Schrödinger, Klein-Gordon and Dirac equations, atomi c wave functions and Operator Product Expansion

Yu Jia (贾宇)

IHEP, Beijing



In collaboration with Yingsheng Huang and Rui Yu Based on **arXiv: 1809.09023, 1812.11957, 1901.04971** 

Kavli IPMU, University of





## **Outline of the talk**

- **Review of universal electron-nucleus coalescence behavior of atomic wave function**
- > Brief introduction to EFT and OPE modern tools of QFT
- Non-relativistic Coulomb-Schrödinger EFT Standard QFT for atomic physics
- Rigorous proof of an OPE relation to all orders in perturbation theory
- > 90-year puzzle about wave function at the origin for KG and Dirac hydrogen
- > Insight from Schrödinger perturbation theory in QM UV div. and Renormalization
- > OPE and RGE in nonrelativistic EFT implementing relativistic corrections
- Summary

# 梦回唐朝一穿越回物理学的黄金年代 一英雄辈出的 1920 年代

- Golden age of physics, many young heroes in deve ping quantum mechanics
- Non-relativistic wave mechanics, relativistic wave echanics were invented in almost same time – fina y give way to more fundamental framework: Quan m Field Theory

QFT = Special Relativity + Quantum Mechanics





 Application of single-particle wave mechanics (Scl<sup>Figure: Erwin Schrödinger (left), Paul</sup> ödinger, Klein-Gordon and Dirac equations) to hy drogen spectroscopy plays a vital role in shaping the modern physics Triumph of QM in early days Schrödinger equation with Coulomb potentia I: the standard theory for atomic physics and quantum chemistry

 $H_{\text{Coul}}\Psi = E\Psi$ 

$$H_{\text{Coul}} = -\sum_{i=1}^{N} \frac{\boldsymbol{\nabla}_{i}^{2}}{2m} - \sum_{i=1}^{N} \frac{Z\alpha}{r_{i}} + \sum_{j>i=1}^{N} \frac{\alpha}{r_{ij}}$$

Standard Model of atomic physics









Orientation: electron-nucleus coaelesence be havior [KG equation with a Coulomb potentia ] (Schrödinger, 1926, unpublished note)

$$\begin{bmatrix} \left(E + \frac{Ze^2}{4\pi r}\right)^2 + \hbar^2 c^2 \nabla^2 - m^2 c^4 \end{bmatrix} \Psi(\mathbf{r}) = 0. \qquad \Psi_{nlm}(\mathbf{r}) = R_{nl}(r) Y_{lm}(\hat{\mathbf{r}}),$$

$$E_{nl} = mc^2 \left\{ 1 + \frac{Z^2 \alpha^2}{\left(n - l - \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - Z^2 \alpha^2}\right)^2} \right\}^{-\frac{1}{2}} \qquad Wrong fine structure,$$

$$= mc^2 \left\{ 1 - \frac{Z^2 \alpha^2}{2n^2} - \frac{Z^4 \alpha^4}{2n^4} \left(\frac{n}{l + \frac{1}{2}} - \frac{3}{4}\right) + \cdots \right\}, \qquad \rho = (2/n) \text{ (r /a0), a0 is Bohr radius}$$

For S-wave hydrogen atom, KG wave function at short-distance scales as

$$R_{n0}^{\rm KG}(r) \approx R_{n0}^{\rm Sch}(0) \left(\frac{\rho}{2}\right)^{\sqrt{\frac{1}{4} - Z^2 \alpha^2} - \frac{1}{2}} \approx R_{n0}^{\rm Sch}(0) \left(\frac{\rho}{2}\right)^{-Z^2 \alpha^2} = R_{n0}^{\rm Sch}(0) \left(1 - Z^2 \alpha^2 \ln r + \cdots\right),$$

Long-standing puzzle: why KG wave function at the origin diverges? And so weakly (logarithmically)?

Orientation: electron-nucleus coaelesence be havior: Dirac equation with a Coulomb potent ial (Darwin and Gordon 1928)

$$\begin{aligned} (-i\hbar c\alpha \cdot \nabla + \beta m c^{2} - \frac{Z\alpha c}{r})\Psi &= E\Psi \\ E_{nj} &= mc^{2} \left\{ 1 + \frac{Z^{2}\alpha^{2}}{\left(n - j - \frac{1}{2} + \sqrt{\left(j + \frac{1}{2}\right)^{2} - Z^{2}\alpha^{2}}\right)^{2}} \right\}^{-\frac{1}{2}} \\ &= mc^{2} \left\{ 1 - \frac{Z^{2}\alpha^{2}}{2n^{2}} - \frac{Z^{4}\alpha^{4}}{2n^{4}} \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4}\right) + \cdots \right\}, \end{aligned}$$

For  $nS_{1/2}$  hydrogen taom, Dirac wave function at short-distance scales as

$$f_{n0}^{\text{Dirac}}(r) \approx R_{n0}^{\text{Sch}}(0) \left(\frac{\rho}{2}\right)^{\sqrt{1-Z^2\alpha^2}-1} \approx R_{n0}^{\text{Sch}}(0) \left(\frac{\rho}{2}\right)^{-Z^2\alpha^2 over2} = R_{n0}^{\text{Sch}}(0) \left(1 - \frac{Z^2\alpha^2}{2}\ln r + \cdots\right),$$

Long-standing puzzle since 1928:

why Dirac wave function at the origin diverges? and so weakly (logarithmically)? What is the physics behind?

Universal behavior of wave function near the origin in Schrödinger hydrogen (S-wave)

Expand the radial wave function near the origin ( $r << a_0$ )

$$R_{n0}^{Schr}(r) \propto \begin{cases} 1 - \alpha mrZ + \frac{1}{2}\alpha^2 m^2 r^2 Z^2 + \cdots & (n = 1) \\ 1 - \alpha mrZ + \frac{3}{8}\alpha^2 m^2 r^2 Z^2 + \cdots & (n = 2) \\ 1 - \alpha mrZ + \frac{19}{54}\alpha^2 m^2 r^2 Z^2 + \cdots & (n = 3) \\ 1 - \alpha mrZ + \frac{11}{32}\alpha^2 m^2 r^2 Z^2 + \cdots & (n = 4) \end{cases}$$

Non-universal



Universal behavior of wave function near the origin in Klein-Gordon hydrogen (S-wave)

Non-universal

$$R_{n0}^{KG}(r) \propto \begin{cases} 1 - \alpha mrZ + \frac{1}{2}\alpha^{2}m^{2}r^{2}Z^{2} - Z^{2}\alpha^{2}\log(Z\alpha mr) + Z^{3}\alpha^{3}mr\log(Z\alpha mr) + \cdots & (n = 1) \\ 1 - \alpha mrZ + \frac{3}{8}\alpha^{2}m^{2}r^{2}Z^{2} - Z^{2}\alpha^{2}\log(Z\alpha mr) + Z^{3}\alpha^{3}mr\log(Z\alpha mr) + \cdots & (n = 2) \\ 1 - \alpha mrZ + \frac{19}{54}\alpha^{2}m^{2}r^{2}Z^{2} - Z^{2}\alpha^{2}\log(Z\alpha mr) + Z^{3}\alpha^{3}mr\log(Z\alpha mr) + \cdots & (n = 3) \\ 1 - \alpha mrZ + \frac{11}{32}\alpha^{2}m^{2}r^{2}Z^{2} - Z^{2}\alpha^{2}\log(Z\alpha mr) + Z^{3}\alpha^{3}mr\log(Z\alpha mr) + \cdots & (n = 4) \end{cases}$$





Universal behavior of wave function near the origin in Dirac hydrogen (The  $nS_{1/2}$  state)

Non-universal

$$R_{n0}^{Dirac}(r) \propto \begin{cases} 1 - \alpha mrZ + \frac{1}{5}\alpha^2 m^2 r^2 Z^2 - \frac{Z^2 \alpha^2 \log(\alpha mrZ)}{2} + \frac{Z^3 \alpha^3 mr \log(\alpha mrZ)}{2} + \cdots & (n = 1) \\ 1 - \alpha mrZ + \frac{3}{8}\alpha^2 m^2 r^2 Z^2 - \frac{Z^2 \alpha^2 \log(\alpha mrZ)}{2} + \frac{Z^3 \alpha^3 mr \log(\alpha mrZ)}{2} + \cdots & (n = 2) \\ 1 - \alpha mrZ + \frac{19}{54} d^2 m^2 r^2 Z^2 - \frac{Z^2 \alpha^2 \log(\alpha mrZ)}{2} + \frac{Z^3 \alpha^3 mr \log(\alpha mrZ)}{2} + \cdots & (n = 3) \\ 1 - \alpha mrZ + \frac{11}{32} \alpha^2 m^2 r^2 Z^2 - \frac{Z^2 \alpha^2 \log(\alpha mrZ)}{2} + \frac{Z^3 \alpha^3 mr \log(\alpha mrZ)}{2} + \cdots & (n = 4) \end{cases}$$



#### Explicit forms of Schrodinger, KG and Dirac ra dial wave functions for S-wave hydrogen



Why various w.f. exhibit universal short-distance behavior for a given orbital angular momentum l? What is the physics behind the divergence, and the universality?

# Thanks to X. D. Ji for very inspiring disc usions that lead to this study

One afternoon in fall of 2011 at Maryland, *Xiangdong* informed me that the wave function near the origin in Dirac equation logarithmically diverges... And likely to be related with renormalization effect...



It takes me for seven years to finally figure out how to solve this puzzle

#### Peter Lepage's pedagogical 1997 Summer School lecture: How to renormalize Schrödinger equation

-- Lots of inspiration from Lepage's 1997 Summer School lecture

HOW TO RENORMALIZE THE SCHRÖDINGER EQUATION Lectures at the VIII Jorge André Swieca Summer School (Brazil, Feb. 1997)

> G. P. LEPAGE Newman Laboratory of Nuclear Studies, Cornell University Ithaca, NY 14853 E-mail: gpl@mail.ns.cornell.edu

These lectures illustrate the key ideas of modern renormalization theory and effective field theories in the context of simple nonrelativistic quantum mechanics and the Schrödinger equation. They also discuss problems in QED, QCD and nuclear physics for which rigorous potential models can be derived using renormalization techniques. They end with an analysis of nucleon-nucleon scattering based effective theory.

#### 1 Renormalization Revisited

These lectures are about effective field theories — low-energy approximations to arbitrary high-energy physics — and therefore they are about modern renormalization theory.<sup>1</sup>

Despite the complexity of most textbook accounts, renormalization is based upon a very familiar and simple idea: a probe of wavelength  $\lambda$  is insensitive to details of structure at distances much smaller than  $\lambda$ . This means that we can mimic the *real* short-distance structure of the target and probe by *simple* short-distance structure. For example, a complicated current source  $\mathbf{J}(\mathbf{r},t)$ of size d that generates radiation with wavelengths  $\lambda \gg d$  is accurately mimicked by a sum of point-like multipole currents (E1, M1, etc). In thinking about the long-wavelength radiation it is generally much easier to treat the source as a sum of multipoles than to deal with the true current directly. This is particularly true since usually only one or two multipoles are needed for sufficient accuracy. The multipole expansion is a simple example of a renormalization analysis.

In a quantum field theory, QED for example, the quantum fluctuations probe arbitrarily short distances. This is evident when one computes radiative corrections in perturbation theory. Ultraviolet divergences, coming from loop momenta  $k \to \infty$  (or wavelengths  $\lambda \to 0$ ), result in infinite contributions radiative corrections seem infinitely sensitive to short distance behavior. Even ignoring the infinities, this poses a serious conceptual problem since we don't really know what happens as  $k \to \infty$ . For example, there might be new supersymmetric interactions, or superstring properties might become important, or electrons and muons might have internal structure. The situation is saved



#### 2.6 Operators and the Operator Product Expansion

So far we have used our effective theory to compute binding energies and phase shifts. We now examine quantities that depend in detail on the wavefunctions. Consider, for example, the matrix element  $\langle n | \mathbf{p}^4 | n \rangle$ , which might be important if we wished to include relativistic corrections in our potential model. In Table 3 I list values of this matrix element for several S-states both for the true theory, and for our corrected theory (with a=1). The values disagree by more than a factor of two, even for very low-energy states, despite the fact that the two theories agree on the corresponding binding energies to several digits.

The problem is that the operator in the effective theory that corresponds to  $\mathbf{p}^4$  in the true theory is not  $\mathbf{p}^4$ . As is true of the hamiltonian, there are local corrections to  $\mathbf{p}^4$  in the effective theory. Thus, for any S state, we expect

$$\langle \mathbf{p}^4 \rangle_{\rm true} = Z \langle \mathbf{p}^4 \rangle_{\rm eff} + \frac{\gamma}{a} \langle \delta_a^3(\mathbf{r}) \rangle_{\rm eff} + \eta \, a \, \langle \nabla^2 \delta_a^3(\mathbf{r}) \rangle_{\rm eff} + \mathcal{O}(a^3) \tag{15}$$

arXiv:nucl-th/9706029v1 12 Jun 1997

### Lots of efforts by two of my students in t he past three years



レエスス 学士学位论文 论文题目: 薛定谔方程的有效理论和重整化研究

作	者	姓	名	黄应生
专			业	物理学
指	导	教	师	贾宇,李世渊

2016 Y.-S. Huang Bachelor thesis





### Part 1: Schrödinger wave function

## EFT and OPE

Coalescence behavior of atomic wave function

- electron-electron coalescence (Kato, 1957; Hofmann, et al., 2013)
- electron-nucleus coalescence (Löwdin, 1954; Kato, 1957; Hofmann, et al., 2013)
- two-electron and nucleus coalescence (Fournais, et al., 2005)
- molecule coalescence (Kolos, 1960; Pack, 1966, ...)
- more...
- a general N-fermion coalescence analysis (Hoffmann-Ostenhof, et al., 1992)

# **Electron-electron coalescence**

Hamiltonian:

$$H_{\text{Coul}} = -\sum_{i=1}^{N} \frac{\boldsymbol{\nabla}_{i}^{2}}{2m} - \sum_{i=1}^{N} \frac{Z\alpha}{r_{i}} + \sum_{j>i=1}^{N} \frac{\alpha}{r_{ij}}$$

• Kato's Cusp condition (S-wave) (Kato, 1957):  $\frac{\partial \Psi}{\partial r_{12}}\Big|_{r_{12}=0} = \gamma \Psi(r_{12}=0)$ 

Leads to:

$$\psi = 1 - \sum_{l=1}^{N} \sum_{i=1}^{n} mZ\alpha r_{il} + \sum_{i>j=1}^{n} \frac{m\alpha r_{ij}}{2} + \mathcal{O}(r^2)$$

# Beyond Kato's cusp conditi on

**Arbitrary orbital angular momentum** (Löwdin, 1954):

$$R_{nl}(x) = \frac{x^{l}}{l!} \frac{d^{l} R_{nl}}{dx^{l}}(0) \left[1 - \frac{1}{l+1} \frac{x}{a_{0}} + \mathcal{O}(x/a_{0})^{2}\right].$$

Three-particle coalescence: (Fournais et al. 2005):

$$F = -\sum_{l=1}^{N} \sum_{i=1}^{n} mZ\alpha r_{il} + \sum_{i>j=1}^{n} \frac{m\alpha r_{ij}}{2} + \frac{2-\pi}{6\pi} \sum_{l=1}^{N} \sum_{i>j=1}^{n} m^2 Z\alpha^2 \mathbf{r}_{il} \cdot \mathbf{r}_{jl} \log \left(m^2 (r_{il}^2 + r_{jl}^2)\right)$$
$$\psi = e^F \phi$$
Two electrons approach the nucleus for an arbitrary atom

How to understand this coalescence be havior of wave function from QFT?

In the field-theoretical context, the Bethe-Salpeter wave function can be viewed as the vacuum-to-atom matrix elements of two nonlocal field operator!

$$\Psi_{nlm}(\mathbf{x}) = \langle 0 | \psi(\mathbf{x}) N(0) | nlm \rangle,$$

This suggests that the coalescence behavior can be inferred from OPE: Wilson coefficients are universal!

OPE is operator relation, does not depend on external states, thus applies to an arbitrary atom!

# Principle of EFT

- Identifying relevant degree of freedom
- Symmetry as building guidance
- Power counting
- Long-range effects is insensitive about short range physics;
- Short-range effects encoded by Wilson coefficients
- Nonrenormalizable theory is renormalizable

QCD and EFT summer school, 有效理话的基本idea: Shanghai, 2018/informal note insensitive to UV ·低能(长轻)物理不依赖高能(延轻)物理 到细节; · 象位于成党起的能标的物理自由度, 红彩的迎 underlying physics: uncertainty principle 用-些参教视划。 Local operators EFT és essential ingredients: 1. Scale separation: 了角定了统的UV能标和IR能标 2. Identify active (effective) degrees of freedom: 确定理论常保留的重要的、有效的自由度

3. Impose a UV cutoff; A 所有有到理话都有一个运用范围 (不再追求 Thony of Everyth 4. Speafy the symmetries of EFT. 利用对新性的差有效建治所有可能的相互作用 5. Dimensional Analysis : Power counting. 如何组织计算,使之满足小参数展开的指定,群度. Don't fool yourself!

EFT 成为了物理学研究的基本范式 (pavadigm). EFT 提供了对renormalization 最全面的理解. "No theory can work at all scales, even sering theory! Standard Model must break down long before hitting Planck scale. · 即使我的知道Junderlying theory,但EFT (可能增一时) 提供了更加有起的描述手段。

创计: QED是所有量子的子和condensed matter 物理 5 & underlying theory. 但基于库伯劳的萨定谔方程可guantum chemisery and atomic physics I 30 f 2d! 载于电子-声子相互作用的分体验治子建解 Superosuductivity 更有起! QCD是描述强相互作用的基本理论 例子2: 但 Chiral perturbation theory 建体了建备 low-enery hadronic physics 更为有社场 建治框架 [以元,N很多有社自由度]

Nonrenormalizable cheories are renormalizable/prediceive. 在GFT的框架下, renormalization 莺味着, 职使 我们不理解 UV (1071)的物理,我们依然 可以做出model-independent 强意, 因为the effects of short-distance physics can be localizable in terms of Wilson coefficients in EFTs. Wilm 了教习从 {从安验值fit. ChpT/SMEFT (J从UV建始指手 HQGT/NRQGD/ (已年) /NRQの/SCET 24

H. Greorgi (1989): In this picture, the presence of infinities in quantum field theory is neither a disaster, nor an asset. It is simply a reminder of practical limitation - we do not know what happens at distances much smaller than those we can look at directly. 送话: All QFTs are EFTs!

Related reasoning: 正前意原子能级, 不需知道度子自 专克肢子结构, 只需到适度子的-些bulk properties: (4) mass, chavge, spin-z, 4p=2.793 Mg (反常游短), ... EFI example I. [最好的学习是通过examples] 静电势的多极距展开(multipole expansion) (even not a QFT) localized elecenic charge distribution, with densing Per) R test charge scale hierrohy: iszsize & d d << R

$$V = \int d^{1}\vec{r} \frac{g(\vec{r})}{|\vec{a}|} = \int d^{2}r \frac{g(\vec{r})}{\sqrt{R^{2}+2Rr\cos\theta+r^{2}}}$$
  

$$= \vec{r} \vec{r} \vec{k} \vec{k} \vec{k} \cdot \vec{k}$$
  

$$M = \int |\vec{r}| \wedge d \ll R, \quad f = \int a_{r}^{2}r \cos\theta + r^{2} \vec{k} \cdot \vec{k}$$
  

$$M \approx \int_{N=0}^{\infty} \frac{1}{R^{n+1}} \int d^{2}r \quad \gamma^{n} \quad g(\vec{r}) \quad Rn(\cos\theta)$$
  

$$= \frac{q}{R} + \frac{p}{R^{2}} + \frac{q}{R^{2}} + \cdots$$
  

$$= \frac{q}{R} + \frac{p}{R^{2}} + \frac{q}{R^{2}} + \cdots$$
  

$$= \frac{q}{R} + \frac{q}{R^{2}} + \frac{q}{R^{2}} + \cdots$$
  

$$= \int a_{r}^{2}r + \frac{q}{R^{2}} + \frac{q}{R^{2}} + \cdots$$
  

$$= \int a_{r}^{2}r + \frac{q}{R^{2}} + \frac{q}{R^{2}} + \cdots$$
  

$$= \int a_{r}^{2}r + \frac{q}{R^{2}} + \frac{q}{R^{2}} + \cdots$$
  

$$= \int a_{r}^{2}r + \frac{q}{R^{2}} + \frac{q}{R^{2}} + \cdots$$
  

$$= \int a_{r}^{2}r + \frac{q}{R^{2}} + \frac{q}{R^{2}} + \cdots$$
  

$$= \int a_{r}^{2}r + \frac{q}{R^{2}} + \frac{q}{R^{2}} + \cdots$$
  

$$= \int a_{r}^{2}r + \frac{q}{R^{2}} + \frac{q}{R^{2}} + \cdots$$
  

$$= \int a_{r}^{2}r + \frac{q}{R^{2}} + \frac{q}{R^{2}} + \cdots$$

EFT example 2: 気原レー量レカ学致言 Underlying cheory: Dirac equation (in Coulomb potential) (it gt + g) y= - itc V. J y + mc 2 g y birec 星子化的束缚态能级为: Parwin, Grordon (1928) mc +  $(n-j-\frac{1}{2}+\sqrt{(j+\frac{1}{2})^2-\alpha^2})^2$ 

 $\approx mc^{2} \left[ 1 - \frac{\alpha}{2n^{2}} - \frac{\alpha}{2n^{4}} \left( \frac{n}{2^{2} + \frac{1}{2}} - \frac{3}{4} \right) + \cdots \right]$ fine - structure Bohr A6 JA cutoff: 12me Schrödinger eguation: valid at p<me 有到建语: -> taken as perenvbactor, recover  $i = H_{sch} = H_{sch} + H_{sch}$ 0 =  $\frac{\overline{P}}{2me} - \frac{\sqrt{2}}{7}$  Contomb hamiltonia 4sch = 4space & 4spin OH = Provent - et B. ExP- et V. E 8 mec2 - 4 mec2 B. ExP- et V. E sph-orbital vel. con.  $\frac{\overline{P}^{4}}{3m_{b}^{2}c^{2}} - \frac{\chi}{2\gamma^{3}m_{b}^{2}}\overline{L}\cdot\overline{S} + \frac{\overline{T}\chi}{2m_{b}^{2}c^{2}}S^{3}(\overline{r})$ 5H =

EFT Example 3: Weak interaceon: 4-fermon interaceon. contract a point P1 = 1-85  $\mathcal{M}(\mu \neq e v_{\mu} \overline{v_{e}}) = \left(\frac{g_{2}}{\sqrt{2}}\right) \left[\overline{u}(R_{\nu_{\mu}}) \mathcal{T}_{L}^{\mu} u(P_{\mu})\right] \left[\overline{u}(R_{e}) \mathcal{T}_{\mu} P_{L} v(P_{ve})\right]$ 

 $\times (P_{\mu} - R_{\nu_{\mu}})^2 - M_{w}^2$ 

13 3 Pr = mr << Mw, W boson is highly virtual, can not propagate far,  $(P_{\mu}-R_{\nu_{\mu}})^2-M_{w}^2 \approx -\frac{1}{M_{w}^2}$ 

M(n+eV, Ve) = - 4GF [u(Pvp) rh PL U(Pp)][u(Pe) X, PLV(Pve)] Fermi constant GF = 92 12 = 2M2. Effective weak Hamiltonian: Hw = - Lw = 4GI [V, r^P. W][= V, P. Ve]

EFT example 4: Light-by-Light scattering YY - YY えみ船とるEr PRIZ EY LL Me underlying theory 我们可以从Q的作用是中轻掉电子场。 (Enler, Heisenberg, Kockel 1936) LQED (Y, Y, An) -> LEH (An)

$$\begin{split} &\stackrel{\text{(a)}}{=} \stackrel{\text{(b)}}{=} \stackrel{\text{(b)}}{=} \stackrel{\text{(c)}}{=} \stackrel{\text{(c)}}{=}$$

EFT example 5: GR as low-energy EFT of Quantum Gravity  
PRAPHIG JWLAL Einstein - Hilbert action HE 4,  
SEH = 
$$\int d^{\phi}x \sqrt{-g} \left(-\frac{2}{K^2R}\right)$$
. (Ponoghue 1935)  
SEH =  $\int d^{\phi}x \sqrt{-g} \left(-\frac{2}{K^2R}\right)$ .  $K = \sqrt{32 \times G_{TV}}$   
 $S = 5_{EH} + S_{Marker.}$   
 $S = 0 \Rightarrow R_{\mu\nu} - \frac{1}{2}R_{\mu\nu}^2 = 8 \times G_{NV} T_{\mu\nu}$   
 $R_{\mu\nu} - \frac{1}{2}R_{\mu\nu}^2 = 8 \times G_{\mu\nu}^2 = 8$ 

Allowed by general coordinate transformation symmetry. Similarly, write down the most general interaction terms allowed by symmetry for matter sector One hop consevens to Newton's law: A't graviton m 6 post-Newtonian Quantum  $V(r) = -\frac{G_{W}m_{1}m_{L}}{\gamma} \left[ 1 + \frac{3}{6} \frac{G_{W}(m_{1}+m_{2})}{\gamma c^{2}} + \frac{41}{10\pi} \frac{G_{W}h}{\gamma^{2}c^{2}} \right].$ non-analytic + CI GAN S'CT)

35

EFT example 6: (量钢分析) Rayleigh scattering: Why the sky is blue ? 可见充和大气中的原子预制, 涉及多flength scales. 1) 可见光 波长入~5000A >> 原子的size~ 儿个A 国的原子可以作为总科子处设; 2) 可见无子能量《原子的激发能, 国地只零孝属 充于和中地原子的了单性友好. 3) 原子九手是静止的, 可以用非相话性的场锋乘描述 Leff = 4 + (~ 2+ + 2M) 4 - & Fro Fru + Lint 原子不带电荷, は妻子教, 著通导教

36
Uci) Gauge invariance demands 
$$F_{AV} = (\vec{e}, \vec{B})$$
  
Lint =  $a_0^3 \psi^{\dagger} \psi (c_1 \vec{E}' + c_2 \vec{B}'^2) + \cdots$   
Nore  $[\psi_{AP}] = \frac{3}{2}, \ C \downarrow ] = \psi$   $a_0 : \ c_1 : 2e \ of \ atom.$   
 $(\vec{e} \sim -\vec{A}, \ \vec{B} \sim \nabla \times \vec{A})$   
 $\mathcal{S}_{Rayleigh} \propto a_0^6 \vec{E}_Y^4$ 

Simple dimensional analysis reproduces the famous Er<sup>4</sup> dependence of the Rayleigh scattering X section, thus explains why sky is the! Shine severgeh of EFT

## EFT for atoms (analogue of heavy-quark bound states)

 Effective Lagrangian: NRQED (Caswell & Lepage, 1986)+HNET (similar to HQET, E. Eichten, Hill & H. Georgi, 1990)

$$\begin{split} & \underbrace{\mathcal{L}}_{\text{VUCUUV}} \mathcal{L} = \mathcal{L}_{\text{Max}} + \mathcal{L}_{\text{NRQED}} + \mathcal{L}_{\text{HNET}} + \delta \mathcal{L}_{\text{contact}} \\ & \mathcal{L}_{\text{Max}} = -\frac{1}{4} d_{\gamma} F_{\mu\nu} F^{\mu\nu} + \cdots, \end{split}$$

$$\mathcal{L}_{\text{NRQED}} = \psi^{\dagger} \left\{ i D_{0} + \frac{D^{2}}{2m} + \frac{D^{4}}{8m^{3}} + c_{D} e \frac{[\nabla \cdot \mathbf{E}]}{8m^{2}} + c_{F} e \frac{\sigma \cdot \mathbf{B}}{2m} + i c_{S} e \frac{(\mathbf{D} \times \mathbf{E} - \mathbf{E} \times \mathbf{D}) \cdot \sigma}{8m^{2}} + \cdots \right\} \psi$$

$$\mathcal{L}_{\text{HNET}} = N^{\dagger} i D_{0} N + \cdots, \\ \delta \mathcal{L}_{\text{contact}} = \frac{c_{4}}{m^{2}} \psi^{\dagger} \psi N^{\dagger} N + \cdots$$
where
$$D^{\mu} = \partial^{\mu} + i e A^{\mu}.$$

### EFT for Schrödinger atoms

• **Coulomb-Schrödinger EFT** for atoms:

$$\mathcal{L}_{\text{Coul-Schr}} = \psi^{\dagger} \left\{ i D_0 + \frac{\nabla^2}{2m} \right\} \psi + N^{\dagger} i D_0 N + \frac{1}{2} \left( \nabla A^0 \right)^2.$$

Field theoretical realization of Schrodinger eq.

$$H_{\text{Coul}} = -\sum_{i=1}^{N} \frac{\nabla_i^2}{2m} - \sum_{i=1}^{N} \frac{Z\alpha}{r_i} + \sum_{j>i=1}^{N} \frac{\alpha}{r_{ij}} \quad H_{\text{Coul}}\Psi = E\Psi$$

Coulomb gauge (only retain instantaneous Coulomb poten tial)

- □ No dynamic photons (set **A**=0): so will not see Lamb shift
- No relativistic corrections included

### Feynman rules in NREFT

The nucleus propagator is defined as

$$D_N(k) \equiv \frac{i}{k^0 + i\epsilon}.$$

Nucleus HNET propagator

NRQED electron propagator  $D_e(k)\equiv rac{1}{k^0-k}$ 

$$(k) \equiv \frac{i}{k^0 - \frac{\mathbf{k}^2}{2m} + i\epsilon}.$$

The photon propagator in Coulomb gauge is defined as

$$D_{00}(k) \equiv \frac{i}{\mathbf{k}^2}, \qquad \text{Instantaneous Coulomb photon}$$
$$D_{ij}(k) \equiv \frac{i}{k^2 + i\epsilon} (\delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2}), \qquad \underbrace{i \neq 0, j \neq 0}_{\substack{i \neq 0, j \neq 0}} \qquad \text{Not needed}$$
in this work!

Only ladder diagrams survives in NREFT calculation

 All crossed ladder diagrams are zero due to the co ntour integral.





Vanish with single pole!

Operator Product Expansion (Wil son, 1969; Zimmermann, 1971)

OPE assumes the following form:

$$T\phi(x)\phi(0) \sim \sum_{\mathcal{O}} C_{\mathcal{O}}(x^{\mu})[\mathcal{O}(0)]_R$$



Applied in various areas of particle physics (light-cone expansion, Minkowski spacetime, and Euclidean OPE)

Can be used to defined the renormalized composite lo cal operators.

# Proof of OPE using path integrals (s ee Weinberg, QFT Vol. 2)

$$\langle T\{A_1(x_1), A_2(x_2), \dots B_1(y_1), B_2(y_2) \dots \} \rangle_0$$
  
=  $\int \left[ \prod_{\ell, z} d\phi_{\ell}(z) \right] a_1(x_1) a_2(x_2) \cdots b_1(y_1) b_2(y_2) \cdots \exp(iI[\phi]),$ 







$$I = \int_{z \in B(R)} d^4 z \, \mathscr{L}(z) + \int_{z \notin B(R)} d^4 z \, \mathscr{L}(z) \, .$$

Locality of action is crucial for existence of OPE

## Proof of OPE (QFT, Weinberg)

$$\langle T\{A_{1}(x_{1}), A_{2}(x_{2}), \dots B_{1}(y_{1}), B_{2}(y_{2}) \dots \} \rangle_{0}$$

$$= \int \left[ \prod_{z \notin B(R), \ell} d\phi_{\ell}(z) \right] b_{1}(y_{1}) b_{2}(y_{2}) \dots \exp\left(i \int_{z \notin B(R)} \mathscr{L}(z)\right)$$

$$\times \int \left[ \prod_{z \in B(R), \ell} d\phi_{\ell}(z) \right] a_{1}(x_{1}) a_{2}(x_{2}) \dots \exp\left(i \int_{z \in B(R)} \mathscr{L}(z)\right)$$

$$\langle T\{A_{1}(x_{1}), A_{2}(x_{2}), \dots B_{1}(y_{1}), B_{2}(y_{2}) \dots \} \rangle_{0} \rightarrow \int \left[ \prod_{\ell, z} d\phi_{\ell}(z) \right]$$

$$\times b_{1}(y_{1}) b_{2}(y_{2}) \dots \exp\left(i \int \mathscr{L}(z)\right)$$

$$\times \sum_{O} U_{O}^{A_{1},A_{2},\dots} (x_{1} - x, x_{2} - x, \dots) o(x)$$

$$= \sum_{O} U_{O}^{A_{1},A_{2},\dots} (x_{1} - x, x_{2} - x, \dots) \langle T\{O(x), B_{1}(y_{1}), B_{2}(y_{2}) \dots \} \rangle_{0}$$

# OPE: an important tool in high ener gy physics

**DIS:**   $T[J^{\mu}(x)J^{\nu}(0)] = \sum C_{i}(x^{2},\mu^{2}) x_{\mu_{1}} \dots x_{\mu_{n}} \mathcal{O}_{i}^{\mu\nu\mu_{1}\dots\mu_{n}}(\mu),$ Twist expansion  $O_{q,V}^{\mu_{1}\dots\mu_{n}} = \frac{1}{2} \left(\frac{i}{2}\right)^{n-1} \mathcal{S}\left\{\bar{q} \gamma^{\mu_{1}} \stackrel{\leftrightarrow}{D}^{\mu_{2}} \dots \stackrel{\leftrightarrow}{D}^{\mu_{n}} q\right\},$ 

$$O_{q,A}^{\mu_1\cdots\mu_n} = \frac{1}{2} \left(\frac{i}{2}\right)^{n-1} \mathcal{S}\left\{\bar{q} \gamma^{\mu_1} \stackrel{\leftrightarrow}{D}^{\mu_2} \cdots \stackrel{\leftrightarrow}{D}^{\mu_n} \gamma_5 q\right\},\,$$

QCD (SVZ) Sum rule

Shifman et al., 1978

OPE + dispersion relation: useful phenomenological model to predict some hadronic nonperturbative quantities.

The essential idea of OPE is factorization: momentum fl ow of Green function: separate hard and soft (lucidly ex plained by John Collins, text on Renormalization)

Hard momentum



Soft momentum

Factorization property of Green function





Consider a  $\phi^4$  theory

$$\mathscr{L} = \partial \phi^2 / 2 - m^2 \phi^2 / 2 - g \phi^4 / 24 + \text{counterterms.}$$

we may have OPE

A toy example! 
$$T\phi(x)\phi(0) \sim \sum_{0} C_{0}(x^{\mu})[\mathcal{O}(0)]$$

To derive the exact Wilson coefficient  $C_{\mathcal{O}}$ , we consider Green function  $\langle 0 | T \phi(x) \phi(0) \tilde{\phi}(p_1) \tilde{\phi}(p_2) | 0 \rangle$ .

At leading order we have disconnected diagrams



which gives

$$\frac{i}{p_1^2 - m^2} \frac{i}{p_2^2 - m^2} \left[ \exp(-ip_1 \cdot x) + \exp(-ip_2 \cdot x) \right].$$
47

Expanding it at x = 0

$$\frac{i}{p_1^2 - m^2} \frac{i}{p_2^2 - m^2} [2 - i(p_1 + p_2) \cdot x - (p_1 \cdot x^2 + p_2 \cdot x^2)/2 + \cdots].$$

which is equivalent to

$$T\phi(x)\phi(0) = \phi^2(0) + \frac{1}{2}x^{\mu}\partial_{\mu}\phi^2 + \frac{1}{2}x^{\mu}x^{\nu}\phi\partial_{\mu}\partial_{\nu}\phi + \cdots$$

However this is only the leading contribution. For next-to-leading contribution, we have the following 1-loop diagram



where the diagram l.h.s is

$$\frac{i^2}{(p_1^2 - m^2)(p_2^2 - m^2)} ig \int \frac{d^4q}{(2\pi)^4} \frac{e^{-iq \cdot x}}{(q^2 - m^2)[(q - p_1 - p_2)^2 - m^2]}.$$

The Wilson coefficient we actually care for is

$$T\phi(x)\phi(0)\sim C_{\phi^2}(x)[\phi^2],$$
  
$$C_{\phi^2}=1+(g/16\pi^2)c_1(x^2).$$
 which is extracted via 1-loop diagram (c)

$$\frac{1}{(p_1^2 - m^2)(p_2^2 - m^2)} \frac{-\mathrm{i}g}{(2\pi)^4} \times \left\{ \int d^4q \frac{\mathrm{e}^{\mathrm{i}q \cdot x} - 1}{(q^2 - m^2)[(q - p_1 - p_2)^2 - m^2]} - \mathrm{UV} \, \mathrm{divergence} \right\}.$$

The contribution of order 1 from large q is

$$c_1(x) = \frac{1}{2\pi^2} \left\{ \frac{i}{(2\pi\mu)^{d-4}} \int d^d q \frac{(e^{iq \cdot x} - 1)}{(q^2)^2} + \frac{2}{d-4} \right\}.$$

while the rest are of order |x|.

Using Schwinger parametrization

$$1/(q^2)^2 = \int_0^\infty dz z e^{-z(-q^2)}$$

one could determine  $c_1$  to be

$$c_1(x) = \frac{1}{2} [\gamma + \ln(-\pi^2 \mu^2 x^2)].$$

## Previous application of OPE to atomic p hysics

#### Braaten & Platter, PRL (2008)



PRL 100, 205301 (2008)

PHYSICAL REVIEW LETTERS

week ending 23 MAY 2008

#### Exact Relations for a Strongly Interacting Fermi Gas from the Operator Product Expansion



Eric Braaten\* and Lucas Platter\*

Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA (Received 12 March 2008; published 21 May 2008)

The momentum distribution in a Fermi gas with two spin states and a large scattering length has a tail that falls off like  $1/k^4$  at large momentum k, as pointed out by Tan. He used novel methods to derive exact relations between the coefficient of the tail in the momentum distribution and various other properties of the system. We present simple derivations of these relations using the operator product expansion for quantum fields. We identify the coefficient as the integral over space of the expectation value of a local operator that measures the density of pairs.

DOI: 10.1103/PhysRevLett.100.205301

PACS numbers: 67.85.Lm, 03.75.Nt, 31.15.-p, 34.50.-s

### **OPE for electron Coulomb gas**

#### Hofmann, Barth and Zwerger in 2013

PHYSICAL REVIEW B 87, 235125 (2013)

#### Short-distance properties of Coulomb systems

Johannes Hofmann,<sup>1,\*</sup> Marcus Barth,<sup>2,†</sup> and Wilhelm Zwerger<sup>2</sup> <sup>1</sup>Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Centre for Mathematical Sciences, Cambridge CB3 0WA, United Kingdom <sup>2</sup>Technische Universität München, Physik Department, James-Franck-Strasse, 85748 Garching, Germany (Received 15 April 2013; revised manuscript received 27 May 2013; published 20 June 2013)

We use the operator product expansion to derive exact results for the momentum distribution and the static structure factor at high momentum for a jellium model of electrons in both two and three dimensions. It is shown that independent of the precise state of the Coulomb system and for arbitrary temperatures, the asymptotic behavior is a power law in the momentum, whose strength is determined by the contact value of the pair distribution function g(0). The power-law tails are quantum effects which vanish in the classical limit  $\hbar \rightarrow 0$ . A leading-order virial expansion shows that the classical and the high-temperature limit do not agree.

DOI: 10.1103/PhysRevB.87.235125

PACS number(s): 71.10.Ca, 05.30.Fk, 31.15.-p

### Why starting from HNET+NRQED?

- Necessary for manifesting the OPE operator relation!!!
- With external Coulomb potential, it is impossible to write down the OPE.

 Nucleus infinitely heavy. Electron moves sl owly. Still local QFT

### **OPE relation for coalescence**

Naïve Taylor expansion:

 $\psi(\mathbf{x})N(\mathbf{0}) = [\psi N](\mathbf{0}) + \mathbf{x} \cdot [\nabla \psi N](\mathbf{0}) + \cdots$ 

#### This is incomplete!!!

Correct expansion in coordinate space:  $\psi(\mathbf{x})N(\mathbf{0}) = (1 - mZ\alpha|\mathbf{x}|)[\psi N](\mathbf{0}) + (1 - mZ\alpha|\mathbf{x}|/2)\mathbf{x} \cdot [\nabla \psi N](\mathbf{0}) + \cdots$ 

And momentum space:  

$$\widetilde{\psi}(\mathbf{q})N(\mathbf{0}) \equiv \int d^3 \mathbf{x} e^{-i\mathbf{q}\cdot\mathbf{x}} \psi(\mathbf{x})N(\mathbf{0})$$

$$= \frac{8\pi Z \alpha m}{\mathbf{q}^4} [\psi N](\mathbf{0}) - \frac{16i\pi Z \alpha m}{\mathbf{q}^6} \mathbf{q} \cdot [\nabla \psi N](\mathbf{0}) + \cdots$$

### Determine Wilson coefficients

First define 4-point connected Green functions  $\Gamma\left(\mathbf{q}; \, \mathbf{p}, E \equiv p^{0} + k^{0}\right) \equiv \int d^{4}y \, d^{4}z \, e^{-ip \cdot y - ik \cdot z} \langle 0 | T\{\widetilde{\psi}(\mathbf{q}) N(\mathbf{0}) \psi^{\dagger}(y) N^{\dagger}(z)\} | 0 \rangle_{\mathrm{amp}},$   $\Gamma_{S}(\mathbf{p}, E) \equiv \int d^{4}y d^{4}z \, e^{-ip \cdot y - ik \cdot z} \langle 0 | T\{[\psi N](\mathbf{0}) \psi^{\dagger}(y) N^{\dagger}(z)\} | 0 \rangle_{\mathrm{amp}}$ 

There're only ladder diagrams defined as r.h.s.





Momentum space: Asymptotic behavior of 4-point Green function as the injected momentum q->m gets hard

- Leading diagram is th e tree diagram.
- Integrand is expanded given q~m.



Figure: The tree-level amputated Green function  $\Gamma^{(1)}$ .

$$\Gamma^{(1)} = Ze^{2} \int \frac{dq^{0}}{2\pi} \frac{i}{q^{0} - \frac{q^{2}}{2m} + i\epsilon} \frac{i}{E - q^{0} + i\epsilon} \frac{i}{|q - p|^{2}}$$
$$= Ze^{2}(-2m) \frac{i}{q^{2} - 2mE - i\epsilon} \frac{i}{|q - p|^{2}}$$
$$\frac{q \rightarrow m}{q^{4}} \frac{8\pi mZ\alpha}{q^{4}} + \cdots, \qquad (20)$$

**Factorized form** 

Define a n-ladder diagram

$$\Gamma^{(n)}(\mathbf{q}; \mathbf{p}, E) = \sum_{i=1}^{n} \tilde{C}^{(i)}(\mathbf{q}) \Gamma_{S}^{R(n-i)}(\mathbf{p}, E)$$

#### The factorized form is seen.

Diagrammatically, the 1<sup>st</sup> order

$$q \uparrow | = q \downarrow | = q \uparrow | = q \downarrow | = q \downarrow$$

## Proof to all orders by method of ind uction

- Analyse the loop momentum  $l_n$ :
- Hard: qSoftSoft:  $q^{-4}$
- Keep leading region: Soft



Figure: Reexpressing the four-point Green function  $\Gamma^{(n+1)}$  with n + 1 Coulomb ladders a one loop integral involving the Green function containing *n*-ladder. *H* and *S* indicate whether the loop momentum is hard or soft. The crossed dot marks composite operator  $[\psi N]$ .

### **OPE in coordinate space**

 Coordinate space Green function (additional diagr am abandoned in momentum space as disconnecte d gives 1)

 $\Gamma_{x}(\mathbf{x};\mathbf{p},E) \equiv \int d^{4}y \, d^{4}z \, e^{-i\mathbf{p}\cdot y - i\mathbf{k}\cdot z} \langle 0|T\{\psi(\mathbf{x})N(\mathbf{0})\psi^{\dagger}(y)N^{\dagger}(z)\}|0\rangle_{\mathrm{amp}}$ 

Given Fourier integral:

$$\int\!\!rac{d^3 \mathbf{q}}{(2\pi)^3}\,rac{e^{i\mathbf{q}\cdot\mathbf{x}}-1}{\mathbf{q}^4}=-rac{1}{8\pi}|\mathbf{x}|$$

Coordinate Wilson coefficient:

Use 
$$\Gamma^{(n)}(\mathbf{q}; \mathbf{p}, E) = \sum_{i=1}^{n} \tilde{C}^{(i)}(\mathbf{q})\Gamma_{S}^{R(n-i)}(\mathbf{p}, E)$$
 as n=1, gives:  
- $mZ\alpha|\mathbf{x}|$ .

### P-wave hydrogen-like atom

- Similar to S-wave
- The only difference is the local operator  $[\nabla \psi N](0)$
- Subtraction to get coordinate Wilson coefficient is different:  $\int \frac{d^3 q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{x}} - i\mathbf{q}\cdot\mathbf{x}}{q^6} \mathbf{q} = -\frac{i}{32\pi} |\mathbf{x}| \mathbf{x}$ gives  $-\frac{mZ\alpha|\mathbf{x}|\mathbf{x}}{2}$ .

### Application to hydrogen-like atoms

Matrix element definition of wave function  $\Psi_{nlm}(\mathbf{x}) = \langle 0 | \psi(\mathbf{x}) N(\mathbf{0}) | nlm \rangle$ 

gives 
$$(a_0 \equiv 1/mZ\alpha)$$
  
 $R_{n0}(x) = R_{n0}(0) \left[1 - \frac{x}{a_0} + \mathcal{O}(x/a_0)^2\right]$   
 $\tilde{R}_{n0}(q)(2\pi)^{-3/2} = 2^2 R_{n0}(0) \frac{(2\pi)}{a_0 q^4} + \mathcal{O}\left(\frac{1}{a_0 q}\right)^2$   
 $R_{n1}(x) = x \frac{dR_{n1}}{dx}(0) \left[1 - \frac{1}{2} \frac{x}{a_0} + \mathcal{O}(x/a_0)^2\right]$   
 $\tilde{R}_{n1}(q)(2\pi)^{-3/2} = 2^3 \frac{dR_{n1}(0)}{dx} \frac{(2\pi)}{a_0 q^5} + \mathcal{O}\left(\frac{1}{a_0 q}\right)^2$ 

### Compare with the old knowledge

• Our results agree with the old QM results:

$$R_{nl}(x) = \frac{x'}{l!} \frac{d' R_{nl}}{dx'}(0) \left[ 1 - \frac{1}{l+1} \frac{x}{a_0} + \mathcal{O}(x/a_0)^2 \right] \quad \text{(Löwdin, 1954)}$$
$$\tilde{R}_{nl}(q) = 2^{l+2} \frac{dR_{nl}^{l}(0)}{d'x} \frac{(2\pi)^{\frac{5}{2}}}{a_0 q^{l+4}} + \mathcal{O}\left(\frac{1}{a_0 q}\right)^2 \qquad \text{(Bethe & Salpeter, 1957)}$$



### Part 2: Klein-Gordon and Dirac

### EFT and OPE

$$\mathbf{Klein-Gordon equation}$$

$$\mathbf{F}$$

$$\begin{bmatrix} \left(E + \frac{Ze^2}{4\pi r}\right)^2 + \hbar^2 c^2 \nabla^2 - m^2 c^4 \end{bmatrix} \Psi(\mathbf{r}) = 0.$$

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

$$\begin{bmatrix} \frac{d^2}{dr^2} + \frac{Z^2 \alpha^2 - l(l+1)}{r^2} + \frac{2Z\alpha E}{\hbar cr} + \frac{E^2 - m^2 c^4}{\hbar^2 c^2} \end{bmatrix} r R_{nl}(r) = 0,$$

$$R_{nl}(r) = N_{nl} \rho^{l'} e^{-\frac{\rho}{2}} {}_1 F_1(l' + 1 - \lambda, 2l' + 2; \rho),$$

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

40.1

Near-the origin behavior of S-wave hydr ogen KG wave function

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

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

$$l'(l'+1) = l(l+1) - Z^2 \alpha^2,$$

$$l' \equiv -\frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - Z^2 \alpha^2}$$

# Expanding the wave function near origin

Expanding ( $\rho$ )<sup>s<sub>i</sub></sup> gives

$$R_{n0}^{\rm KG}(r) \approx R_{n0}^{\rm Sch}(0)\rho^{\sqrt{\frac{1}{4} - Z^2\alpha^2} - \frac{1}{2}} \approx R_{n0}^{\rm Sch}(0)\rho^{-Z^2\alpha^2} = R_{n0}^{\rm Sch}(0)\left(1 - Z^2\alpha^2\ln\frac{2r}{na_0} + \cdots\right)$$

Expanding the rest gives Schrödinger results

 $1 - \alpha mrZ$ 

Sum up to

$$R_{n0}^{\rm KG}(r) = R_{n0}^{\rm Sch}(0)(1 - mZ\alpha r) \left(1 - Z^2\alpha^2 \ln \frac{2r}{na_0} + \cdots\right)$$

## S-wave Klein-Gordon wave functions ne ar the origin

Wave function near the origin:



Perturbation theory in QM

#### Hamiltonian:

$$\begin{split} H_{\text{eff}} &= H_0 + \Delta H = H_0 + H_{\text{kin}} + H_{\text{Darwin}}, \\ H_0 &= -\frac{\boldsymbol{\nabla}^2}{2m} - \frac{Ze^2}{4\pi r}, \\ H_{\text{kin}} &= -\frac{\boldsymbol{\nabla}^4}{8m^3c^2}, \qquad H_{\text{Darwin}} = \frac{1}{32m^4c^4} \left[ \boldsymbol{\nabla}^2, \left[ \frac{Ze^2}{4\pi r}, \boldsymbol{\nabla}^2 \right] \right] \end{split}$$

Energy

$$\begin{split} \Delta E_{nl}^{(1)} \Big|_{\rm kin} &= \langle nl | H_{\rm kin} | nl \rangle = -mc^2 \frac{Z^4 \alpha^4}{2n^4} \left( \frac{n}{l+\frac{1}{2}} - \frac{3}{4} \right) \\ \Delta E_{nl}^{(1)} \Big|_{\rm Darwin} &= \langle nl | H_{\rm Darwin} | nl \rangle = 0. \end{split}$$

## Wave function correction

First-order QM perturbation

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

- Coutinuum spectrum gives UV divergence
- Coutinuum Coulomb wave function

$$\begin{aligned} R_{k0}^{\rm Sch}(r) &= \sqrt{\frac{8\pi mcZ\alpha k}{1 - e^{\frac{-2\pi mcZ\alpha}{k}}}} e^{-ikr} {}_{1}F_{1}\left(1 + \frac{imcZ\alpha}{k}, 2; 2ikr\right), \qquad E_{k0} = \frac{k^{2}}{2m}, \\ \int dr \, r^{2}R_{k0}^{\rm Sch}(r) R_{k'0}^{\rm Sch}(r) &= 2\pi\delta(k - k'). \end{aligned}$$

## Continuum matrix element

$$\langle k0|H_{\rm kin}|10\rangle = -2Z^3\alpha^3\sqrt{\frac{\pi k}{2\left(1-e^{-\frac{2\pi mZ\alpha}{k}}\right)}}\left[1-\frac{2m^2Z^2\alpha^2\cosh\frac{\pi mZ\alpha}{k}\exp\left(\frac{2mZ\alpha}{k}\tan^{-1}\frac{mZ\alpha}{k}\right)}{k^2+m^2Z^2\alpha^2}\right]$$

$$\xrightarrow{k \to \infty} -\sqrt{mZ\alpha}Z^3\alpha^3\left(\frac{k}{mZ\alpha} + \frac{\pi}{2} + \cdots\right),\tag{17a}$$

$$\langle k0 | H_{\text{Darwin}} | 10 \rangle = -\frac{Z^3 \alpha^3}{4} \sqrt{\frac{\pi k}{2(1 - e^{-\frac{2\pi mZ\alpha}{k}})}} \left(\frac{k^2}{m^2} + Z^2 \alpha^2\right)$$

$$\xrightarrow{k \to \infty} -\sqrt{mZ\alpha} \frac{Z^3 \alpha^3}{8m^2} \left(\frac{k^3}{mZ\alpha} + \frac{\pi k^2}{2} + \frac{(24 + \pi^2)k(mZ\alpha)}{24} + \frac{\pi(\pi^2 - 24)(mZ\alpha)^2}{48} + \cdots\right),$$
(17b)

Must impose a UV cutoff, yields divergence

$$\begin{split} \Delta R_{10}^{(1)}(0)\Big|_{\rm kin} \ &= \ R_{10}^{\rm Sch}(0) \left(\frac{Z\alpha\Lambda}{\pi m} + Z^2\alpha^2\ln\Lambda + {\rm finite}\right),\\ \Delta R_{10}^{(1)}(0)\Big|_{\rm Darwin} \ &= \ R_{10}^{\rm Sch}(0) \left(\frac{Z\alpha\Lambda^3}{24\pi m^3} + \frac{Z^2\alpha^2\Lambda^2}{16m^2} + \frac{Z^3\alpha^3\pi\Lambda}{24m} + {\rm finite}\right). \end{split}$$

Scalar QED+HNET and OPE: an unsuccessful attempt!

Lagrangian:

$$\mathcal{L} = (D_{\mu}\phi)^{\dagger}D^{\mu}\phi - m^{2}\phi^{\dagger}\phi + N^{\dagger}iD_{0}N - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}$$
$$D^{\mu} = \partial^{\mu} + ieA^{\mu}: D^{\mu}_{\mu} = \partial^{\mu} - iZeA^{\mu}$$

$$D^{\mu} = \partial^{\mu} + ieA^{\mu}; D^{\mu}_{N} = \partial^{\mu} - iZeA^{\mu}$$

OPE relations defined as:

 $\phi_R(\mathbf{r})N_R(\mathbf{0}) = (1+C(\mathbf{r}))[\phi N]_R(\mathbf{0}) + \cdots,$ 

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

### **Renormalize Local Operators**

### Definition:

$$egin{aligned} &[\phi N]_R(\mathbf{0})\equiv Z_{\phi N}\phi^0 N^0(\mathbf{0})=Z_{\phi N}\sqrt{Z_\phi Z_N}\phi_R N_R(\mathbf{0})\ &=Z_S\phi_R N_R(\mathbf{0}) \end{aligned}$$

Calculate the following diagrams in both Fe ynman gauge and Coulomb gauge


#### **Renormalize Local Operators**

#### Relation for counterterms

$$\delta_S = \delta_{\phi N} + rac{\delta_\phi}{2} + rac{\delta_N}{2}.$$

	$\delta_{\phi}$	$\delta_N$	$\delta_S$	$\delta_{\phi N}$
Feynman Gauge	$\frac{e^2}{4\pi^2\epsilon}$	$rac{Z^2 e^2}{4\pi^2\epsilon}$	$-\frac{Ze^2}{8\pi^2\epsilon}$	$-\frac{Ze^2}{8\pi^2\epsilon}-\frac{e^2}{8\pi^2\epsilon}-\frac{Z^2e^2}{8\pi^2\epsilon}$
Coulomb Gauge	$rac{e^2}{4\pi^2\epsilon}$	0	$-rac{Ze^2}{4\pi^2\epsilon}$	$-rac{Ze^2}{4\pi^2\epsilon}-rac{e^2}{8\pi^2\epsilon}$

TABLE I: Counterterms in Feynman gauge and Coulomb gauge within MS scheme.

• While  $\delta_{\phi N}$  is gauge-invariant with Z=1, what's related to OPE is  $\delta_{\delta S}$ .

OPE (similar to point-splitting, smearng a local composite operator)

Define  $\tilde{\Gamma}_{\phi}\left(\mathbf{q}; \mathbf{p}, E \equiv k^{0} + p^{0}\right) \equiv \int \frac{d^{3}r}{(2\pi)^{3}} \frac{d^{4}y}{(2\pi)^{4}} \frac{d^{4}z}{(2\pi)^{4}} e^{-i\mathbf{q}\cdot\mathbf{r}} e^{ip\cdot y} e^{ik\cdot z} \langle \Omega | T\left\{\phi(\mathbf{r})N(0)\varphi^{\dagger}(y)N^{\dagger}(z)\right\} | \Omega \rangle_{amp},$   $= \left[ \begin{array}{c} \\ \\ \\ \\ \end{array} \right] + \cdots$ 

FIG. 4: The OPE relation to order  $Z\alpha$  in the momentum space.

74

OPE in coordinate space (Fey nman gauge)

In Feynman gauge, expanding  $\tilde{\Gamma}_{\phi}^{Feyn}$  (q; p,  $k^0$ ,  $p^0$ ) gives

$$\tilde{C}^{Feyn}(\mathbf{q}) = \frac{\pi Z \alpha}{|\mathbf{q}|^3} + \cdots$$

Fourier transform to coordinate space

$$C^{Feyn}(\mathbf{r}) = -\frac{Z\alpha}{2\pi} (\log \mu r + \frac{1}{2} \log \pi e^{\gamma_E}),$$

OPE in coordinate space (Co ulomb gauge)

In Coulomb gauge, expanding  $\tilde{\Gamma}_{\phi}^{Coul}$  (q; p,  $E \equiv k^0 + p^0$ ) ve gives

$$\tilde{C}^{Coul}(\mathbf{q}) = \frac{2\pi Z \alpha}{|\mathbf{q}|^3} + \cdots$$

Fourier transform to coordinate space

$$C^{Coul}(\mathbf{r}) = -\frac{Z\alpha}{\pi}(\log \mu r + \frac{1}{2}\log \pi e^{\gamma_E}),$$

Both gauges give logarithm at 272 order



- Scalar QED + HNET won't work!
- **Drop**  $A^0$

$$\mathcal{L} = (D_0\phi)^{\dagger} D^0\phi - \nabla\phi^{\dagger} \cdot \nabla\phi - m^2\phi^{\dagger}\phi + N^{\dagger}iD_0N + \frac{1}{2}(\nabla A_0)^2$$

Non-relativistic approximation

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

Use with EOM, the following conditions are obtained

$$\tilde{\varphi} = -\frac{iD_0}{2mc^2}(\varphi + \tilde{\varphi}).$$
  $iD_0\varphi = \frac{\nabla^2}{2m}(\varphi + \tilde{\varphi})$ 

# NREFT: our working basis

NREFT Lagrangian:

$$\begin{aligned} \mathcal{L}_{EFT} &= \varphi^{\dagger} \left[ i D_0 + \frac{\boldsymbol{\nabla}^2}{2m} + \frac{\boldsymbol{\nabla}^4}{8m^3} + \frac{\boldsymbol{\nabla}^6}{16m^5} + \frac{e}{32m^4} [\boldsymbol{\nabla}^2, [A_0, \boldsymbol{\nabla}^2]] + \cdots \right] \varphi + N^{\dagger} i D_N^0 N \\ &+ \frac{1}{2} (\boldsymbol{\nabla} A_0)^2 + c_4 \varphi^{\dagger} \varphi N^{\dagger} N + \cdots . \end{aligned}$$



FIG. 7: One-loop diagrams for  $eN \rightarrow eN$  on-shell amplitude from both sQED+HNET and NREFT. The cross represents the  $p^4$  relativistic correction, and the solid square represents the  $c_4$  electronnucleus contact interaction.

• Matching gives 
$$c_4 = \mathcal{O}(Z^3 \alpha^3)$$



• Coordinate space  $\varphi(\mathbf{r})N(\mathbf{0}) = \left(1 - mZ\alpha|\mathbf{r}| - Z^2\alpha^2 \left(\log\left(mZ\alpha|\mathbf{r}|\right) + \frac{1}{2}\log 4\pi e^{\gamma_E - 1}\right) + \cdots\right) [\varphi N]_R(\mathbf{0}) + \cdots$ 

Momentum space

$$ilde{arphi}(\mathbf{q})N(\mathbf{0}) \equiv \int d^3 \mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{x}} \varphi(\mathbf{r})N(\mathbf{0})$$
  
=  $\left(\frac{8\pi mZ\alpha}{\mathbf{q}^4} + \frac{2\pi^2 Z^2 \alpha^2 + \cdots}{\mathbf{q}^3}\right) [\varphi N]_R(\mathbf{0}) + \cdots$ 

Crossed multiplication

$$\tilde{\Gamma}^{(n)}\left(\mathbf{q};\,\mathbf{p},E\right) = \sum_{i=1}^{n} \tilde{C}^{(i)}(\mathbf{q}) F_{R}^{(n-i)}(\mathbf{p},E)$$

# Renormalize local operators

No need include wave function correction, the ren ormalization only involves vertex correction:

 $[\varphi N]_R(\mathbf{0}) = Z_S \varphi N(\mathbf{0})$ 

Define

$$F(\mathbf{p}, E) \equiv \int \frac{d^4y}{(2\pi)^4} \int \frac{d^4z}{(2\pi)^4} e^{ip \cdot y} e^{ik \cdot z} \langle \Omega | T\left\{\varphi N(\mathbf{0})\tilde{\varphi}^{\dagger}(p)\tilde{N}^{\dagger}(k)\right\} | \Omega \rangle_{amp},$$

### Renormalize local operators

- Calculate diagram b and d won't give logarithmic divergence.
- Diagram a and c are finite.
- Calculate diagram e gives logarithmic divergence  $Z^2 \alpha^2 \left(\frac{1}{2\epsilon} + \log \mu\right)$ .
- Diagram f is higher order contribution.



### Renormalize local operators

With MS scheme in dimensional regularization

$$Z_{\mathcal{S}} = 1 - rac{Z^2 lpha^2}{2\epsilon} + \mathcal{O}(lpha^4),$$

#### The anomalous dimension

$$\gamma_{\mathcal{S}} \equiv \frac{d \log Z_{\mathcal{S}}}{d \log \mu} = Z^2 \alpha^2$$

#### Momentum space Wilson coefficient

#### Define

 $\tilde{\Gamma}\left(\mathbf{q};\,\mathbf{p},E\equiv k^{0}+p^{0}\right)\equiv\int\frac{d^{4}y}{(2\pi)^{4}}\int\frac{d^{4}z}{(2\pi)^{4}}e^{ip\cdot y}e^{ik\cdot z}\langle\Omega|T\left\{\tilde{\varphi}(\mathbf{q})N(\mathbf{0})\varphi^{\dagger}(y)N^{\dagger}(z)\right\}|\Omega\rangle_{amp},$ 

- Scales in the problem:
- Hard: m v << q < m,

 $v = Z\alpha << 1$ 

Soft:  $p \sim mv$ ,  $E \sim mv \wedge 2$ 

Leading scaling behavior of diagrams: d ouble-layer form of OPE



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  $\mathbf{p}^4$  kinetic term, Darwin term and contact interaction, respectively

$$\widetilde{\Gamma}(\mathbf{q}; \mathbf{p}, E) \xrightarrow{q \to m} \frac{1}{\mathbf{q}^4} \text{ and } \frac{1}{|\mathbf{q}|^3},$$



FIG. 9: The factorization of momentum-space four-point function into hard and soft parts through order  $Z^2 \alpha^2$ .

## **OPE** relation (coordinate space)

$$= \left( \bigwedge_{c} + \text{UVCT} \right) + \left( \bigwedge_{c} - \bigwedge_{c} \right) + \left( \bigwedge_{c} - \bigwedge_{c} - \text{UVCT} \right) + \cdots$$

## Wilson coefficient

Momentum space

$$\tilde{C}^{(2)}(\mathbf{q}) = \frac{2\pi^2 Z^2 \alpha^2}{|\mathbf{q}|^3}.$$

Coordinate space

$$C^{(2)}(\mathbf{r}) = -Z^2 \alpha^2 \left( \log \mu |\mathbf{r}| + \frac{1}{2} \log 4\pi e^{\gamma_E - 1} \right),$$

# Renormalization Group Equation: Resumble methods and the leading logarithm:

 $\gamma_{\mathcal{S}} = Z^2 \alpha^2 + \mathcal{O}(Z^4 \alpha^4)$ 

*RGE* for local composite S-wave operator:

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

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



RGE for S-wave Wilson coefficient of OPE:

$$\mu \frac{d\mathcal{C}(r)}{d\mu} + \mathcal{C}(r)\gamma_{\mathcal{S}} = 0. \qquad (\mu \frac{d}{d\mu} - r \frac{d}{dr})\mathcal{C}(\mu r) = 0. \text{ Define } r \equiv r_0\kappa,$$
  

$$\kappa \frac{d\mathcal{C}(r_0\kappa)}{d\kappa} + \mathcal{C}(r_0\kappa)\gamma_{\mathcal{S}} = 0.$$
  

$$\mathcal{C}(r) = \mathcal{C}(r_0)\kappa^{-Z^2\alpha^2} = \mathcal{C}(r_0)\left(\frac{r}{r_0}\right)^{-Z^2\alpha^2} \text{ Choosing } r_0 = a_0 \text{ as the Bohr radius}$$

Fully reproduce the near-the origin anomalous scaling  $R_{n0}^{\text{KG}}(r) \approx R_{n0}^{\text{Sch}}(0)\rho^{\sqrt{\frac{1}{4}-Z^2\alpha^2}-\frac{1}{2}} \approx R_{n0}^{\text{Sch}}(0)\rho^{-Z^2\alpha^2}$  of KG wf.

#### Dirac wave function of hydrogen

$$\left(-i\hbar c\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}+\beta mc^2-\frac{Ze^2}{4\pi r}\right)\Psi=E\Psi,$$

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

We focus on the large component of Dirac wave functions for the j=1/2, positive parity hydrogen

$$\Psi_{n\frac{1}{2}m}(\mathbf{r}) = \begin{pmatrix} F_n(r)\sqrt{\frac{1}{4\pi}}\,\xi_m\\ G_n(r)\sqrt{\frac{3}{4\pi}}\sigma\cdot\hat{\mathbf{r}}\,\xi_m \end{pmatrix},$$

$$F_n(r) \approx R_n^{\rm Sch}(0) \left(\frac{2r}{na_0}\right)^{-\frac{Z^2 \alpha^2}{2}},$$

where  $a_0 = \hbar/(mcZ\alpha)$  is the Bohr radius, and  $R_n^{\rm Sch}(0)$ represents the radial Schrödinger wave function at the origin for the nS hydrogen state. We have also taken the nonrelativistic approximation  $\sqrt{1 - Z^2\alpha^2} \approx 1 - Z^2\alpha^2/2$ in the exponent. The singularity has noticeable effect only when  $r \leq \frac{na_0}{2} \exp(-2/Z^2\alpha^2) \sim \frac{na_0}{2} 10^{-16300/Z^2}$  [14], which is even many orders shorter than the length scale related to the QED Landau pole!

### **Dirac wave function**

Wave function origin behavior of large component

$$F_n(r) \approx R_n^{\rm Sch}(0) \left(\frac{2r}{na_0}\right)^{-\frac{Z^2\alpha^2}{2}}, \label{eq:Fn}$$

• Expand the large component spinor:

$$\lim_{r \to 0} F_n(r) = R_n^{\rm Sch}(0) \left(1 - r/a_0\right) \left(1 - \frac{Z^2 \alpha^2}{2} \ln r + \cdots\right).$$

- Divergence can be reproduced by perturbative QM
- Kinetic correction + Darwin term+ spin orbit



#### Correct OPE formulated in NRQED+HNET

$$\mathcal{L}_{\text{NREFT}} = \psi^{\dagger} \left\{ iD_{0} + \frac{\nabla^{2}}{2m} + \frac{\nabla^{4}}{8m^{3}} + iC_{2}e^{\frac{\nabla^{2}}{2m}} + iC_{2}e^{\frac{\nabla^{2}}{4m^{2}}} + iC_{2}e^{\frac{\sigma}{2}} \cdot (\nabla A^{0} \times \nabla) + \cdots \right\} \psi$$

$$+ N^{\dagger}iD^{0}N + \frac{c_{4}}{m^{2}}\psi^{\dagger}\psi N^{\dagger}N + \frac{1}{2}(\nabla A^{0})^{2} + \cdots$$

$$\lim_{r \to \frac{1}{m}} \psi(\mathbf{r})N(0) = \mathcal{C}(r)[\psi N]_{R}(0) + \cdots , \qquad (18)$$

$$\mathcal{C}(r) = 1 - mZ\alpha r - \frac{Z^{2}\alpha^{2}}{2}(\ln\mu r + \operatorname{const}) + \mathcal{O}(Z^{3}\alpha^{3}).$$

$$\widetilde{\psi}(\mathbf{q})N(0) \equiv \int d^{3}\mathbf{r} \, e^{-i\mathbf{q}\cdot\mathbf{r}}\varphi(\mathbf{r})N(0)$$

$$\to \widetilde{C}(q)[\psi N]_{R}(0) + \cdots , \qquad (19)$$

$$\widetilde{C}(q) = \frac{8\pi mZ\alpha + \mathcal{O}(Z^{3}\alpha^{3})}{q^{4}} - \frac{\pi^{2}Z^{2}\alpha^{2} + \mathcal{O}(Z^{4}\alpha^{4})}{|\mathbf{q}|^{3}}, \qquad (19)$$

## Summary

- EFT combined with OPE offers new insights for deeper understanding coalesc ence behavior of atomic wave functions.
  - It can be extended to study multi-particle coalescence behaviors.
- Applied in relativistic Klein-Gordon and Dirac equations, solving long-standin g puzzle about the anomalous scaling behavior of the hydrogen wave function s near the origin
- Leading logarithms are resummed with the aid of RGE
- Lesson: To succeed, one must start from NREFT, not the UV-completed relati vistic QED+HNET
- KG and Dirac equation as r<1/m becomes untrustworthy... why? 94</p>



#### Thanks for your attention!