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Title	Scale dependence of the retarded van der Waals potential
Author(s)	Miyao, Tadahiro; Spohn, Herbert
Citation	Journal of Mathematical Physics, 53(9), 095215 https://doi.org/10.1063/1.4745911
Issue Date	2012-09
Doc URL	https://hdl.handle.net/2115/50790
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Type	journal article
File Information	JMP53-9_095215.pdf

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Citation: J. Math. Phys. **53**, 095215 (2012); doi: 10.1063/1.4745911
View online: http://dx.doi.org/10.1063/1.4745911
View Table of Contents: http://jmp.aip.org/resource/1/JMAPAQ/v53/i9
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JOURNAL OF MATHEMATICAL PHYSICS **53**, 095215 (2012)

Scale dependence of the retarded van der Waals potential

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(Received 4 May 2012; accepted 30 July 2012; published online 29 August 2012)

We study the ground state energy for a system of two hydrogen atoms coupled to the quantized Maxwell field in the limit $\alpha \to 0$ together with the relative distance between the atoms increasing as $\alpha^{-\gamma}R$, $\gamma > 0$. In particular we determine explicitly the crossover function from the R^{-6} van der Waals potential to the R^{-7} retarded van der Waals potential, which takes place at scale $\alpha^{-2}R$. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4745911]

We dedicate our contribution to Elliott Lieb with greatest admiration and deep gratitude for what he has taught us, and whole generations, about quantum mechanics and statistical physics.

I. INTRODUCTION

In a now very famous contribution, Casimir and Polder[1] investigate the ground state energy, $E(R)$, of a system of two hydrogen atoms for which the two immobile nuclei are separated by a distance R and the two spinless electrons are coupled through the quantized Maxwell field according to non-relativistic QED. In the approximation where the quantum fluctuations of the Maxwell field are ignored, only the electrostatic Coulomb interaction remains. In this case $E(R) - E(\infty) \approx -R^{-6}$, the ubiquitous van der Waals potential, which has been discovered on thermodynamic grounds way before the advent of quantum mechanics. The R^{-6} behavior is well understood quantum mechanically[2] and has been proved in great generality by Lieb and Thirring.[3] Casimir and Polder use fourth order perturbation theory to argue that because of retardation effects the true asymptotic behavior is in fact $E(R) - E(\infty) \approx -R^{-7}$ for large R. Their argument has been reworked many times and extended to arbitrary atoms and molecules, see for example.[4–9] It is generally agreed that for two *neutral* molecules A, B it holds

$$E(R) - E(\infty) \cong -\frac{23}{4\pi}\alpha_A\alpha_B R^{-7} \tag{1.1}$$

for large R. Here α_A, α_B, are the electric dipole moments of molecule A, B. The numerical prefactor is universal ($23/4\pi$ is the value in Gaussian units).

Equation (1.1) is based on perturbation theory and thus holds only for small coupling. With improved experimental techniques, there has been a renewed interest to explore a wider regime. One still finds the R^{-7} power law, but the prefactor is now a bilinear form in the electric and magnetic dipole moments. To be consistent, in principle, these moments have to be computed for the single molecule in isolation but still coupled to its own quantized radiation field. All atomic/molecular properties appear through the electric and magnetic dipole moments. As in (1.1), the remaining coefficients are universal. In particular the coefficient $23/4\pi$ for electric dipole-electric dipole contribution persists. To mention only the most recent work: in Refs. 11 and 12 the retarded van der Waals potential is computed in the framework of macroscopic QED. The approach in Ref. 13 is based on the standard non-relativistic QED Hamiltonian, but uses the representation in terms of a functional integral. Conceptually, this has the advantage that $E(\infty)$ is subtracted without error and

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that $1/R$ turns into a small parameter explicitly showing up in the action. Thus $1/R$ can be used as an expansion parameter, which is more physical than the conventional coupling strength to the Maxwell field.

In the framework of non-relativistic QED the existence of a ground state, for arbitrary R and coupling strength, has been established in the break through contribution of Griesemer, Lieb, and Loss.[10,14] To determine the leading, large R asymptotics of $E(R)$ seem to be a difficult problem, even for small, but fixed, coupling. In view of this situation we develop here a novel approach somewhat closer in spirit to the original Casimir-Polder considerations. As interaction strength we use the fine structure constant α and regard the ground state energy, $E(R) = E_\alpha(R)$, as depending both on R and α. We then study the limit of small coupling with an approximately adjusted scale of R, more precisely we consider the limit

$$E_\alpha(\alpha^{-\gamma} R) - E_\alpha(\infty), \quad \gamma \geq 0, \tag{1.2}$$

as $\alpha \to 0$. Depending on the value γ distinct features of $E_\alpha(R)$ will become visible. In particular, we will find an explicit formula for the crossover from R^{-6} to R^{-7}, which occurs at scale α^{-2}.

In Sec. 2 we define the Hamiltonians and provide an overview on the dependence on γ. There are two special values. At $\gamma = 1$ one crosses from core dominated behavior to the $-R^{-6}$ van der Waals and at $\gamma = 2$ one crosses from $-R^{-6}$ to $-R^{-7}$. The corresponding crossover function is computed explicitly and seems to be novel. Sections III and IV provide proofs and point out open problems.

II. HAMILTONIANS AND MAIN RESULTS

Let us first consider a single hydrogen atom with an infinitely heavy nucleus located at the origin. The nucleus has charge e, $e > 0$, the electron has charge $-e$. We will use units in which $\hbar = 1$, $c = 1$, and the bare mass of the electron $m = 1$. Then the fine-structure constant is $\alpha = e^2/4\pi$. Let x, p be position and momentum of the spinless electron. Then the non-relativistic QED Hamiltonian for this system reads

$$H_{1,\alpha} = \tfrac{1}{2} :\big(p - eA(x)\big)^2: -e^2 V_\varphi(x) + H_{\mathrm{f}}\,. \tag{2.1}$$

The electrons and the nuclei are assumed to have the same prescribed charge distribution φ with the following properties: φ is normalized, $\int \mathrm{d}x\, \varphi(x) = 1$, rotation invariant, $\varphi(x) = \varphi_{\mathrm{rad}}(|x|)$, and of rapid decrease. Denoting Fourier transform by $\hat{\varphi}$, the potential V_φ is the smeared Coulomb potential

$$V_\varphi(x) = \int_{\mathbb{R}^3} \mathrm{d}k\, |\hat{\varphi}(k)|^2 |k|^{-2} \mathrm{e}^{-\mathrm{i}k\cdot x}\,. \tag{2.2}$$

$A(x)$ is the quantized vector potential and H_{f} is the field energy. These are defined through a two-component Bose field $a(k,\lambda)$, $k \in \mathbb{R}^3$, $\lambda = 1, 2$, with commutation relation

$$[a(k,\lambda), a(k',\lambda')^*] = \delta_{\lambda\lambda'}\delta(k - k'). \tag{2.3}$$

Explicitly

$$H_{\mathrm{f}} = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \mathrm{d}k\, \omega(k) a(k,\lambda)^* a(k,\lambda) \tag{2.4}$$

with dispersion relation

$$\omega(k) = |k| \tag{2.5}$$

and

$$\begin{aligned} A(x) &= \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \mathrm{d}k\, \hat{\varphi}(k) \frac{1}{\sqrt{2\omega(k)}} \varepsilon(k,\lambda)\big(\mathrm{e}^{\mathrm{i}k\cdot x} a(k,\lambda) + \mathrm{e}^{-\mathrm{i}k\cdot x} a(k,\lambda)^*\big) \\ &= A^+(x) + A^-(x) \end{aligned} \tag{2.6}$$

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with the standard dreibein $\varepsilon(k,1)$, $\varepsilon(k,2)$, $\hat{k} = k/|k|$. $:\cdot:$ denotes normal ordering, which will be of use later on. Thus the Hilbert space for H is

$$\mathcal{H} = L^2(\mathbb{R}^3_x) \otimes \mathfrak{F}\,, \tag{2.7}$$

where $\mathfrak{F}$ is the bosonic Fock space over $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$. From the quantization of the classical system of charges coupled to the Maxwell field it follows that for the smearing of $A(x)$ and of V_φ the same charge distribution has to be used. We refer to Ref. 15 for details. The ground state energy of $H_{1,\alpha}$ is denoted by $E_{1,\alpha}$.

To investigate the van der Waals potential one considers two hydrogen atoms, one located at 0 and the other at $r = (0, 0, R)$, $R \geq 0$. It will be convenient to define the position of the second electron relative to r. Then x_1, $x_2 + r$ are positions and p_1, p_2 the momenta of the two electrons. The two-electron Hamiltonian reads

$$\begin{aligned} H_R =& \tfrac{1}{2} :\big(p_1 - eA(x_1)\big)^2: -e^2 V_\varphi(x_1) + \tfrac{1}{2} :\big(p_2 - eA(x_2 + r)\big)^2: -e^2 V_\varphi(x_2) \\ &+ H_{\mathrm{f}} + e^2 V_R(x_1, x_2) \end{aligned} \tag{2.8}$$

with the interaction potential

$$\begin{aligned} V_R(x_1, x_2) &= -V_\varphi(x_1 - r) - V_\varphi(x_2 + r) + V_\varphi(r) + V_\varphi(r + x_2 - x_1) \\ &= \int_{\mathbb{R}^3} \mathrm{d}k\, |\hat{\varphi}(k)|^2 \mathrm{e}^{\mathrm{i}k\cdot r} |k|^{-2} (1 - \mathrm{e}^{-\mathrm{i}k\cdot x_1})(1 - \mathrm{e}^{\mathrm{i}k\cdot x_2})\,. \end{aligned} \tag{2.9}$$

H_R acts on the Hilbert space $L^2(\mathbb{R}^3_{x_1}) \otimes L^2(\mathbb{R}^3_{x_2}) \otimes \mathfrak{F}$. H_R has a unique ground state with energy $E_\alpha(R)$. It is known that $\lim_{R\to\infty} E_\alpha(R) = 2E_{1,\alpha}$.

We plan to study $E_\alpha(\alpha^{-\gamma}R)$ in the limit of small α and consider first the hydrogen atom. In the limit $\alpha \to 0$ the Bohr radius is order α^{-1} and the energy is order $-\alpha^2$. Hence it is convenient to switch to atomic coordinates which amounts to the unitary transformation

$$\begin{aligned} &U^* a(k,\lambda) U = \alpha^{-3} a(\alpha^{-2}k, \lambda)\,, \quad U^* x U = \alpha^{-1} x\,, \quad U^* p U = \alpha p\,, \\ &U^* x_j U = \alpha^{-1} x_j\,, \quad U^* p_j U = \alpha p_j\,, \quad j = 1, 2\,. \end{aligned} \tag{2.10}$$

Then

$$U^* H_{1,\alpha} U = \alpha^2 \Big(\tfrac{1}{2} :\big(p - \sqrt{4\pi}\alpha^{3/2} A_\alpha(x)\big)^2: - V_\alpha(x) + H_{\mathrm{f}} \Big) \tag{2.11}$$

with

$$V_\alpha(x) = 4\pi \int_{\mathbb{R}^3} \mathrm{d}k\, |\hat{\varphi}(\alpha k)|^2 |k|^{-2} \mathrm{e}^{-\mathrm{i}k\cdot x} \tag{2.12}$$

and

$$\begin{aligned} A_\alpha(x) &= \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \mathrm{d}k\, \hat{\varphi}(\alpha^2 k) \frac{1}{\sqrt{2|k|}} \varepsilon(k,\lambda) \big(\mathrm{e}^{\mathrm{i}\alpha k\cdot x} a(k,\lambda) + \mathrm{e}^{-\mathrm{i}\alpha k\cdot x} a(k,\lambda)^* \big) \\ &= A^+_\alpha(x) + A^-_\alpha(x)\,. \end{aligned} \tag{2.13}$$

We note that

$$\alpha^3 [A^+_\alpha(x), A^-_\alpha(x)] = \alpha^3 \int_{\mathbb{R}^3} \mathrm{d}k\, |\hat{\varphi}(\alpha^2 k)|^2 |k|^{-1} = \mathcal{O}(\alpha^{-1})\,. \tag{2.14}$$

Thus normal ordering is introduced to subtract these more singular contributions.

Correspondingly, the atomic scale Hamiltonian for two hydrogen atoms separated by a distance $\alpha^{-1}R$ reads

$$\begin{aligned} U^* H_{\alpha^{-1}R} U =& \alpha^2 \Big(\tfrac{1}{2} :\big(p_1 - \sqrt{4\pi}\alpha^{3/2} A_\alpha(x_1)\big)^2: + \tfrac{1}{2} :\big(p_2 - \sqrt{4\pi}\alpha^{3/2} A_\alpha(x_2 + r)\big)^2: \\ &- V_\alpha(x_1) - V_\alpha(x_2) + V_{\alpha,R}(x_1, x_2) + H_{\mathrm{f}} \Big)\,. \end{aligned} \tag{2.15}$$

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2.1 The scale $0 \le \gamma \le 1$

For $\gamma = 1$, instead of considering merely the ground state energy, a more complete picture would be the strong convergence of resolvents. For the smeared Coulomb potentials it holds

$$\lim_{\alpha\to 0} \sup_x |V_\alpha(x) - |x|^{-1}| = 0\,, \tag{2.16}$$

$$\lim_{\alpha\to 0} \sup_{x_1,x_2} \big| V_{\alpha,R}(x_1,x_2) - \big(- |x_1+r|^{-1} - |x_2+r|^{-1} + R^{-1} + |r+x_2-x_1|^{-1}\big)\big| = 0\,. \tag{2.17}$$

Thus the issue of strong resolvent convergence is reduced to the study of the free particle Hamiltonian

$$T_{1,\alpha} = \tfrac{1}{2} :\big(p - \sqrt{4\pi}\alpha^{3/2} A_\alpha(x)\big)^2: + H_{\rm f} \tag{2.18}$$

and correspondingly for two free electrons, with Hamiltonian denoted by $T_{2,\alpha}$. Note that the norm of the coupling function in (2.18) diverges as $\alpha^{-1/2}$. Thus the limit $\alpha \to 0$ is singular. On the other hand the recent estimate[17] of the ground state energy $E^0_{1,\alpha}$ of $T_{1,\alpha}$ establishes that $E^0_{1,\alpha} = -a_0 + a_3\alpha + \mathcal{O}(\alpha^2)$. For us only the coefficient a_0 is of interest, which is given by

$$a_0 = (2\pi)^2 \big\langle A_1^+(0)\cdot A_1^+(0)\Omega, \big(\tfrac{1}{2}P_{\rm f}^2 + H_{\rm f}\big)^{-1} A_1^+(0)\cdot A_1^+(0)\Omega\big\rangle\,. \tag{2.19}$$

Here Ω denotes the Fock vacuum and $P_{\rm f}$ is the field momentum,

$$P_{\rm f} = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} {\rm d}k\, k a(k,\lambda)^* a(k,\lambda)\,. \tag{2.20}$$

With this information one arrives at

Conjecture 2.1: In the sense of strong convergence of resolvents,

$$\lim_{\alpha\to 0} T_{1,\alpha} = \tfrac{1}{2}p^2 + H_{\rm f} - a_0\,, \tag{2.21}$$

$$\lim_{\alpha\to 0} T_{2,\alpha} = \tfrac{1}{2}p_1^2 + \tfrac{1}{2}p_2^2 + H_{\rm f} - 2a_0\,. \tag{2.22}$$

To our surprise, this limit has apparently never been investigated. In Sec. 4 we provide some arguments towards the validity of Conjecture 2.1. If it holds, then by (2.16) and (2.17) we conclude that

$$\begin{aligned}\lim_{\alpha\to 0} \alpha^{-2} U^* H_{1,\alpha} U &= \frac{1}{2}p^2 - \frac{1}{|x|} + H_{\rm f} - a_0 \\ &= H_{\rm hy} + H_{\rm f} - a_0\,,\end{aligned} \tag{2.23}$$

and

$$\begin{aligned}\lim_{\alpha\to 0} \alpha^{-2} U^* H_{\alpha^{-1}R} U &= \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 - |x_1|^{-1} - |x_2|^{-1} - |x_1 - r|^{-1} - |x_2 + r|^{-1} \\ &\quad + R^{-1} + |r + x_2 - x_1|^{-1} + H_{\rm f} - 2a_0 \\ &= H_{2,R} + H_{\rm f} - 2a_0\end{aligned} \tag{2.24}$$

in the sense of strong resolvent convergence. Denoting the ground state energy of $H_{2,R}$ by $E_{2,R}$, in particular it holds

$$\gamma = 1: \qquad \lim_{\alpha\to 0} \alpha^{-2} E_\alpha(\alpha^{-1}R) = E_{2,R} - 2a_0\,. \tag{2.25}$$

Note that

$$\lim_{R\to 0} (E_{2,R} - R^{-1}) = E_{\rm he} \tag{2.26}$$

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with $E_{\rm he}$ the ground state of the helium atom, while

$$\lim_{R\to\infty} R^6(E_{2,R} - 2E_{\rm hy}) = -a_{\rm VW}\,, \tag{2.27}$$

where $a_{\rm VW}$ is the strength of the van der Waals potential

$$a_{\rm VW} = 6\int_0^\infty {\rm d}t\, \left|\tfrac{1}{3}\langle\psi_0, x\cdot {\rm e}^{-t(H_{\rm hy}-E_{\rm hy})}x\psi_0\rangle\right|^2 \tag{2.28}$$

with $H_{\rm hy}\psi_0 = E_{\rm hy}\psi_0, E_{\rm hy} = -1/2$. Thus we conclude that on the distance scale $\alpha^{-1}R$ the energy $\alpha^2 E_{2,R}$ describes the crossover to the $-R^{-6}$ potential.

For completeness we list the even smaller distance scales,

$$\gamma = 0: \qquad E_\alpha(R) \cong \alpha V_\alpha(R) + \alpha^2(E_{\rm he} - 2a_0)\,, \tag{2.29}$$

$$0 < \gamma < 1: \qquad E_\alpha(\alpha^{-\gamma}R) \cong \alpha^{1+\gamma}R^{-1} + \alpha^2(E_{\rm he} - 2a_0)\,. \tag{2.30}$$

2.2 The scale $\gamma \geq 1$

To go beyond the distance scale $\alpha^{-1}R$ is a more difficult problem and we have only partial results. We expect that the range $1 < \gamma < 2$ is dominated by the van der Waals potential, i.e.,

$$1 < \gamma < 2: \qquad E_\alpha(\alpha^{-\gamma}R) \cong \alpha^{6\gamma-4}a_{\rm VW}R^{-6} + 2E_{1,\alpha}\,. \tag{2.31}$$

The retardation of the van der Waals potential first appears at scale α^{-2}. More precisely

$$\gamma = 2: \qquad E_\alpha(\alpha^{-2}R) \cong -\alpha^8 h_{\rm co}(R) + 2E_{1,\alpha}\,, \tag{2.32}$$

where the crossover function $h_{\rm co}$ is defined by

$$\begin{aligned} &h_{\rm co}(R) \\ &= \pi^{-1}\int_0^\infty {\rm d}u\left(\tfrac{1}{3}\langle\psi_0, x\cdot(H_{\rm hy}-E_{\rm hy})\big((H_{\rm hy}-E_{\rm hy})^2 + (u/2)^2\big)^{-1}x\psi_0\rangle\right)^2 {\rm e}^{-Ru} \\ &\qquad \times\left\{2^{-3}R^{-2}u^4 + 2^{-1}R^{-3}u^3 + 5\cdot 2^{-1}R^{-4}u^2 + 6R^{-5}u + 6R^{-6}\right\}. \end{aligned} \tag{2.33}$$

At small distances

$$h_{\rm co}(R) \cong a_{\rm VW}R^{-6}, \quad \text{as } R\to 0\,, \tag{2.34}$$

and at large distances

$$h_{\rm co}(R) \cong a_{\rm CP}R^{-7}, \quad \text{as } R\to\infty\,. \tag{2.35}$$

Here the strength of the retarded van der Waals potential is

$$a_{\rm CP} = \frac{23}{4\pi}(\alpha_{\rm hy})^2\,, \quad \alpha_{\rm hy} = \frac{2}{3}\langle\psi_{\rm hy}, x\cdot(H_{\rm hy}-E_{\rm hy})^{-1}x\psi_{\rm hy}\rangle = \frac{9}{2}\,. \tag{2.36}$$

We conclude that at scale $\alpha^{-2}R$ the ground state energy crosses from the van der Waals potential to the retarded one as specified by $h_{\rm co}$.

At even larger scales one expects the exact power low R^{-7},

$$\gamma > 2: \qquad E_\alpha(\alpha^{-\gamma}R) \cong -\alpha^{7\gamma-6}a_{\rm CP}R^{-7} + 2E_{1,\alpha}\,. \tag{2.37}$$

The hydrogen atom ground state has been estimated up to $\mathcal{O}(\alpha^5\log\alpha^{-1})$ (Ref. 18) based on a method originally devised by Hainzl and Seiringer.[19] It is rather natural to use similar methods for the case of two hydrogen atoms. If more modestly we strive for a precision of order α^3, then the scale will be limited to $\alpha^{-6/5}$, unless there is a more direct way to accomplish the subtraction. At scale α^{-2} the first term is order α^8. There is no hope to control $E_{1,\alpha}$ with such a precision and one has to look for alternative schemes.

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III. THE $\gamma = 2$ CROSSOVER FUNCTION

Our main goal is to derive the crossover function of (2.33). The starting point is the functional integral representation of $E_\alpha(R) - E_\alpha(\infty)$, as the logarithm of a partition function to be evaluated in the limit of large "volume," $[-T, T]$ with $T \to \infty$, see Ref. 13. In this paper we consider only the second cumulant of the action, assuming that higher cumulants decay at least as R^{-8} for $R \to \infty$. The functional integration is defined with respect to two independent ground state processes for the Hamiltonian H of (2.1) and thus still includes the coupling to the radiation field. On the basis of our conjecture, for small coupling we replace H by

$$\alpha^2\big(H_\alpha + H_{\mathrm{f}} - a_0\big)\,, \quad H_\alpha = \tfrac{1}{2}p^2 - V_\alpha(x)\,. \tag{3.1}$$

Denoting both approximations by $[\cdots]_{\mathrm{cu}}$ we have

$$[E_\alpha(R) - E_\alpha(\infty)]_{\mathrm{cu}} = -2(2\pi\alpha)^2\big(I_2(R) + I_3(R) + I_4(R)\big)\,, \tag{3.2}$$

where the coefficients are given in (39), respectively, (47), (52) of Ref. 13 with the understanding that H is replaced by $\alpha^2(H_\alpha + H_{\mathrm{f}} - a_0)$. Equation (3.2) should be regarded as the definition of the left-hand side. I_2, I_3, I_4 are explicitly given integrals with two three-dimensional momentum integrations and, respectively, 1, 2, 3 time integrations, compare with (3.3) below. I_2 and I_3 are not displayed here. Required is an asymptotic analysis of the integrals I_2, I_3, and I_4. In fact, in the scalings of (2.31), (2.32), (2.37), the contribution of I_2 and I_3 vanish as $\alpha \to 0$. The details are lengthy and will not be recorded here. In the following we focus only on the relevant contribution I_4.

For notational simplicity, we replace $H_\alpha - \inf \mathrm{spec}(H_\alpha)$ by H_α in the remainder of this section. Then the ground state ψ_α is defined through $H_\alpha\psi_\alpha = 0$. Similarly, $H_{\mathrm{hy}} - E_{\mathrm{hy}}$ is replaced by H_{hy}. Hence $H_{\mathrm{hy}}\psi_{\mathrm{hy}} = 0$. According to (52) of Ref. 13, $I_4(R)$ is defined by

$$\begin{aligned} I_4(R) = \alpha^6 \int_{\mathbb{R}^3} \mathrm{d}t_1\mathrm{d}t_2\mathrm{d}t_3 \sum_{\lambda_1,\lambda_2} \int_{\mathbb{R}^6} \mathrm{d}k_1\mathrm{d}k_2 |\hat{\varphi}(\alpha^2 k_1)|^2 |\hat{\varphi}(\alpha^2 k_2)|^2 \mathrm{e}^{\mathrm{i}(k_1+k_2)\cdot r\alpha^2} \\ \times \tfrac{1}{4}\omega_1\omega_2\, \mathrm{e}^{-\omega_1|t_1+t_2+t_3|}\mathrm{e}^{-\omega_2|t_3|} \\ \times \big\langle \psi_\alpha, (\varepsilon_1\cdot x)H_\alpha \mathrm{e}^{-\mathrm{i}k_1\cdot x\alpha} H_\alpha^{-2}\, \mathrm{e}^{-|t_1|H_\alpha}\, \mathrm{e}^{-\mathrm{i}k_2\cdot x\alpha} H_\alpha(\varepsilon_2\cdot x)\psi_\alpha\big\rangle \\ \times \big\langle \psi_\alpha, (\varepsilon_1\cdot x)H_\alpha \mathrm{e}^{\mathrm{i}k_1\cdot x\alpha} H_\alpha^{-2}\, \mathrm{e}^{-|t_2|H_\alpha}\, \mathrm{e}^{\mathrm{i}k_2\cdot x\alpha} H_\alpha(\varepsilon_2\cdot x)\psi_\alpha\big\rangle\,, \end{aligned} \tag{3.3}$$

where now the inner product is in $L^2(\mathbb{R}^3_x)$. The asymptotics of integrals as (3.3) have been studied before,[23] but only in the dipole approximation, which amounts to setting $\alpha = 0$ in the factors $\exp(\pm k_j \cdot x\alpha)$, $j = 1, 2$. The handling without dipole approximation is novel.

Proposition 3.1: Assume that the smearing function φ is radial, continuous, and of compact support.
(i) Let $1 < \gamma < 2$. Then

$$\lim_{\alpha\to 0} \alpha^{6-6\gamma}(4\pi)^{-2} I_4(\alpha^{-\gamma}R) = a_{\mathrm{VW}} R^{-6}\,. \tag{3.4}$$

(ii) Let $\gamma = 2$. Then

$$\lim_{\alpha\to 0} \alpha^{-6} I_4(\alpha^{-2}R) = h_{\mathrm{co}}(R)\,. \tag{3.5}$$

(iii) Let $\gamma > 2$. Then

$$\lim_{\alpha\to 0} \alpha^{8-7\gamma}(4\pi)^{-2} I_4(\alpha^{-\gamma}R) = \frac{23}{4\pi}(a_{\mathrm{hy}})^2 R^{-7}\,. \tag{3.6}$$

Using (3.2) the proposition supports the claims of Sec. 2.

Proof: For better readability we subdivide our proof into several steps. But before we remark that, within the current proof, compact support of φ is required.

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Step 1 (Rewriting): We scale $k_j \rightsquigarrow \alpha^{\gamma-2}k_j$ and $t_3 \rightsquigarrow \alpha^{2-\gamma}t_3$. Then

$$
\begin{aligned}
&I_4(\alpha^{-\gamma}R)\\
&\quad= \alpha^{7\gamma-8}\int_{\mathbb{R}^3}\mathrm{d}t_1\mathrm{d}t_2\mathrm{d}t_3\sum_{\lambda_1,\lambda_2}\int_{\mathbb{R}^6}\mathrm{d}k_1\mathrm{d}k_2|\hat{\varphi}(\alpha^\gamma k_1)|^2|\hat{\varphi}(\alpha^\gamma k_2)|^2\\
&\qquad\times \mathrm{e}^{\mathrm{i}(k_1+k_2)\cdot r}\,\tfrac{1}{4}\omega_1\omega_2\,\mathrm{e}^{-\alpha^{\gamma-2}\omega_1|t_1+t_2+\alpha^{2-\gamma}t_3|}\mathrm{e}^{-\omega_2|t_3|}\\
&\qquad\times\big\langle\psi_\alpha,(\varepsilon_1\cdot x)H_\alpha\mathrm{e}^{-\mathrm{i}\alpha^{\gamma-1}k_1\cdot x}H_\alpha^{-2}\,\mathrm{e}^{-|t_1|H_\alpha}\,\mathrm{e}^{-\mathrm{i}\alpha^{\gamma-1}k_2\cdot x}H_\alpha(\varepsilon_2\cdot x)\psi_\alpha\big\rangle\\
&\qquad\times\big\langle\psi_\alpha,(\varepsilon_1\cdot x)H_\alpha\mathrm{e}^{\mathrm{i}\alpha^{\gamma-1}k_1\cdot x}H_\alpha^{-2}\,\mathrm{e}^{-|t_2|H_\alpha}\,\mathrm{e}^{\mathrm{i}\alpha^{\gamma-1}k_2\cdot x}H_\alpha(\varepsilon_2\cdot x)\psi_\alpha\big\rangle\,.
\end{aligned}
\tag{3.7}
$$

Let us note the following equality,

$$
\begin{aligned}
&\int_{\mathbb{R}^3}\mathrm{d}t_1\mathrm{d}t_2\mathrm{d}t_3\,\mathrm{e}^{-\omega_1\alpha^{\gamma-2}|t_1+t_2+\alpha^{2-\gamma}t_3|}\mathrm{e}^{-\omega_2|t_3|}\mathrm{e}^{-\lambda_1|t_1|}\mathrm{e}^{-\lambda_2|t_2|}\\
&\quad=(2\pi)^{-1}\alpha^{2-\gamma}\int_{\mathbb{R}}\mathrm{d}u\,\frac{2\omega_1}{\omega_1^2+\alpha^{4-2\gamma}u^2}\cdot\frac{2\omega_2}{\omega_2^2+\alpha^{4-2\gamma}u^2}\cdot\frac{2\lambda_1}{\lambda_1^2+u^2}\cdot\frac{2\lambda_2}{\lambda_2^2+u^2}\,,
\end{aligned}
\tag{3.8}
$$

which is proven by using the Fourier transform

$$
(2\pi)^{-1}\int_{\mathbb{R}}\mathrm{d}u\,\mathrm{e}^{-\mathrm{i}ut}\frac{2\omega}{\omega^2+u^2}=\mathrm{e}^{-\omega|t|}\,. \tag{3.9}
$$

Viewing λ_1 and λ_2 as spectral parameters for H_α, one arrives at

$$
\begin{aligned}
I_4(\alpha^{-\gamma}R)&=\alpha^{6\gamma-6}(2\pi)^{-1}\int_{\mathbb{R}}\mathrm{d}u\int_{\mathbb{R}^6}\mathrm{d}k_1\mathrm{d}k_2\,|\hat{\varphi}(\alpha^\gamma k_1)|^2|\hat{\varphi}(\alpha^\gamma k_2)|^2\\
&\quad\times\mathrm{e}^{\mathrm{i}(k_1+k_2)\cdot r}\frac{k_1^2}{k_1^2+\alpha^{4-2\gamma}u^2}\cdot\frac{k_2^2}{k_2^2+\alpha^{4-2\gamma}u^2}\\
&\quad\times2\big\langle\psi_\alpha,(\varepsilon_1\cdot x)H_\alpha\mathrm{e}^{-\mathrm{i}k_1\cdot x\alpha}H_\alpha^{-1}\,(H_\alpha^2+u^2)^{-1}\,\mathrm{e}^{-\mathrm{i}k_2\cdot x\alpha}H_\alpha(\varepsilon_2\cdot x)\psi_\alpha\big\rangle\\
&\quad\times2\big\langle\psi_\alpha,(\varepsilon_1\cdot x)H_\alpha\mathrm{e}^{\mathrm{i}k_1\cdot x\alpha}H_\alpha^{-1}(H_\alpha^2+u^2)^{-1}\,\mathrm{e}^{\mathrm{i}k_2\cdot x\alpha}H_\alpha(\varepsilon_2\cdot x)\psi_\alpha\big\rangle\,.
\end{aligned}
\tag{3.10}
$$

Next we use

$$
H_\alpha(\varepsilon\cdot x)\psi_\alpha=[H_\alpha,\varepsilon\cdot x]\psi_\alpha=\mathrm{i}\varepsilon\cdot p\psi_\alpha \tag{3.11}
$$

and also introduce the integral kernel of $(\mathbb{1}-P_\alpha)H_\alpha^{-1}(H_\alpha^2+u^2)^{-1}$ as

$$
K_{u,\alpha}(x,x')=\langle x|(\mathbb{1}-P_\alpha)H_\alpha^{-1}(H_\alpha^2+u^2)^{-1}|x'\rangle \tag{3.12}
$$

with P_α the projection onto ψ_α. Note that $\langle(\varepsilon\cdot p)\psi_\alpha,\mathrm{e}^{\mathrm{i}k\cdot x}\psi_\alpha\rangle=0$, which allows one to insert $\mathbb{1}-P_\alpha$. Since H_α has a spectral gap, uniformly in α, $K_{u,\alpha}$ is bounded and $\langle\phi,K_{u,\alpha}\phi\rangle\cong C\langle\phi,\phi\rangle u^{-2}$ for $u\to\infty$. With this notation we arrive at the starting representation of I_4,

$$
\begin{aligned}
I_4(\alpha^{-\gamma}R)&=\alpha^{6\gamma-6}(2\pi)^{-1}4\int_{\mathbb{R}}\mathrm{d}u\int_{\mathbb{R}^6}\mathrm{d}k_1\mathrm{d}k_2\,|\hat{\varphi}(\alpha^\gamma k_1)|^2|\hat{\varphi}(\alpha^\gamma k_2)|^2\\
&\quad\times k_1^2(k_1^2+\alpha^{4-2\gamma}u^2)^{-1}k_2^2(k_2^2+\alpha^{4-2\gamma}u^2)^{-1}\\
&\quad\times\Big(\sum_{\lambda_1,\lambda_2}\int_{\mathbb{R}^{12}}\mathrm{d}x\mathrm{d}x'\mathrm{d}y\mathrm{d}y'K_{u,\alpha}(x,x')K_{u,\alpha}(y,y')\mathrm{e}^{\mathrm{i}k_1\cdot(r+\alpha^{\gamma-1}(y-x))}\mathrm{e}^{\mathrm{i}k_2\cdot(r+\alpha^{\gamma-1}(y'-x'))}\\
&\quad\times(\varepsilon_1\cdot p_x)(\varepsilon_1\cdot p_y)(\varepsilon_2\cdot p_{x'})(\varepsilon_2\cdot p_{y'})\psi_\alpha(x)\psi_\alpha(y)\psi_\alpha(x')\psi_\alpha(y')\Big)\,.
\end{aligned}
\tag{3.13}
$$

Step 2 (Error estimate for vanishing phase): We deal with the set on which the phase in (3.13) is close to 0 and define

$$
\Lambda_{r,\alpha}=\Big\{(x,y)\in\mathbb{R}^3\times\mathbb{R}^3\,\Big|\,|r+\alpha^{\gamma-1}(y-x)|\geq\tfrac{1}{2}R\Big\}\,, \tag{3.14}
$$

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correspondingly $\Lambda'_{r,\alpha}$ with x, y replaced by x', y'. $\tilde{I}_4$ is I_4 from (3.13) with the integration restricted to $\Lambda_{r,\alpha} \times \Lambda'_{r,\alpha}$. The error term equals $I_4^{\text{error}} = I_4 - \tilde{I}_4$. We use the Cauchy-Schwarz inequality inside (3.13) and perform the u, k_1, k_2 integrations. Since $K_{u,\alpha}$ is bounded, this yields

$$|I_4^{\text{error}}(\alpha^{-\gamma} R)| \leq C\alpha^{-4\gamma-8} \int_{\mathbb{R}^6} \mathrm{d}k_1 \mathrm{d}k_2 |k_1|^2 |k_2|^2 |\hat{\varphi}(k_1)|^2 |\hat{\varphi}(k_2)|^2 \times \Big(\int_{\mathbb{R}^6 \setminus \Lambda_{r,\alpha}} \mathrm{d}x \mathrm{d}y |\nabla \psi_\alpha(x)|^2 |\nabla \psi_\alpha(y)|^2 \Big)^{1/2}. \tag{3.15}$$

The ground state ψ_α has the exponential decay. Therefore

$$|I_4^{\text{error}}(\alpha^{-\gamma} R)| \leq C\alpha^{-4\gamma-8} \mathrm{e}^{-\kappa R \alpha^{1-\gamma}}, \tag{3.16}$$

which tends to 0 as $\alpha \to 0$. In the remainder we will study $\tilde{I}_4$.

Step 3 (Angular integration): The k_1, k_2 integrations are done in spherical coordinates setting $\mathrm{d}k_j = w_j^2 \mathrm{d}w_j \mathrm{d}\Omega_j$, $j = 1, 2$. Let $Q(k) = \mathbb{1} - |\hat{k}\rangle\langle\hat{k}|$ be the transverse projection. Then the angular part reads

$$\int \mathrm{d}\Omega_1 \, \mathrm{e}^{\mathrm{i}k_1 \cdot a_1} Q(k_1) \otimes \int \mathrm{d}\Omega_2 \, \mathrm{e}^{\mathrm{i}k_2 \cdot a_2} Q(k_2) \tag{3.17}$$

with

$$a_1 = r + \alpha^{\gamma-1}(y - x), \quad a_2 = r + \alpha^{\gamma-1}(y' - x'). \tag{3.18}$$

We omit the index and compute $\int \mathrm{d}\Omega \, \mathrm{e}^{\mathrm{i}k \cdot a} Q(k)$ for general a.

Let O_a be an orthogonal transformation in $\mathbb{R}^3$ such that $\mathsf{O}_a a = |a| e_3$, where $e_3 = (0, 0, 1)^T$. Then

$$\begin{aligned} \int \mathrm{d}\Omega \, \mathrm{e}^{\mathrm{i}k \cdot a} Q(k) &= \int \mathrm{d}\Omega \, \mathrm{e}^{\mathrm{i}k \cdot \mathsf{O}_a a} \mathsf{O}_a^{-1} Q(k) \mathsf{O}_a \\ &= 2\pi \int_0^\pi \mathrm{d}\vartheta \, \sin\vartheta \, \mathrm{e}^{\mathrm{i}|k||a|\cos\vartheta} \mathsf{O}_a^{-1} \tilde{B}(\vartheta) \mathsf{O}_a, \end{aligned} \tag{3.19}$$

where $\tilde{B}_{ij}(\vartheta) = \delta_{ij} \tilde{b}_j(\vartheta)$, $i, j = 1, 2, 3$, with

$$\tilde{b}_1(\vartheta) = \tilde{b}_2(\vartheta) = \frac{1}{2}(1 + (\cos\vartheta)^2), \quad \tilde{b}_3(\vartheta) = 1 - (\cos\vartheta)^2. \tag{3.20}$$

Integrating over ϑ yields

$$\int \mathrm{d}\Omega \, \mathrm{e}^{\mathrm{i}k \cdot a} Q(k) = 2\pi \mathsf{O}_a^{-1} B(|k||a|) \mathsf{O}_a, \tag{3.21}$$

where $B_{ij}(s) = \delta_{ij} b_j(s)$ with

$$b_1(s) = b_2(s) = \hat{g}(s) - \hat{g}''(s), \quad b_3(s) = 2(\hat{g}(s) + \hat{g}''(s)), \quad \hat{g}(s) = s^{-1} \sin s. \tag{3.22}$$

Thus, for $j = 1, 2$,

$$\int \mathrm{d}\Omega_j \, \mathrm{e}^{\mathrm{i}k_j \cdot a_j} Q(k_j) = 2\pi \mathsf{O}_{a_j}^{-1} B(|k_j||a_j|) \mathsf{O}_{a_j}. \tag{3.23}$$

Step 4 (Radial integration): The radial integrations are of the form

$$\tfrac{1}{2} \int_{\mathbb{R}} \mathrm{d}w \hat{\varrho}(\alpha^\gamma w) w^4 (w^2 + \alpha^{4\gamma-2} u^2)^{-1} f(|a||w|) \tag{3.24}$$

with $f(s) = \hat{g}(s) = s^{-1} \sin s$ or $\hat{g}''(s) = 2s^{-3} \sin s - 2s^{-2} \cos s - s^{-1} \sin s$. Here $\hat{\varrho}(|k|) = |\hat{\varphi}(k)|^2$ and we extended $\hat{\varrho}$ to $\mathbb{R}$ by reflection at 0. We introduce a new function ρ by

$$\rho(v) = (2\pi)^{-1/2} \int_{\mathbb{R}} \mathrm{d}w \hat{\varrho}(w) \mathrm{e}^{\mathrm{i}vw}. \tag{3.25}$$

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Then one has

$$\int_{\mathbb{R}} \mathrm{d}v \rho(v) = (2\pi)^{1/2} \hat{\varrho}(0) = (2\pi)^{-5/2} . \tag{3.26}$$

Let $\sigma(|x|) = \varphi * \varphi(x)$. Then

$$\rho(v) = (2\pi)^{-3/2} \int_v^\infty \mathrm{d}r \, r\sigma(r) \tag{3.27}$$

for $v \geq 0$. Since φ is continuous and of compact support, $\rho \in C^1(\mathbb{R})$ and ρ has compact support.

We plan to use Plancherel's theorem in (3.24) and obtain, in the sense of distributions,

$$\begin{aligned} c_1(v; |a|, u) &= (2\pi)^{-1/2} \int_{\mathbb{R}} \mathrm{d}w \, \mathrm{e}^{\mathrm{i}vw} w^3 (w^2 + u^2)^{-1} |a|^{-1} \sin(|a|w) \\ &= (4|a|)^{-1} (2\pi)^{1/2} \Big(-2\delta'(v + |a|) - u^2 \mathrm{sgn}(v + |a|) \, \mathrm{e}^{-|u||v+|a||} \\ &\quad + 2\delta'(v - |a|) + u^2 \mathrm{sgn}(v - |a|) \, \mathrm{e}^{-|u||v-|a||} \Big) , \end{aligned} \tag{3.28}$$

$$\begin{aligned} c_2(v; |a|, u) &= (2\pi)^{-1/2} \int_{\mathbb{R}} \mathrm{d}w \, \mathrm{e}^{\mathrm{i}vw} w (w^2 + u^2)^{-1} |a|^{-3} \sin(|a|w) \\ &= (4|a|^3)^{-1} (2\pi)^{1/2} \Big(\mathrm{sgn}(v + |a|) \, \mathrm{e}^{-|u||v+|a||} - \mathrm{sgn}(v - |a|) \, \mathrm{e}^{-|u||v-|a||} \Big) , \end{aligned} \tag{3.29}$$

$$\begin{aligned} c_3(v; |a|, u) &= (2\pi)^{-1/2} \int_{\mathbb{R}} \mathrm{d}w \, \mathrm{e}^{\mathrm{i}vw} w^2 (w^2 + u^2)^{-1} |a|^{-2} \cos(|a|w) \\ &= (4|a|^2)^{-1} (2\pi)^{1/2} \Big(2\delta(v + |a|) - |u| \, \mathrm{e}^{-|u||v+|a||} \\ &\quad + 2\delta(v - |a|) - |u| \, \mathrm{e}^{-|u||v-|a||} \Big) \end{aligned} \tag{3.30}$$

with the sign function $\mathrm{sgn}(t) = 1$ for $t \geq 0$, $\mathrm{sgn}(t) = -1$ for $t < 0$. Since $\rho \in C^1$, Plancherel's theorem yields

$$\begin{aligned} d_1(|a|, u, \alpha) &= \int_{\mathbb{R}} \mathrm{d}v \alpha^{-\gamma} \rho(\alpha^{-\gamma} v) \big(c_1(v; |a|, u) - c_2(v; |a|, u) + c_3(v; |a|, u) \big), \\ d_2(|a|, u, \alpha) &= d_1(|a|, u, \alpha) , \\ d_3(|a|, u, \alpha) &= \int_{\mathbb{R}} \mathrm{d}v \alpha^{-\gamma} \rho(\alpha^{-\gamma} v) 2 \big(c_2(v; |a|, u) - c_3(v; |a|, u) \big) \end{aligned} \tag{3.31}$$

and

$$D_{ij}(|a|, u, \alpha) = (2\pi) \delta_{ij} d_j(|a|, u, \alpha) . \tag{3.32}$$

We now combine all terms. The ground state ψ_α is invariant under rotations. It is convenient to write

$$\psi_\alpha(x) = \psi_{\alpha,\mathrm{rad}}(|x|) , \quad \nabla \psi_\alpha(x) = \psi'_{\alpha,\mathrm{rad}}(|x|) \hat{x} , \tag{3.33}$$

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where $\hat{x} = x/|x|$. Then (3.13) becomes

$$\begin{aligned}
&\tilde{I}_4(\alpha^{-\gamma} R) \\
&\quad = \alpha^{6\gamma-6}(2\pi)^{-1} 4 \int_{\mathbb{R}} \mathrm{d}u \int_{\Lambda_{r,\alpha}\times\Lambda'_{r,\alpha}} \mathrm{d}x\mathrm{d}y\mathrm{d}x'\mathrm{d}y' \\
&\qquad \times\Big(\hat{x}\cdot \mathsf{O}^{-1}_{r+\alpha^{\gamma-1}(y-x)} D\big(|r+\alpha^{\gamma-1}(y-x)|, \alpha^{2-\gamma}u, \alpha\big)\mathsf{O}_{r+\alpha^{\gamma-1}(y-x)}\hat{y}\Big) \\
&\qquad \times\Big(\hat{x}'\cdot \mathsf{O}^{-1}_{r+\alpha^{\gamma-1}(y'-x')} D\big(|r+\alpha^{\gamma-1}(y'-x')|, \alpha^{2-\gamma}u, \alpha\big)\mathsf{O}_{r+\alpha^{\gamma-1}(y'-x')}\hat{y}'\Big) \\
&\qquad \times \psi'_{\alpha,\mathrm{rad}}(|x|)\psi'_{\alpha,\mathrm{rad}}(|x'|)\psi'_{\alpha,\mathrm{rad}}(|y|)\psi'_{\alpha,\mathrm{rad}}(|y'|)K_{u,\alpha}(x,x')K_{u,\alpha}(y,y')\,. \qquad (3.34)
\end{aligned}$$

Step 5 (The limit $\alpha \to 0$): c_1, c_2, c_3 contain terms proportional to δ and δ'. Since, by assumption, ϱ has compact support and since $|a_j|$ is bounded away from zero on the prescribed domain of integration, these terms vanish for α sufficiently small. Thus only the regular terms, containing the exponential function, have still to be considered.

We have to discuss the cases $1 < \gamma < 2$ and $\gamma \geq 2$ separately.

$1 < \gamma < 2$. As before we use the uniform bound from $K_{u,\alpha}$. Therefore, the terms proportional to u^0, u, u^2 have a uniformly integrable bound in u. By dominated convergence only the term proportional to u^0 does not vanish as $\alpha \to 0$. The terms proportional to u^3, u^4 are bounded as

$$(1+u^2)^{-2}\big((\alpha^{2-\gamma}u)^4 + (\alpha^{2-\gamma}|u|)^3\big)\,\mathrm{e}^{-\kappa\alpha^{2-\gamma}|u|} \leq C\alpha^{3(2-\gamma)}\,\mathrm{e}^{-\kappa(2-\gamma)|u|} \qquad (3.35)$$

with $\kappa \geq \kappa_0 > 0$ uniformly in α. Thus the integral over u vanishes as $\alpha \to 0$.

We are left with the products of the u^0 terms. As $\alpha \to 0$, the matrix $\mathsf{O}_{r+\alpha^{\gamma-1}(y-x)}$ tends to the unit matrix. Thus we conclude

$$\begin{aligned}
&\lim_{\alpha\to 0} \alpha^{6-6\gamma}\tilde{I}_4(\alpha^{-\gamma}R) \\
&\quad = (2\pi)^{-1}4\Big((2\pi)^{3/2}(2R^3)^{-1}\tfrac{1}{2}\int_{\mathbb{R}} \mathrm{d}v\rho(v)\Big)^2 \\
&\qquad \times \int_{\mathbb{R}} \mathrm{d}u \int_{\mathbb{R}^{12}} \mathrm{d}x\mathrm{d}x'\mathrm{d}y\mathrm{d}y'\big(\hat{x}_1\hat{y}_1 + \hat{x}_2\hat{y}_2 + 2\hat{x}_3\hat{y}_3\big)\big(\hat{x}'_1\hat{y}'_1 + \hat{x}'_2\hat{y}'_2 + 2\hat{x}'_3\hat{y}'_3\big) \\
&\qquad \times \psi'_{\mathrm{hy,rad}}(|x|)\psi'_{\mathrm{hy,rad}}(|x'|)\psi'_{\mathrm{hy,rad}}(|y|)\psi'_{\mathrm{hy,rad}}(|y'|)K_{u,0}(x,x')K_{u,0}(y,y')\,. \qquad (3.36)
\end{aligned}$$

Using the rotational invariance of $K_{u,0}$ one arrives at

$$\begin{aligned}
\lim_{\alpha\to 0} \alpha^{6-6\gamma}\tilde{I}_4(\alpha^{-\gamma}R) &= (2\pi)^{-3}2^{-1}3R^{-6}\int_{\mathbb{R}} \mathrm{d}u\big(\tfrac{1}{3}\langle\psi_{\mathrm{hy}}, x\cdot H_{\mathrm{hy}}(H_{\mathrm{hy}}^2+u^2)^{-1}x\psi_{\mathrm{hy}}\rangle\big)^2 \\
&= (2\pi)^{-2}2^{-2}a_{\mathrm{VW}}R^{-6}. \qquad (3.37)
\end{aligned}$$

$2 \leq \gamma$. We substitute u by $\alpha^{\gamma-2}u$. The uniform bound now results from the exponential terms $\exp[-|u|v \pm |a|]$, using that

$$\int_{\mathbb{R}} \mathrm{d}v|\rho(v)|\mathrm{e}^{-|u||\alpha^{\gamma}v\pm|a||} \leq C\mathrm{e}^{-\kappa|u|} \qquad (3.38)$$

uniformly in α, provided α is sufficiently small, since $\rho(v)$ has compact support by the assumption. In the limit $\alpha \to 0$ one obtains a formula which has the same structure as in (3.36). Only the coefficients in front of $\hat{x}_j$, $\hat{y}_j$ and $\hat{x}'_j$, $\hat{y}'_j$ are now different.

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For $\gamma = 2$, one obtains

$$\lim_{\alpha\to 0} \alpha^{-6}\tilde{I}_4(\alpha^{-2}R) = (2\pi)^2\Big(\int_{\mathbb{R}} \mathrm{d}v\rho(v)\Big)^2 \times \int_{\mathbb{R}} \mathrm{d}u\Big(\beta_1^2 + 3\beta_2^2 + 3\beta_3^2 - 2\beta_1\beta_2 - 6\beta_2\beta_3 + 2\beta_1\beta_3\Big)2\mathrm{e}^{-2R|u|} \times \Big(\tfrac{1}{3}\big\langle\psi_{\mathrm{hy}}, x\cdot(\mathbb{1} - P_{\mathrm{hy}})H_{\mathrm{hy}}(H_{\mathrm{hy}}^2 + u^2)^{-1}x\psi_{\mathrm{hy}}\big\rangle\Big)^2 \tag{3.39}$$

with $\beta_1 = -R^{-1}u^2$, $\beta_2 = R^{-3}$, $\beta_3 = -R^{-2}|u|$, which yields

$$\lim_{\alpha\to 0} \alpha^{-6}\tilde{I}_4(\alpha^{-2}R) = (2\pi)^{-2}2^{-1}h_{\mathrm{co}}(R)\,. \tag{3.40}$$

For $\gamma > 2$, one has the same expression except that from the rescaling of $\mathrm{d}u$ one picks up the factor $\alpha^{\gamma-2}$ and that the factor $(\mathbb{1} - P_{\mathrm{hy}})(H_{\mathrm{hy}}^2 + u^2)^{-1}$ now reads $(\mathbb{1} - P_{\mathrm{hy}})(H_{\mathrm{hy}}^2 + (\alpha^{\gamma-2}u)^2)^{-1}$, which is still uniformly bounded in u. Hence

$$\lim_{\alpha\to 0} \alpha^{8-7\gamma}\tilde{I}_4(\alpha^{-\gamma}R) = (2\pi)^{-2}2^{-1}a_{\mathrm{CP}}R^{-7}\,. \tag{3.41}$$

This concludes the proof of Proposition 3.1. □

IV. STRONG RESOLVENT CONVERGENCE

We discuss the limit $\alpha \to 0$ for a free electron coupled to the radiation field on the scale set by the hydrogen atom. Then the energies are of order α^2 and Hamiltonian on that scale reads

$$T_{1,\alpha} = \tfrac{1}{2} :\big(p - \sqrt{4\pi}\alpha^{3/2}A_\alpha(x)\big)^2: + H_{\mathrm{f}}\,. \tag{4.1}$$

The coupling function in (4.1) is

$$g_\alpha(k,\lambda) = \sqrt{4\pi}\alpha^{3/2}\hat{\varphi}(\alpha^2 k)\frac{1}{\sqrt{2\omega}}\mathrm{e}^{\mathrm{i}\alpha k\cdot x}\varepsilon(k,\lambda). \tag{4.2}$$

Note that $\|g_\alpha\| \cong \alpha^{-1/2}$, which makes the limit $\alpha \to 0$ singular.

The ultraviolet cutoff as α^{-2} corresponds to a charge distribution localized on the relativistic scale. If the charge distribution would have a width of the order of the Bohr radius, then $\hat{\varphi}(\alpha^2 k)$ would have to be replaced by $\hat{\varphi}(\alpha k)$. Thus it is natural to introduce the parameter δ with $0 \le \delta < 1$ and to define $T_{1,\alpha}^{(\delta)}$ by (4.1) with $\hat{\varphi}(\alpha^2 k)$ substituted through $\hat{\varphi}(\alpha^{2-\delta}k)$. If $0 < \delta < 1$, our arguments in Secs. 2 and 3 would not be altered, except for $a_0 = 0$. But now the resolvent convergence can be established.

Proposition 4.1: Let $0 < \delta < 2$. *Then, in the sense of strong convergence of resolvents*,

$$\lim_{\alpha\to 0} T_{1,\alpha}^{(\delta)} = \tfrac{1}{2}p^2 + H_{\mathrm{f}}\,. \tag{4.3}$$

Proof: Let

$$T_{1.\alpha}^{(\delta)} = \tfrac{1}{2} :\big(p - \sqrt{4\pi}\alpha^{3/2}A_{\alpha,\delta}(x)\big)^2: + H_{\mathrm{f}} = T_0 + B_{\alpha,\delta}\,, \tag{4.4}$$

where

$$T_0 = \tfrac{1}{2}p^2 + H_{\mathrm{f}}\,,$$
$$B_{\alpha,\delta} = -\sqrt{4\pi}\alpha^{3/2}p\cdot(A_{\alpha,\delta}^+(x) + A_{\alpha,\delta}^-(x)) + 2\pi\alpha^3\big(A_{\alpha,\delta}^+(x)\cdot A_{\alpha,\delta}^+(x) + 2A_{\alpha,\delta}^+(x)\cdot A_{\alpha,\delta}^-(x) + A_{\alpha,\delta}^-(x)\cdot A_{\alpha,\delta}^-(x)\big)\,. \tag{4.5}$$

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The coupling function of $A_{\alpha,\,\delta}(x)$ is given by

$$g_{\alpha,\delta}(k,\lambda) = \hat{\varphi}(\alpha^{2-\delta}k)\frac{1}{\sqrt{2\omega}}\mathrm{e}^{\mathrm{i}\alpha k\cdot x}\varepsilon(k,\lambda)\,. \tag{4.6}$$

If it can be shown that

$$|\langle\phi,\,B_{\alpha,\delta}\phi\rangle| \le C(\alpha)\|(T_0+\mathbb{1})^{1/2}\phi\|\,,\quad C(\alpha)\to 0\ \text{ as }\ \alpha\to 0\,, \tag{4.7}$$

for all $\phi\in\mathrm{dom}(T_0^{1/2})$, then one concludes $T_{1,\alpha}^{(\delta)}\to\frac{1}{2}p^2+H_{\mathrm{f}}$ as $\alpha\to 0$ in the norm resolvent sense by the general theorem [Ref. 20, Theorem 8.25], as based on the famous Nelson's argument.[21] To prove (4.7), we apply the standard bounds

$$\|a(f)\psi\| \le \|\omega^{-1/2}f\|\|(H_{\mathrm{f}}+\mathbb{1})^{1/2}\psi\|\,, \tag{4.8}$$

$$\|a(f)^*\psi\|^2 \le (\|f\|^2+\|\omega^{-1/2}f\|^2)\|(H_{\mathrm{f}}+\mathbb{1})^{1/2}\psi\|^2\,. \tag{4.9}$$

As to $A^-_{\alpha,\delta}(x)$, the bound (4.8) translates to

$$\alpha^{3/2}\|A^-_{\alpha,\delta}(x)\psi\| \le \alpha^{3/2}\|\omega^{-1/2}g_{\alpha,\delta}\|\|(T_0+\mathbb{1})^{1/2}\psi\| \tag{4.10}$$

$$\le \mathcal{O}(\alpha^{(1+\delta)/2})\|(T_0+\mathbb{1})^{1/2}\psi\|\,. \tag{4.11}$$

Similarly, $A^-_{\alpha,\delta}\cdot A^-_{\alpha,\delta}$ can be estimated as

$$\begin{aligned}
&\alpha^3\|(H_{\mathrm{f}}+\mathbb{1})^{-1/2}A^-_{\alpha,\delta}(x)\cdot A^-_{\alpha,\delta}(x)\psi\| \\
&\quad\le \alpha^3\|A^+_{\alpha,\delta}(H_{\mathrm{f}}+\mathbb{1})^{-1/2}\|\|A^-_{\alpha,\delta}(H_{\mathrm{f}}+\mathbb{1})^{-1/2}\|\|(H_{\mathrm{f}}+\mathbb{1})^{1/2}\psi\| \\
&\quad\le \alpha^3(\|g_{\alpha,\delta}\|^2+\|\omega^{-1/2}g_{\alpha,\delta}\|^2)^{1/2}\|\omega^{-1/2}g_{\alpha,\delta}\|\|(H_{\mathrm{f}}+\mathbb{1})^{1/2}\psi\| \\
&\quad\le \mathcal{O}(\alpha^{3\delta/2})\|(H_{\mathrm{f}}+\mathbb{1})^{1/2}\psi\|\,.
\end{aligned} \tag{4.12}$$

Thus we arrive at

$$\alpha^{3/2}|\langle\phi,\,p\cdot A^-_{\alpha,\delta}\phi\rangle| \le \mathcal{O}(\alpha^{(1+\delta)/2})\|(T_0+\mathbb{1})^{1/2}\phi\|^2 \tag{4.13}$$

and

$$\begin{aligned}
\alpha^3|\langle\phi,\,A^-_{\alpha,\delta}(x)\cdot A^-_{\alpha,\delta}(x)\phi\rangle| &\le \alpha^3\|(H_{\mathrm{f}}+\mathbb{1})^{1/2}\phi\|\|(H_{\mathrm{f}}+\mathbb{1})^{-1/2}A^-_{\alpha,\delta}\cdot A^-_{\alpha,\delta}\phi\| \\
&\le \mathcal{O}(\alpha^{3\delta/2})\|(T_0+\mathbb{1})^{1/2}\phi\|^2
\end{aligned} \tag{4.14}$$

for each $\phi\in\mathrm{dom}(T_0^{1/2})$. Hence (4.7) is satisfied and the assertion follows. □

The case $\delta=0$ is physically distinguished, but Nelson's argument fails and no other functional analytic method seems to be available. We devise an alternative approach based on functional integrals, which clearly displays that $\delta=0$ is on the borderline. In our context functional integration is explained in Ref. 15, Chapter 14, and at greater depth in Ref. 22. The propagator $\mathrm{e}^{-\tau T_{1,\alpha}}$ can be written as an integral with respect to Brownian motion for the particle and a Gaussian space-time measure for the Maxwell field. It is convenient to pick for ψ the particular form

$$\psi = \phi\otimes W(f)\Omega\,. \tag{4.15}$$

Here $\phi\in L^2(\mathbb{R}^3)$, Ω is the Fock vacuum, and $W(f)$ is the Weyl operator

$$W(f) = \mathrm{e}^{(a(f)^*-a(f))}\,,\quad f\in L^2(\mathbb{R}^3)\otimes\mathbb{C}^2\,. \tag{4.16}$$

Note that the linear span of these vectors is dense in $L^2(\mathbb{R}^3)\otimes\mathfrak{F}$. Integrating over the Maxwell field one arrives at the following expression:

$$\langle\psi,\,\mathrm{e}^{-\tau T_{1,\alpha}}\psi\rangle = \mathbb{E}_{\mathrm{W}}\big(\phi(q_0)^*\phi(q_\tau)\,\mathrm{e}^{-\mathscr{A}}\big)\,, \tag{4.17}$$

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where $t \mapsto q_t$ is a path in $\mathbb{R}^3$ and $\mathbb{E}_{\mathrm{W}}$ denotes average over the Wiener measure. The action $\mathscr{A}$ results from the Gaussian integration over the Maxwell field and consists of a sum of three pieces,

$$\mathscr{A} = \mathscr{A}_1 + \mathscr{A}_2 + \mathscr{A}_3 \,. \tag{4.18}$$

$\mathscr{A}_1$ is the piece corresponding to $f = 0$,

$$\mathscr{A}_1 = 4\pi\alpha^3 \int_0^\tau \int_0^t \mathrm{d}q_t \cdot W_\alpha(q_t - q_s, t - s)\, \mathrm{d}q_s \tag{4.19}$$

with the photon propagator

$$W_\alpha(x, t) = \int_{\mathbb{R}^3} \mathrm{d}k |\hat{\varphi}(\alpha^2 k)|^2 \frac{1}{2\omega(k)} \mathrm{e}^{\mathrm{i}k\cdot x\alpha} \mathrm{e}^{-\omega(k)|t|} Q(k) \tag{4.20}$$

and $Q(k) = 1\!\!1 - |\hat{k}\rangle\langle\hat{k}|$, the transverse projection. Equation (4.19) is an iterated Ito integral. It avoids the diagonal $\{s = t\}$ in accordance with the Wick ordering $::$. $\mathscr{A}_3$ reflects the term coming from $W(f)$,

$$\mathscr{A}_3 = \int_{\mathbb{R}^3} \mathrm{d}k \frac{1}{\omega}(1 + \mathrm{e}^{-\omega\tau}) \hat{f}^*(k) \cdot Q(k) \hat{f}(k) \,. \tag{4.21}$$

Note that $\mathscr{A}_3$ does not depend on q_t and α. Finally, the cross term $\mathscr{A}_2$ reads

$$\mathscr{A}_2 = -\mathrm{i}\sqrt{4\pi}\alpha^{3/2} \int_0^\tau \int_{\mathbb{R}^3} \mathrm{d}k\, \hat{\varphi}(\alpha^2 k) \frac{1}{\sqrt{2\omega}} \mathrm{e}^{\mathrm{i}k\cdot q_t\alpha} \left(\mathrm{e}^{-\omega t} + \mathrm{e}^{-\omega(\tau - t)}\right) \mathrm{d}q_t \cdot Q(k) \hat{f}(k) \,. \tag{4.22}$$

We will argue that $\mathscr{A}_2 \to 0$ and $(q_\tau, \mathscr{A}_1)$ jointly tends to a Gaussian as $\alpha \to 0$. The complete argument uses the martingale central limit theorem and the uniform lower bound on the energy for the control of the exponential moments.[16]

The cross term is small, since for the expectation $\mathbb{E}_0$ with respect to standard Brownian motion starting at $q_0 = 0$ it holds

$$\begin{aligned} \mathbb{E}_0\left(|\mathscr{A}_2|^2\right) &= 4\pi\alpha^3 \int_0^\tau \int_{\mathbb{R}^6} \mathrm{d}k_1 \mathrm{d}k_2\, \hat{\varphi}(\alpha^2 k_1)\hat{\varphi}(\alpha^2 k_2)(2|k_1|2|k_2|)^{-1/2} \\ &\qquad \times \mathrm{e}^{-(\alpha^2 \frac{1}{2}(k_1+k_2)^2 + |k_1| + |k_2|)t} \hat{f}(k_1) \cdot Q(k_1) Q(k_2) \hat{f}(k_2) \\ &\le \alpha\pi \|\hat{\varphi}\omega^{-1}\|^2 \|\hat{f}\|^2 \,. \end{aligned} \tag{4.23}$$

Ignoring the cross term one arrives at

$$\left\langle \phi \otimes W(f)\Omega, \mathrm{e}^{-\tau T_{1,\alpha}} \phi \otimes W(f)\Omega \right\rangle = \mathbb{E}_{\mathrm{W}}\left(\phi(q_0)^* \phi(q_\tau)\, \mathrm{e}^{-\mathscr{A}_1}\right) \mathrm{e}^{-\mathscr{A}_3} + \mathcal{O}(\alpha) \,. \tag{4.24}$$

It is now convenient to rewrite (4.24) using that $\mathscr{A}_1$ depends only on the increments. Then

$$\left\langle \phi \otimes W(f)\Omega, \mathrm{e}^{-\tau T_{1,\alpha}} \phi \otimes W(f)\Omega \right\rangle = \int_{\mathbb{R}^3} \mathrm{d}k |\hat{\phi}(k)|^2 \mathbb{E}_0\left(\mathrm{e}^{-\mathscr{A}_1} \mathrm{e}^{\mathrm{i}k\cdot q_\tau}\right) \mathrm{e}^{-\mathscr{A}_3} + \mathcal{O}(\alpha) \,, \tag{4.25}$$

To turn to $\mathscr{A}_1$ we first note that $\mathbb{E}_0(\mathscr{A}_1) = 0$ by Ito calculus. Second, we use the Brownian motion scaling $q_t = \alpha q_{t/\alpha^2}$ to rewrite $\mathscr{A}_1$ as

$$\mathscr{A}_1 = 4\pi\alpha \int_{0 \le s < t \le \tau/\alpha^2} \mathrm{d}q_t \cdot W_1(q_t - q_s, t - s)\, \mathrm{d}q_s \,. \tag{4.26}$$

By definition W_1 does not depend on α. W_1 decays as $(t - s)^{-2}$, which should provide enough independence for a central limit theorem hold. Thus the key input is that $(\mathscr{A}_1, q_\tau)$ jointly converge to a Gaussian as $\alpha \to 0$. One checks that

$$\mathbb{E}_0(\mathscr{A}_1 q_\tau) = 0 \,. \tag{4.27}$$

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Hence the assumption is that

$$\lim_{\alpha\to 0} \mathscr{A}_1 = \xi_{\mathrm{G}} \tag{4.28}$$

with ξ_{G} a centered Gaussian random variable independent of q_τ. To complete our argument we compute the variance of $\mathscr{A}_1$,

$$\begin{aligned}
&\mathbb{E}_0\big(\mathscr{A}_1^2\big) \\
&\quad = (4\pi\alpha)^2 \int_{0\le s_1<t_1\le\tau/\alpha^2} \int_{0\le s_2<t_2\le\tau/\alpha^2} \mathbb{E}_0\big(\big(\mathrm{d}q_{t_1}\cdot W_1(q_{t_1}-q_{s_1},t_1-s_1)\,\mathrm{d}q_{s_1}\big) \\
&\qquad\qquad\qquad\qquad \times\big(\mathrm{d}q_{t_2}\cdot W_1(q_{t_2}-q_{s_2},t_2-s_2)\,\mathrm{d}q_{s_2}\big)\big) \\
&\quad = (4\pi\alpha)^2 \int_{0\le s<t\le\tau/\alpha^2} \mathbb{E}_0\big(\mathrm{Tr}\big(W_1(q_t-q_s,t-s)^2\big)\big)\,\mathrm{d}s\mathrm{d}t\,.
\end{aligned} \tag{4.29}$$

Hence

$$\begin{aligned}
\lim_{\alpha\to 0}\mathbb{E}_0\big(\mathscr{A}_1^2\big) &= (4\pi)^2\int_0^\infty \mathrm{d}t \int_{\mathbb{R}^6} \mathrm{d}k_1\mathrm{d}k_2\,|\hat\varphi(k_1)|^2|\hat\varphi(k_2)|^2(2|k_1|2|k_2|)^{-1} \\
&\qquad \times\exp\Big\{-\frac{1}{2}\Big((k_1+k_2)^2+|k_1|+|k_2|\Big)t\Big\}\mathrm{Tr}(Q(k_1)Q(k_2)) \\
&= 2a_0\tau\,.
\end{aligned} \tag{4.30}$$

Returning to (4.24) one concludes that

$$\begin{aligned}
\lim_{\alpha\to 0}\big\langle\phi\otimes W(f)\Omega,\mathrm{e}^{-\tau T_{1,\alpha}}\phi\otimes W(f)\Omega\big\rangle &= \int_{\mathbb{R}^3}\mathrm{d}k\,|\hat\phi(k)|^2\mathbb{E}_0(\mathrm{e}^{\mathrm{i}k\cdot q_\tau})\mathbb{E}(\mathrm{e}^{\xi_{\mathrm{G}}})\,\mathrm{e}^{-\mathscr{A}_3} \\
&= \big\langle\phi\otimes W(f)\Omega,\mathrm{e}^{-\tau((p^2/2)+H_{\mathrm{f}}-a_0)}\phi\otimes W(f)\Omega\big\rangle\,.
\end{aligned} \tag{4.31}$$

If one reintroduces the parameter δ from above, then the variance vanishes provide $\delta > 0$, in accordance with Proposition 4.1.

ACKNOWLEDGMENTS

We thank Stefan Teufel for raising the question on scale dependence, Mario Koppen for discussions on the asymptotic analysis, and Alessandro Pizzo for pointing at Nelson's theorem on resolvent convergence. T.M. was supported by KAKENHI (20554421).

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