{(1)}(r) = \lim_{r \to \frac{1}{m}} \Gamma_{10a}^{(1)}(r; p, E) - G_{7a}^{(1)}(p, E)
\]

\[
= \int \frac{d^3q}{(2\pi)^3} \tilde{\Gamma}_{10a}^{(1)}(q; p, E) (e^{iq\cdot r} - 1) \bigg|_{q \text{ hard}} \approx \int \frac{d^3q}{(2\pi)^3} \tilde{c}^{(1)}(q) (e^{iq\cdot r} - 1)
\]

\[
= 8\pi m Z\alpha \int \frac{d^3q}{(2\pi)^3} \frac{e^{iq\cdot r} - 1}{q^2} = -mZ\alpha r. \quad (98)
\]
We have used the Fourier representation (91) and
\[ G^{(n)}(\mathbf{p}, E) = \int \frac{d^3q}{(2\pi)^3} \tilde{\Gamma}^{(n)}(\mathbf{q}; \mathbf{p}, E), \quad \text{for } n \geq 1. \] (99)

Furthermore, in the second line of (98), we have used (82) and (83) to keep only the leading asymptotic form of \( \tilde{\Gamma}^{(1)} \) in the \( \mathbf{q} \rightarrow m \) limit, since Wilson coefficient stems from the hard loop momentum region. Notice the subtraction term automatically guarantees \( c^{(1)}(r) \) to be IR finite, which is a consequence of \( c^{(0)}(r) = 1 \). This analytic expression of \( c^{(1)}(r) \) was first obtained within the Coulomb-Schrödinger EFT [4].

2. Deciphering \( c^{(2)}(r) \)

From (94) and (98), we have inferred that \( c^{(0)} \) and \( c^{(1)} \) to be 1 and \(-mZ\alpha r\), respectively. We proceed to deduce the expression of \( c^{(2)}(r) \). In accordance with (95), higher-order Wilson coefficients account for the difference between the full four-point Green function and the three-point Green functions multiplied by lower-order Wilson coefficients. In particular, the difference solely comes from the hard loop region. In the following, we will explicitly analyze the asymptotic behaviors of \( \Gamma^{(2)}(\mathbf{r}; \mathbf{p}, E) \) in the limit \( r \rightarrow \frac{1}{m} \), by identifying the hard loop momentum and expanding the integrands accordingly. This analysis would lead to the OPE structure as exhibited by (95), where the hard part renders the Wilson coefficients, and the soft part is absorbed by the three-point Green function \( G^{(1)}(\mathbf{p}, E) \).

Using (85), (91) and (69), we find the difference between \( \Gamma^{(2)}_{10b} \) and \( G^{(2)}_{\gamma_\alpha} \) to be

\[
\Gamma^{(2)}_{10b}(\mathbf{r}; \mathbf{p}, E) - c^{(0)}(r)G^{(2)}_{\gamma_\alpha}(\mathbf{p}, E) = Z^2 e^4 \mu^2 \int \frac{d^Dq}{2\pi} D_e(q)D_N(k+p-q)(e^{i\mathbf{q}\cdot\mathbf{r}} - 1) \\
\times \int \frac{d^{D-1}l}{(2\pi)^D} D_e(l)D_{00}(p-l)D_N(k+p-l)D_{00}(l-q) \\
= 4m^2 Z^2 e^4 \mu^2 \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \frac{1}{q^2 + \kappa^2} \int \frac{d^{D-1}l}{(2\pi)^{D-1}} \frac{1}{(1 - q^2)(1 - p^2)(l^2 + \kappa^2)}.
\] (100)

Eq. (100) in the limit \( r \rightarrow \frac{1}{m} \) is dominated by the situation when \( \mathbf{q} \) becomes hard. More specifically, one should consider two situations: the top loop is hard and bottom loop is soft, as well as both loop momenta are hard,

\[
\Gamma^{(2)}_{10b}(\mathbf{r}; \mathbf{p}, E) - G^{(2)}_{\gamma_\alpha}(\mathbf{p}, E) \approx \left[ 2mZe^2 \mu^\epsilon \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \frac{e^{i\mathbf{q}\cdot\mathbf{r}} - 1}{\mathbf{q}^4} \right] G^{(1)}_{\gamma_\alpha}(\mathbf{p}, E) \bigg|_{\mathbf{q} \text{ hard, } \mathbf{1} \text{ soft}} \\
+ \left( 4m^2 Z^2 e^4 \mu^2 \int \frac{d^{D-1}q}{(2\pi)^{D-1}} \int \frac{d^{D-1}l}{(2\pi)^{D-1}} \frac{e^{i\mathbf{q}\cdot\mathbf{r}} - 1}{(1 - q^2)(l^2 + \kappa^2)} \right) \bigg|_{\mathbf{q} \text{ hard, } \mathbf{l} \text{ soft}} \\
= c^{(1)}(r) G^{(1)}_{\gamma_\alpha}(\mathbf{p}, E) + \mathcal{O}(r^2),
\] (101)

which only involves the known Wilson coefficient at order \( Z\alpha \), as is represented in the parenthesis of the second line in Fig. 10b). The both-loop-hard regions yield a contribution subleading in \( r \), thus can be neglected according to our assumption (96). Note (101) is compatible with (95), with the conclusion \( c^{(2)}(r) = 0 \) from this diagram.
Finally let us turn to Fig. 10c), the most interesting order-$Z^2\alpha^2$ diagram where a $p^4$ relativistic correction inserted on the lower loop. With the aid of (87), (91) and (73), we find the difference between $\Gamma_{10c}^{(2)}$ and $\mathcal{G}_{7e}^{(2)}$ to be

$$\Gamma_{10c}^{(2)}(\mathbf{r}; \mathbf{p}, E) - c^{(0)}(r) \left( \mathcal{G}_{7e}^{(2)}(\mathbf{p}, E) + UVCT \right)$$

$$= Z^2 e^4 \mu^2 \left[ \int \frac{d^D q}{(2\pi)^D} D_e(q) D_N(k + p - q) \int \frac{dP}{(2\pi)^D} (e^{i\mathbf{q} \cdot \mathbf{x}} - 1) \right]$$

$$\times D_e(l) D_{00}(p - l) D_N(k + p - l) D_{00}(l - q) \frac{l^4}{8m^3} - \delta Z_S \mathcal{G}^{(0)}$$

$$= Z^2 e^4 \mu^2 \left[ \int \frac{d^D q}{(2\pi)^D-1} \frac{e^{i\mathbf{q} \cdot \mathbf{x}} - 1}{q^2 + \kappa^2} \int \frac{d^D-1 l}{(2\pi)^D-1} \frac{l^4}{(1 - \mathbf{p})^2(1 - \mathbf{q})^2 l^2 + \kappa^2 l^2} \right] - \delta Z_S,$$

where $\delta Z_S$ is the UV counterterm to renormalize the composite operator $\varphi N$. Its value in the MS prescription is given in (74).

Similar to (100), in the limit $r \to \frac{1}{\alpha}$ (102) is again dominated by the situation when $\mathbf{q}$ becomes hard. Specifically, we consider two situations: the top loop is hard and bottom loop is soft, as well as both loop momenta are hard,

$$\Gamma_{10c}^{(2)}(\mathbf{r}; \mathbf{p}, E) - \mathcal{G}_{7eR}^{(2)}(\mathbf{p}, E) \approx \left( 2mZ e^2 \mu^4 \int \frac{d^D-1 q}{(2\pi)^D-1} \frac{e^{i\mathbf{q} \cdot \mathbf{x}} - 1}{q^4} \right) \left. \mathcal{G}_{7b}^{(1)}(\mathbf{p}; E) \right|_{\mathbf{q}, \text{hard}, \text{1 soft}}$$

$$+ \left[ \mu^2 e^4 \int \frac{d^D-1 q}{(2\pi)^D-1} \int \frac{d^D-1 l}{(2\pi)^D-1} \frac{e^{i\mathbf{q} \cdot \mathbf{x}} - 1}{q^2 l^2 (1 - \mathbf{q})^2 - \delta Z_S} \right]_{\mathbf{q}, \text{1 hard}}$$

$$= c^{(1)}(r) \mathcal{G}_{7b}^{(1)}(\mathbf{p}, E) + c^{(2)}(r) \mathcal{G}^{(0)}(\mathbf{p}, E),$$

where the desired Wilson coefficient at order $Z^2\alpha^2$ reads

$$c^{(2)}(\mu, r) \bigg|_{\text{MS}} = \mu^2 e^4 \int \frac{d^D-1 q}{(2\pi)^D-1} \frac{e^{i\mathbf{q} \cdot \mathbf{x}} - 1}{q^2 l^2 (1 - \mathbf{q})^2} - \delta Z_S$$

$$= -16\pi^2 \mu^2 e^4 Z^2\alpha^2 \frac{\Gamma(D-2)}{2} \sin \frac{\pi(D-1)}{2} \int \frac{d^D-1 q}{(2\pi)^D-1} \frac{e^{i\mathbf{q} \cdot \mathbf{r}} - 1}{|\mathbf{q}|^{D-D} + Z^2\alpha^2}$$

$$= -Z^2\alpha^2 \left( \ln \mu r + \frac{\gamma_E - 1 + \ln 4\pi}{2} \right),$$

where the $D$-dimensional expression of $\tilde{c}^{(2)}(q)$ in (88) is used. It is reassuring that $c^{(2)}(r)$ is indeed UV and IR finite, and does contain the $-Z^2\alpha^2 \ln r$ term. The nonlogarithm constant is scheme-dependent, which is largely irrelevant for our purpose. Note we have used the simplest MS scheme to renormalize the local operator $\varphi N$. As indicated in Fig. 10c), this coefficient receive the contribution solely from the regions where both loop momenta become hard. Notice (103) is compatible with (95), with the new piece of Wilson coefficient given in (104).
3. Final expression of the OPE in coordinate space, KG wave function near the origin

It is the time to sew up everything and represent the OPE relation in coordinate space, (76) through the order $Z^2\alpha^2$ explicitly as

$$\varphi(r) N(0) \xrightarrow{r \to \frac{1}{m}} 1 - mZ\alpha r - Z^2\alpha^2 \left( \ln \mu r + \frac{\gamma_E - 1 + \ln 4\pi}{2} \right) + O(Z^3\alpha^3) \right\} [\varphi N]_R(0; \mu) + \cdots.$$  \hfill (105)

This relation holds at operator level, which is the main result of this work. We stress that both the $O(Z^2\alpha^2)$ Wilson coefficient and the renormalized composite operator $[\varphi N]_R$ become scale-dependent. If we continue to analyze the asymptotic behaviors of even higher-order Green functions, it is conceivable that the Wilson coefficients of the form $Z^3\alpha^3 r \ln r$ and $Z^4\alpha^4 \ln^2 r$ should be correctly extracted. However, the explicit verification is beyond the scope of the current work, though we fully trust in the correctness of our approach based on NREFT and OPE.

In (21), we tentatively formulate the KG wave function as the nonlocal vacuum-to-atom matrix element of the sQED and HNET fields at equal time. There we fail to use OPE to account for the correct near-the-origin behavior of the $S$-wave KG wave functions of hydrogen-like atom. Encouragingly, the structure of (105) suggests us to identify the KG wave function of the hydrogen-like atom as the following equal-time matrix element formed by the product of the NRsQED and HNET fields:

$$\Psi_{nlm}(r) \equiv \langle 0 | \varphi(x) N(0) | nlm \rangle.$$ \hfill (106)

When focusing on $S$-wave states, the universal near-the-origin behavior of KG wave functions in (10) and (11), at least to order $Z^2\alpha^2$, are entirely characterized by the Wilson coefficients associated with the leading $S$-wave composite operator $[\varphi N]_R$.

Now we come to the crux of this work. It is usually thought that the Klein-Gordon equation in an external Coulomb field is a genuinely relativistic wave equation, where one is able to probe arbitrary short-distance ($r \to 0$) profile of wave function. Nevertheless, one should note that KG equation in (1) is specifically defined in the rest frame of the nucleus, whose Lorentz covariance is far from obvious. Actually, our OPE-based analysis reveals that KG wave function should be viewed as a secretly nonrelativistic wave function, as represented by (106) rather than by (21). As a consequence, it does not make sense to talk about the near-the-origin behavior of the KG wave function when $r \ll \frac{1}{m}$! On the contrary, when probing the short-range behavior of the wave function, we are only justified to let the minimum value of $r$ approach $\frac{1}{m}$. The reason is simple, since the Compton length of the electron comprises the shortest length scale where nonrelativistic EFT can still make sense.

C. Renormalization Group Equation for Wilson coefficient

In the $r \to \frac{1}{m}$ limit, if the renormalization scale $\mu$ is taken around the inverse Bohr radius, the logarithm $\ln \mu r \approx \ln Z\alpha$ in (105) is potentially large, which might harm the perturbative convergence of fixed-order prediction. The convenient and effective method to resum large logarithms to all orders is via the celebrated renormalization group equation (RGE). Our starting observation is that the atomic Bethe-Salpeter wave function in (106) is obviously independent of the artificial scale $\mu$. When $r$ becomes small, one may invoke the OPE relation (76), and demand that the combination $C(r; \mu)[\varphi N]_R(0; \mu)$ is independent...
of $\mu$. The scale dependence of the composite $S$-wave operator is controlled by the standard RGE:

$$\frac{d[\varphi N]_R}{d\mu} = \gamma_S [\varphi N]_R,$$

(107)

with $\gamma_S = Z^2 \alpha^2 + O(Z^4 \alpha^4)$ being the anomalous dimension for the composite operator $\varphi N$, as given in (75). The solution is

$$[\varphi N]_R(\mu) = [\varphi N]_R(\mu_0) \left( \frac{\mu}{\mu_0} \right)^{Z^2 \alpha^2}.$$

(108)

One readily writes down the following RGE for the $S$-wave Wilson coefficient $C(r)$:

$$\mu \frac{dC(r)}{d\mu} + C(r) \gamma_S = 0.$$

(109)

Note $\mu$ and $r$ always come hand in hand inside the logarithm, dimensional consideration leads to $(\mu \frac{d}{d\mu} - r \frac{d}{dr}) C(\mu r) = 0$. Define $r \equiv r_0 g$, where $r_0$ is a typical length scale of order Bohr radius. We can transform the RGE (109) into the evolution equation that governs the scaling behavior of $C$ near small $r$:

$$\kappa \frac{dC(r_0 \kappa)}{d\kappa} + C(r_0 \kappa) \gamma_S = 0.$$

(110)

The solution of (110) becomes

$$C(r) = C(r_0) \kappa^{-Z^2 \alpha^2} = C(r_0) \left( \frac{r}{r_0} \right)^{-Z^2 \alpha^2},$$

(111)

which has resummed the leading logarithms of $\kappa$ to all orders. As expected, this anomalous scaling behavior is identical to the near-the-origin behavior of the $S$-wave KG wave function encoded in (10). Moreover, if setting $\mu = 1/r_0 = 2/na_0$ for the $nS$ hydrogen-like atom, we have $C(r_0; \mu) = 1$. If we further identify the matrix element $\langle 0 | [\varphi N]_R(0; \mu = 1/r_0) | n00 \rangle$ as the nonrelativistic Coulomb-Schrodinger wave function at the origin, we may even fully reproduce (10):

$$R_{n0}^{KG}(r) \approx C(r; \mu = 1/r_0) \sqrt{4\pi} \langle 0 | [\varphi N]_R(0; \mu = 1/r_0) | n00 \rangle \approx \left( \frac{2r}{na_0} \right)^{-Z^2 \alpha^2} R_{n0}^{Sch}(0).$$

(112)

VIII. SUMMARY

The Klein-Gordon equation in an external Coulomb field marks an important milestone in the early development of relativistic quantum mechanics. It has been known almost a century ago that the $S$-wave KG wave function for hydrogen-like atoms acquires logarithmic divergence near the origin. It is often thought that this divergence is of only academic interest, since this logarithmic singularity becomes relevant only for extremely small $r$. Moreover, the physical origin underlying this divergent near-the-origin behavior is rather poorly understood.
As a sequel of our previous work [4], we employ some modern field-theoretical tools, e.g. EFT and OPE, to solve this long-standing puzzle. We explicitly demonstrate that, by incorporating the relativistic kinetic correction into the nonrelativistic Coulomb-Schrödinger EFT, we are able to provide a novel perspective to look into this universal logarithmic near-the-origin divergence, i.e., which can be interpreted as the Wilson coefficients arising from the product of the nonrelativistic electron field and HQET-like nucleus field. With the aid of renormalization group equation, we can satisfactorily reproduce the anomalous scaling behavior observed in the KG wave function at small $r$.

The folklore says that the Klein-Gordon equation in an external Coulomb field is a relativistic wave equation, where one is allowed to probe the arbitrarily small distance ($r \to 0$) of the wave function. Curiously, our OPE analysis based on relativistic scalar QED utterly fails to reproduce the correct short-distance logarithmic divergence of the KG wave function! This is a clear sign that the KG equation may secretly describe the nonrelativistic rather than relativistic bound-state wave function. In our opinion, it does not make any sense to talk about the near-the-origin behavior of the KG wave function when $r \ll \frac{1}{m}$, contrary to the folklore. Furthermore, when probing the short-range behavior of the wave function, the minimum value of $r$ is frozen at $\frac{1}{m}$, since the Compton length of the electron constitutes the smallest length scale where nonrelativistic EFT can still apply.

In a follow-up work, using the same methodology, we will demonstrate that [3], it is also feasible to employ OPE within nonrelativistic EFT to account for the universal weakly divergent near-the-origin behavior of the Dirac wave functions for the $nS_{1/2}$ hydrogen atom.

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