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ORIGINAL PAPER

Variational justification of the dimensional-scaling method in chemical physics: the H-atom

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Abstract The dimensional scaling (D-scaling) method first originated from quantum chromodynamics by using the spatial dimension D as an order parameter. It later has found many useful applications in chemical physics and other fields. It enables, e.g., the calculation of the energies of the Schrödinger equation with Coulomb potentials without having to solve the partial differential equation (PDE). This is done by imbedding the PDE in a D-dimensional space and by letting D tend to infinity. One can avoid the partial derivatives and then solve instead a reduced-order finite dimensional minimization problem. Nevertheless, mathematical proofs for the D-scaling method remain to be rigorously established. In this paper, we will establish this by examining the D-scaling procedures from the variational point of view. We show how the ground state energy of the hydrogen atom model can be calculated by justifying the singular

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perturbation procedures. In the process, we see in a more clear and mathematical way confirming (Herschbach J Chem Phys 85:838, 1986 Sect. II.A) how the D-dimensional electron wave function "condenses into a particle," the Dirac delta function, located at the unit Bohr radius.

Keywords Dimensional scaling method · Schrodinger equation · Variational justification

1 Introduction

Asymptotic and perturbative expansions lie at the heart of mathematical methods for equations in physics and chemistry. In the absence of a natural parameter about which an asymptotic or perturbation series can be developed, the space dimension D itself can be used as an "order parameter" for such problems to produce $1/D$-expansions. t'Hooft [17], in his study of quantum chromodynamics where there are many color degrees of freedom, first developed $1/D$-expansions and obtained interesting results about strong interactions. Elsewhere in statistical mechanics and field theory, $1/D$-expansions have also successfully led to nice insights and results [4,5,18–20]. In an expository article by Witten [19], he applied the $1/D$-expansion in a heuristic way to H (hydrogen) and He (helium). In doing so he obtained the ground state energy of H with an error of about 60%. Actually, through more refined analysis, the ground state energy of H in any dimension D and in the large D limit (i.e., $D \to \infty$) can be calculated *exactly*; see Herrick and Stillinger [6], also Herschbach [7]. The D-scaling research has undergone rapid progress [8]. For some more recent work, see, for example,

(i) Svidzinsky et al. [14,15], where the "old quantum mechanical model" of Bohr can now be derived by the asymptotics of the D-scaling method;
(ii) The *quantum number dimensional scaling method*, in Murawski and Svidzinsky [12] and Chen et al. [3];
(iii) A long new survey article by Svidzinsky et al. [16].

D-scaling is now an effective working method for the physicists and chemists to study simple atoms and molecules. It is a truly nice tool to have. Nevertheless, from the mathematical point of view, the *justification through rigorous proofs* is always desirable for any method, which are non-trivial for D-scaling, in particular. In doing the rigorous justification, we can put the method on a firm mathematical foundation. It is

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based on this view that we write this paper. Our way for establishing the mathematical rigor is through examining the *singular perturbation* nature of the D-scaling procedures by *calculus of variations*. In going through this process, we are also able to see the mathematical details as to how the D-dimensional electron wave function condenses into a particle, namely, that the probability unit density function tends to the Dirac delta function, located at the unit Bohr radius.

This paper is organized as follows. In Sect. 2, we revisit the D-scaling method for the H-atom as used in chemical physics. In Sect. 3, we formulate variational problems corresponding to the sequence of change variables related to D-scaling, and prove rigorously that the limit of the scaled energies tends to the correct value. Key lemmas are needed which are put in the Appendix. A brief discussion is given in the Summary.

2 Dimensional scaling method for the hydrogen atom

To make this paper properly self-contained and to prepare for the material in Sect. 3, we recall the D-scaling procedures according to the tutorial lecture in [8, Chap. 1].

The Schrödinger equation for a particle in a central force field with potential $V(r)$, using the atomic units, is given by

$$-\frac{1}{2}\nabla^2\Psi(\boldsymbol{r}) + V(r)\Psi(\boldsymbol{r}) = E\Psi(\boldsymbol{r}), \quad \boldsymbol{r} = (x_1, x_2, x_3) \in \mathbb{R}^3. \tag{2.1}$$

Instead of considering Eq. (2.1) in three-dimension, D-scaling goes by imbedding the problem in D-dimension, that is, Eq. (2.2) will be considered instead:

$$\begin{gathered} -\frac{1}{2}\nabla_D^2\Psi_D(\boldsymbol{r}) + V(r)\Psi_D(\boldsymbol{r}) = E_D\Psi_D(\boldsymbol{r}), \\ \boldsymbol{r} = (x_1, x_2, \ldots, x_D) \in \mathbb{R}^D, r = |\boldsymbol{r}|. \end{gathered} \tag{2.2}$$

Introduce the D-dimensional hyperspherical coordinates:

$$\begin{aligned} x_1 &= r\cos\theta_1 \sin\theta_2 \sin\theta_3 \ldots \sin\theta_{D-1}, \\ x_2 &= r\sin\theta_1 \sin\theta_2 \sin\theta_3 \ldots \sin\theta_{D-1}, \\ x_3 &= r\cos\theta_2 \sin\theta_3 \ldots \sin\theta_{D-1}, \\ &\vdots \quad \vdots \\ x_{D-1} &= r\cos\theta_{D-2} \sin\theta_{D-1}, \\ x_D &= r\cos\theta_{D-1}; \quad r \ge 0, \quad 0 \le \theta_1 < 2\pi, \quad 0 \le \theta_j \le \pi, \quad j = 2, 3, \ldots, D-1. \end{aligned}$$

The Jacobian of the transformation is

$$J_D = r^{D-1}\sin^{D-2}\theta_{D-1}\sin\theta_{D-2}^{D-3}\ldots\sin^2\theta_3\sin\theta_2. \tag{2.3}$$

The D-dimensional Laplacian now can be written as

$$\nabla_D^2 = K_{D-1}(r) - \frac{L_{D-1}^2}{r^2} = K_{D-1}(r) - \frac{1}{r^2}\sum_{1\le i<j\le D}\left(x_i\frac{\partial}{\partial x_j} - x_j\frac{\partial}{\partial x_i}\right)^2, \tag{2.4}$$

where

$$\begin{aligned} K_{D-1}(r) &= \frac{1}{r^{D-1}}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right), \\ L_1^2 &= \frac{\partial^2}{\partial\theta_1^2} \\ &\vdots \\ L_k^2 &= -\frac{1}{\sin^{k-1}\theta_k}\frac{\partial}{\partial\theta_k}\left(\sin^{k-1}\theta_k\frac{\partial}{\partial\theta_k}\right) + \frac{1}{\sin^2\theta_k}L_{k-1}^2, \quad \text{for } 2\le k\le D-1. \end{aligned}$$

Eq. (2.1) then becomes

$$-\frac{1}{2}\left[K_{D-1}(r) - \frac{L_{D-1}^2}{r^2}\right]\Psi_D(\boldsymbol{r}) + V(r)\Psi_D(\boldsymbol{r}) = E_D\Psi_D(\boldsymbol{r}). \tag{2.5}$$

The radial and angular variables in (2.5) are separable:

$$\Psi_D(\boldsymbol{r}) = \Psi_D(r,\Omega_{D-1}) = \psi_D(r)Y_D(\Omega_{D-1}), \tag{2.6}$$

where $\Omega_{D-1} = (\theta_1,\theta_2,\ldots,\theta_{D-1})$ denotes the collective angular variables, and $Y_D(\Omega_{D-1})$ is a hyperspherical harmonic function [1,2] satisfying

$$L_{D-1}^2 Y_D(\Omega_{D-1}) = \ell(\ell+D-2)Y_D(\Omega_{D-1}), \quad \ell = 0,1,2,\ldots. \tag{2.7}$$

Using (2.4), (2.5) and (2.6), we obtain

$$\left[-\frac{1}{2}K_{D-1}(r) + \frac{\ell(\ell+D-2)}{2r^2} + V(r)\right]\psi_D(r) = E_D\psi_D(r). \tag{2.8}$$

We now incorporate the Jacobian factor into ψ by making a further change of variables:

$$\psi_D(r)r^{\frac{D-1}{2}} \equiv \phi_D(r) \tag{2.9}$$

so that $|\phi_D(r)|^2$ becomes the *probability density function* with unit weighting factor:

$$\int_{\mathbb{R}_+} |\psi_D(r)|^2 r^{D-1}\,dr = \int_{\mathbb{R}_+} |\phi_D(r)|^2 dr = 1; \quad \mathbb{R}_+ = (0,\infty). \tag{2.10}$$

Upon using (2.9), (2.8) becomes

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{\Lambda(\Lambda+1)}{2r^2}+V(r)\right]\phi_D(r)=E_D\phi_D, \tag{2.11}$$

where

$$\Lambda=\ell+\frac{1}{2}(D-3),\quad D=3,4,5,\ldots,\ell=0,1,2,\ldots\,. \tag{2.12}$$

Henceforth, we specialize mainly to the hydrogen atom, where $V(r)$ in (2.1) is $-1/r$, i.e., we consider

$$-\frac{1}{2}\nabla^2\Psi(\boldsymbol{r})-\frac{1}{r}\Psi(\boldsymbol{r})=E\Psi(\boldsymbol{r}),\quad \boldsymbol{r}=(x_1,x_2,x_3)\in\mathbb{R}^3. \tag{2.13}$$

Then (2.11) becomes

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{\Lambda(\Lambda+1)}{2r^2}-\frac{1}{r}\right]\phi_D(r)=E_D\phi_D(r). \tag{2.14}$$

We can now see that the spatial dimension D is a natural parameter in Λ in (2.12) and, thus, in Eq. (2.11). An expansion in terms of $1/D$ can now be envisaged.

Remark 1 There are several *equivalent* variants for performing the $1/D$ asymptotic expansion for large D; see [7,9,13], e.g.; the scalings used in [7, Eqs. (10)–(13a), p. 839] are

$$r_s=\frac{1}{\Lambda(\Lambda+1)}r,\quad E_s=\Lambda(\Lambda+1)E_D, \tag{2.15}$$

(the subscript s above means "scaled" (variable)) while those used in [13, p. 418] are (in our current notation)

$$r_s=\frac{1}{(2\Lambda-a)^2}r,\quad E_s=(2\Lambda-a)^2E_D, \tag{2.16}$$

for some a to be further chosen later.

Both (2.15) and (2.16), after a proper $\frac{1}{D}$-expansion, will lead to the *exact* value of the ground state energy. In fact, any scaling factor $f(D)$ in the form

$$f(D)=\frac{1}{D^2}\left(A_0+\frac{A_1}{D}+\frac{A_2}{D^2}+\cdots\right);\quad (A_0>0), \tag{2.17}$$

such that

$$r_s=f(D)r,\quad E_s=[f(D)]^{-1}E_D$$

will work. □

Remark 2 Denote the ground state of (2.13) as $\Psi_0(\boldsymbol{r})$. Then it is known that $\Psi_0(\boldsymbol{r})$ is radially symmetric, depending only on $r(=|\boldsymbol{r}|)$:

$$\Psi_0(\boldsymbol{r}) = \frac{1}{2\sqrt{\pi}} e^{-r}, \quad E_0 = -\frac{1}{2}. \tag{2.18}$$

For the hydrogen atom in D-dimension, Eq. (2.13) becomes

$$\begin{aligned} &-\frac{1}{2}\nabla_D^2 \Psi_D(\boldsymbol{r}) - \frac{1}{r}\Psi_D(\boldsymbol{r}) = E_D \Psi_D(\boldsymbol{r}), \\ &\boldsymbol{r} = (x_1, x_2, \ldots, x_D) \in \mathbb{R}^D, \, D = 3, 4, 5, \ldots . \end{aligned} \tag{2.19}$$

Let us denote the ground state of (2.19) as $\Psi_{D,0}(\boldsymbol{r})$. Then it is known [8, p. 13] that

$$\Psi_{D,0}(\boldsymbol{r}) = \frac{2^D}{\sqrt{(D-1)^D (D-1)! \omega_D}} e^{-\frac{2r}{D-1}}, \tag{2.20}$$

$$E_{D,0} = -\frac{2}{(D-1)^2} = \frac{4}{(D-1)^2} E_0, \tag{2.21}$$

$$\int_{\mathbb{R}^D} |\Psi_{D,0}|^2 \, d\boldsymbol{r} = 1, \tag{2.22}$$

where ω_D is the area of the unit sphere $\mathbb{S}^{D-1}$ in D-dimension, given by

$$\omega_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}, \quad (\Gamma: \text{ the gamma function}). \qquad \square$$

At this point, by observing (2.20) and (2.21), we see that the following scalings

$$r_s \equiv \frac{4}{(D-1)^2} r, \quad E_s = \frac{(D-1)^2}{4} E, \tag{2.23}$$

are actually *exact* for any dimension $D \geq 3$. We call the above the "hydrogenic D-scaling." Its use will somehow make our subsequent calculations much more *concise*, so let us use (2.23) in lieu of (2.15)–(2.17) from now on. Then (2.14) becomes

$$\left[-\frac{2}{(D-1)^2} \frac{d^2}{dr_s^2} + \frac{2\Lambda(\Lambda+1)}{(D-1)^2} \frac{1}{r_s^2} - \frac{1}{r_s} \right] \phi_D = E_s \phi_D. \tag{2.24}$$

By letting $D \to \infty$, and using (2.12), we have

$$\lim_{D\to\infty} \frac{2\Lambda(\Lambda+1)}{(D-1)^2} = \frac{1}{2}, \tag{2.25}$$

so (2.24) becomes

$$\left(\frac{1}{2r_s^2} - \frac{1}{r_s}\right)\phi_\infty = E_s\phi_\infty. \tag{2.26}$$

The calculation of the ground state energy now becomes

$$\min_{r_s>0} E_s = \min_{r_s>0}\left(\frac{1}{2r_s^2} - \frac{1}{r_s}\right). \tag{2.27}$$

The minimum thus happens at

$$\frac{d}{dr_s}\left(\frac{1}{2r_s^2} - \frac{1}{r_s}\right) = 0 \Rightarrow r_s = 1,$$

and therefore

$$\min_{r_s>0} E_s = \left(\frac{1}{2r_s^2} - \frac{1}{r_s}\right)\Big|_{r_s=1} = \frac{1}{2} - \frac{1}{1} = -\frac{1}{2}. \tag{2.28}$$

This value $-1/2$ is the *exact ground state energy* of the hydrogen atom (in three-dimension).

The generalization of a PDE from three-dimension to any D-dimension is a relatively straightforward process. However, returning from D-dimension to three-dimension after D tends to infinity is no easy matter in general. This is one of the most fascinating features of D-scaling.

Remark 3 A note on the differential Eq. 2.24 is in order here. The coefficient $-\frac{2}{(D-1)^2}$ of the highest order derivative $\frac{d^2}{dr_s^2}$ is small when D is large. Thus, such a term $-\frac{2}{(D-1)^2}\frac{d^2}{dr_s^2}\phi_D$ constitutes a *singular perturbation*. Usually, a singularly perturbed term may not be cavalierly dropped. For example, in (2.24), if

$$\phi_D(r_s) \sim e^{-Dr_s},$$

then

$$-\frac{2}{(D-1)^2}\frac{d^2}{dr_s^2}\phi_D(r_s) \sim -\frac{2D^2}{(D-1)^2}e^{-Dr_s}$$

and the singularly perturbed term will be equally (or even more) important as (resp., than) the potential terms.

This is an important technical question, which will be resolved in Lemma A.1 in the Appendix. □

Overall, in order to study the calculus of variations procedures for the D-scaling method, we address the key mathematical issues and offer their resolutions as follows:

(i) The uniqueness and rotational invariance of the D-dimensional Schrödinger equation with a central force potential, Eq. (2.2):
$\Rightarrow$ Theorem 3.1;

(ii) The condensation of the (transformed) probability density function $|\phi_D(\boldsymbol{r})|^2$ into the delta distribution $\delta(r-1)$ and the validification of dropping the singular perturbation term:
$\Rightarrow$ Lemma A.1 in the Appendix.

(iii) Calculus of variations procedures to establish the rigor of the limiting process $D \to \infty$:
$\Rightarrow$ Lemma 3.2, Proposition 3.3,..., up to the Main Theorem.

3 Variational justification of the *D*-scaling method

We now proceed to *rigorize* the D-scaling arguments in the preceding section by carefully examining the procedures from the calculus of variations point of view.

The total energy (kinetic and potential energies) of the 3-D hydrogen atom is given by

$$E(\Psi) = \int_{\mathbb{R}^3} \left[\frac{1}{2} \sum_{n=1}^{3} \left| \frac{\partial \Psi}{\partial x_n} \right|^2 - \frac{1}{r} |\Psi|^2 \right] d\boldsymbol{r}. \tag{3.1}$$

The *weak* solutions of the eigenvalue problems of Eq. 2.13 correspond to the critical points of $E(\Psi)$. The ground state $\Psi_0(\boldsymbol{r})$ and ground state energy E_0 given in Eq. 2.18 are the solution to the following minimization problem

$$\inf_{\substack{\Psi \in H^1(\mathbb{R}^3) \\ \int_{\mathbb{R}^3} |\Psi|^2 d\boldsymbol{r} = 1}} E(\Psi), \tag{3.2}$$

where $H^1(\mathbb{R}^D)$ denotes the usual Sobolev space on $\mathbb{R}^D$; here $D = 3$. For the hydrogen atom in D-dimension, define

$$E_D(\Psi) = \int_{\mathbb{R}^D} \left[\frac{1}{2} \sum_{n=1}^{D} \left| \frac{\partial \Psi}{\partial x_n} \right|^2 - \frac{1}{r} |\Psi|^2 \right] d\boldsymbol{r}. \tag{3.3}$$

Thus the critical points of $E(\Psi)$ correspond to the weak solutions of Eq. 2.19. The ground state $\Psi_{D,0}(\boldsymbol{r})$ and ground state energy $E_{D,0}$ given in (2.20) and (2.21) are the solution to the following minimization problem

$$\inf_{\substack{\Psi \in H^1(\mathbb{R}^D) \\ \int_{\mathbb{R}^D} |\Psi|^2 d\boldsymbol{r} = 1}} E_D(\Psi), \tag{3.4}$$

Remark 4 For the information and benefit of the reader who are not mathematicians, we briefly explain the concept of *weak solutions*. A partial differential equation such as (2.1) or (2.2) may not have infinitely differentiable, i.e., C^∞ solutions on the entire space. One of the main reasons is that the potential V may have singularities. For an atom or molecule, the occurrences of *cusps* in the wave function Ψ is well known. Thus, even though the wave function Ψ is continuous, its first order partial derivatives fail to be continuous at the locations where Ψ has cusps. So the first-order partial derivatives $\frac{\partial \Psi}{\partial x_i}$ is only "piecewise" continuous. The same can be said about the second-order partial derivatives $\partial^2\Psi/\partial x_i \partial x_j$. Therefore, Eqs. (2.1) or (2.2) are *not satisfied by* Ψ *pointwise everywhere* in the entire space. However, a function Ψ may satisfy (2.1) or (2.2) *in the sense of calculus of variations*, i.e.,

$$\partial E_D(\Psi) \cdot v = \int \left[\frac{1}{2}\nabla\Psi \cdot \nabla v + V\Psi v\right] d\boldsymbol{r} = E \int \Psi v \, d\boldsymbol{r}$$

for all test functions v, i.e., for all C^∞-smooth functions v on $\mathbb{R}^D$ with compact support. Such a Ψ is called a *weak solution*. For "strongly elliptic" equations such as the Schrödinger equation, a weak solution will also be a "strong solution", i.e., one with the maximal regularity (i.e., integrability and differentiability). □

By using the D-dimensional hyperspherical coordinates introduced in Sect. 2, the total energy $E_D(\Psi)$ defined in (3.3) is then given by

$$E_D(\Psi) = \int\limits_{\mathbb{R}_+ \times \mathbb{S}_{D-1}} \left\{ \frac{1}{2}\left[\left|\frac{\partial \Psi}{\partial r}\right|^2 + \frac{1}{r^2}\sum_{n=1}^{D-1} \frac{1}{\prod_{k=n+1}^{D-1}\sin^2\theta_k}\left|\frac{\partial\Psi}{\partial\theta_n}\right|^2\right] - \frac{1}{r}|\Psi|^2 \right\} J_D d\Omega_{D-1} dr, \tag{3.5}$$

where $\Omega_{D-1} = [0, 2\pi] \times [0, \pi]^{D-2}$, $\prod_{k=D}^{D-1} \sin^2\theta_k \equiv 1$, and J_D is as introduced in Sect. 2. Thus the critical points of $E_D(\Psi)$ correspond to the weak solutions of Eq. 2.5. It is well known that (e.g., [11]) Eq. 2.7 admits $M_{\ell,D} = \dfrac{(2\ell + D - 2)(\ell + D - 3)!}{\ell!(D-2)!}$ linearly independent solutions, and $L^2(\mathbb{S}^{D-1}) = \oplus_{\ell=0}^{\infty} H^\ell(\mathbb{S}^{D-1})$, where $H^\ell(\mathbb{S}^{D-1})$ is the solution space of Eq. 2.7. Let $\{Y_{\ell m}(\Omega_{D-1})\}_{m=0}^{M_{\ell,D}}$ denote an orthonormal basis of $H^\ell(\mathbb{S}^{D-1})$ for each $\ell = 0, 1, 2, \ldots$. Then $\{Y_{\ell m}(\Omega_{D-1})\}$ forms an orthonormal basis for $L^2(\mathbb{S}^{D-1})$.

We will first need the following uniqueness theorem about the rotational symmetry of the ground state in a central force field.

Theorem 3.1 (Uniqueness) (Lieb and Loss [10, p. 280]) *Let* $\Psi_0 \in H^1(\mathbb{R}^D)$ *be a minimizer for*

$$\mathcal{E}(\Psi) \equiv \int\limits_{\mathbb{R}^D} \left\{\frac{1}{2}|\nabla\Psi|^2 + V(\boldsymbol{r})\Psi\right\} d\boldsymbol{r},$$

i.e., $\mathcal{E}(\Psi_0) = E_0 > -\infty$ *and* $\|\Psi_0\|_{L^2(\mathbb{R}^D)} = 1$, *under the assumptions that* $V \in L^1_{loc}(\mathbb{R}^D)$, V *is locally bounded from above, and that* $V|\Psi_0|^2$ *is summable. Then* Ψ_0 *satisfies the Schrödinger equation*

$$-\frac{1}{2}\nabla\Psi + V(\cdot)\Psi = E\Psi \quad \text{on} \quad \mathbb{R}^D$$

with $E = E_0$, $\Psi_0 > 0$ *and* Ψ_0 *is unique up to a constant phase.* □

Applying Theorem 3.1 to the functional E_D given in (3.3) and comparing the right-hand sides of (3.3) and (3.5), we see that the ground state $\Psi_{D,0}$ must satisfy

$$\frac{\partial\Psi_{D,0}}{\partial\theta_j} = 0 \quad \text{for} \quad j = 1, 2, \ldots, D-1,$$

i.e., $\Psi_{D,0}(\cdot)$ is a function of r only: $\Psi_{D,0} = \Psi_{D,0}(r)$. Thus, the minimization problem (3.4) reduces to the following problem

$$E_{D,0} = E_D(\psi_{D,0}) = \inf_{\substack{\psi\in F_D \\ \int_{\mathbb{R}_+}|\psi|^2 r^{D-1}dr=1}} E_D(\psi), \tag{3.6}$$

where by setting $\ell = 0$ (because of rotational symmetry from Lemma 3.1) in (2.8), we have

$$E_D(\psi) \equiv \int_{\mathbb{R}_+} \left[\frac{1}{2}\left|\frac{d\psi}{dr}\right|^2 - \frac{1}{r}|\psi|^2\right] r^{D-1}\, dr, \tag{3.7}$$

$$F_D \equiv \left\{\psi:\ \mathbb{R}_+ \longrightarrow \mathbb{R} \,\middle|\, \psi r^{\frac{D-1}{2}} \in L_2(\mathbb{R}_+),\ \frac{d\psi}{dr} r^{\frac{D-1}{2}} \in L_2(\mathbb{R}_+)\right\}, \tag{3.8}$$

$$\psi_{D,0} = \frac{2^D}{\sqrt{(D-1)^D(D-1)!}} e^{-\frac{2r}{D-1}}. \tag{3.9}$$

The set F_D constitutes a Hilbert space with the inner product

$$\langle\psi_1|\psi_2\rangle_{F_D} \equiv \int_{\mathbb{R}_+} \left[\psi_1^*\psi_2 + \left(\frac{d\psi_1}{dr}\right)^* \left(\frac{d\psi_2}{dr}\right)\right] dr;\ \psi_1, \psi_2 \in F_D;$$

$*$: complex conjugate.

Note that the critical points of $E_D(\psi)$ correspond to the solutions of Eq. 2.8 with $\ell = 0$. It is now natural to introduce the following change of variables which corresponds to (2.9) in the D-scaling method:

$$\begin{aligned} \phi(r) &= \psi(r) r^{\frac{D-1}{2}}, \\ \frac{d\psi}{dr} &= -\left(\frac{D-1}{2}\right) r^{-\frac{D+1}{2}}\phi + r^{-\frac{D-1}{2}}\frac{d\phi}{dr}. \end{aligned} \tag{3.10}$$

Then

$$E_D(\psi) = \int\limits_{\mathbb{R}_+} \frac{1}{2}\Bigg[r^{-(D-1)} \left|\frac{d\phi}{dr}\right|^2 - (D-1)r^{-D}\phi\frac{d\phi}{dr} + \frac{(D-1)^2}{4} r^{-(D+1)}|\phi|^2 - 2r^{-D}|\phi|^2 \Bigg] r^{D-1}\, dr$$
$$= \int\limits_{\mathbb{R}_+} \left[\frac{1}{2}\left|\frac{d\phi}{dr}\right|^2 - \frac{(D-1)}{2r}\phi\frac{d\phi}{dr} + \frac{(D-1)^2}{8r^2}|\phi|^2 - \frac{1}{r}|\phi|^2 \right] dr. \tag{3.11}$$

To perform the integration by parts on the second term in (3.11), we need the following lemma.

Lemma 3.2 *Let $D \geq 3$. If a distribution f on $\mathbb{R}^+$ satisfies*

$$f(r)r^{\frac{D-1}{2}} \in L^2(\mathbb{R}_+), \quad f'(r)r^{\frac{D-1}{2}r} \in L^2(\mathbb{R}_+),$$

then $f \in C(\mathbb{R}_+)$ and

$$\lim_{r\to 0^+} f(r)r^{\frac{D-2}{2}} = 0 \quad and \quad \lim_{r\to\infty} f(r)r^{\frac{D-2}{2}} = 0. \qquad \square$$

The proof of Lemma 3.2 is given in the Appendix.

By Lemma 3.2, if $\psi \in F_D$, then $\phi \in C(\mathbb{R}_+)$ and

$$\lim_{r\to 0+} r^{-\frac{1}{2}}\phi(r) = 0, \quad \lim_{r\to\infty} r^{-\frac{1}{2}}\phi(r) = 0.$$

Thus

$$\int\limits_{\mathbb{R}_+} \frac{1}{r}\phi\frac{d\phi}{dr}dr = \frac{1}{2r}\phi^2(r)\Big|_{r=0}^{r=\infty} + \frac{1}{2}\int\limits_{\mathbb{R}_+} \frac{1}{r^2}\phi^2 dr = \frac{1}{2}\int\limits_{\mathbb{R}_+} \frac{1}{r^2}\phi^2 dr. \tag{3.12}$$

Substituting (3.12) into (3.11), we obtain

$$\widetilde{E}_D(\phi) \overset{def}{=} E_D(\psi) = \int\limits_{\mathbb{R}_+} \left[\frac{1}{2}\left(\frac{d\phi}{dr}\right)^2 + \frac{\Lambda(\Lambda+1)}{2r^2}\phi^2 - \frac{1}{r}\phi^2 \right] dr, \tag{3.13}$$

where $\Lambda = \dfrac{D-3}{2}$, and the variational problem (3.6) becomes

$$\inf_{\substack{\phi \in \widetilde{F} \\ \int_{\mathbb{R}_+} |\phi|^2 dr = 1}} \widetilde{E}_D(\phi), \tag{3.14}$$

where

$$\widetilde{F} = \{\phi\colon\ \mathbb{R}_+ \to \mathbb{R} \mid d\phi/dr \in L^2(\mathbb{R}_+), \phi \in L^2(\mathbb{R}_+), \phi/r \in L^2(\mathbb{R}_+)\}, \tag{3.15}$$

Note that $E_D(\psi)$ in (3.13) depends on D, $\widetilde{F}$ in (3.15) is independent of D. $\widetilde{F}$ also constitutes a Hilbert space with the natural inner product

$$\langle \phi_1 | \phi_2 \rangle_{\widetilde{F}} \equiv \int\limits_{\mathbb{R}_+} \left[\phi_1^*(r)\phi_2(r) + \frac{1}{r^2}\phi_1^*(r)\phi_2(r) + \phi_1'^*(r)\phi_2'(r) \right] dr; \quad \phi_1, \phi_2 \in \widetilde{F}.$$

It is easy to show that if $\phi \in \widetilde{F}$, then (3.13) is finite.

We now further re-scale according to (2.23):

$$\begin{aligned} \widetilde{E}_D(\tilde{\phi}) &= \frac{(D-1)^2}{4} \int\limits_{\mathbb{R}_+} \left[\frac{8}{(D-1)^4} \left(\frac{d\tilde{\phi}}{dr_s} \right)^2 + \frac{8}{(D-1)^4} \Lambda(\Lambda+1) \frac{|\tilde{\phi}|^2}{r_s^2} \right. \\ &\quad \left. - \frac{(D-1)^2}{4 r_s} |\tilde{\phi}|^2 \right] dr_s \\ &= \int\limits_{\mathbb{R}_+} \left[\frac{2}{(D-1)^2} \left(\frac{d\tilde{\phi}}{dr_s} \right)^2 + \frac{2\Lambda(\Lambda+1)}{(D-1)^2} \frac{|\tilde{\phi}|^2}{r_s^2} - \frac{|\tilde{\phi}|^2}{r_s} \right] dr_s, \end{aligned} \tag{3.16}$$

where $\tilde{\phi}(r_s) \equiv \phi\left(\frac{(D-1)^2}{4} r_s\right)$.

Proposition 3.3 *For the variational problem*

$$\inf_{\substack{\phi \in \widetilde{F} \\ \int_{\mathbb{R}_+} \phi^2 dr = 1}} \widetilde{E}_D(\phi) \equiv \lambda_D,$$

we have $\lambda_D \geq -(D-1)^2/[8\Lambda(\Lambda+1)]$.

Proof Choose a fixed $\phi_0 \in \widetilde{F}$ satisfying the normalized unit $L^2(\mathbb{R}_+)$ norm. Then

$$\begin{aligned}\widetilde{E}_D(\phi_0) &= \int\limits_{\mathbb{R}_+} \left[\frac{2}{(D-1)^2} \left(\frac{d\phi_0}{dr} \right)^2 + \frac{2\Lambda(\Lambda+1)}{(D-1)^2} \frac{|\phi_0|^2}{r^2} - \frac{|\phi_0|^2}{r} \right] dr \\ &\geq \int\limits_{\mathbb{R}_+} \left[\frac{2\Lambda(\Lambda+1)}{(D-1)^2} \frac{1}{r^2} - \frac{1}{r} \right] |\phi_0|^2 dr \\ &\geq \min_{r\in\mathbb{R}_+} W_D(r) \int\limits_{\mathbb{R}_+} |\phi_0|^2 dr \\ &= \min_{r\in\mathbb{R}_+} W_D(r),\end{aligned}$$

where

$$W_D(r) \equiv \frac{2\Lambda(\Lambda+1)}{(D-1)^2} \frac{1}{r^2} - \frac{1}{r}, \tag{3.17}$$

with a unique minimum happening at

$$W_D'(r_{D,\min}) = 0, \quad r_{D,\min} = \frac{4\Lambda(\Lambda+1)}{(D-1)^2} > 0, \tag{3.18}$$

such that

$$W_D(r_{D,\min}) = -\frac{(D-1)^2}{8\Lambda(\Lambda+1)}. \tag{3.19}$$

The proof is complete. □

Corollary 3.4 *We have*

$$\lim_{D\to\infty} \lambda_D \geq -1/2, \quad \lim_{D\to\infty} r_{D,\min} = 1.$$

Proof Straightforward verification, by using (2.12), (3.18) and (3.19). □

Now, denote

$$\psi_D(r) \equiv \frac{2^D}{\sqrt{(D-1)^D(D-1)!}} e^{-\frac{2r}{D-1}}. \tag{3.20}$$

This $\psi_D(r)$ is related to $\Psi_{D,0}(\boldsymbol{r})$ in (2.20) by dropping the angular factor $(\omega_{D-1})^{-1/2}$. (This angular factor $(\omega_{D-1})^{-1/2}$ is dropped in (3.20) for the obvious reason of normalization requirement, because the angular factor is quotient out in $\inf[E_D(\psi)/\|\phi\|_{L^2(\mathbb{R}_+)}]$.) The function (3.20), after the hydrogenic D-scaling (2.23), becomes

$$\tilde{\phi}_D(r_s) = \frac{(D-1)^{D/2}}{\sqrt{(D-1)!}} r_s^{\frac{D-1}{2}} e^{-(\frac{D-1}{2})r_s}. \tag{3.21}$$

Since r_s is just a dummy variable, we write r_s simply as r. By Lemma A.1 from the Appendix, we have, in the sense of distributions,

$$\lim_{D\to\infty} \tilde{\phi}_D^2(r) = \delta(r-1), \tag{3.22}$$

$$\lim_{D\to\infty} \left[\left(\frac{2}{D-1}\right)\tilde{\phi}'_D(r)\right]^2 = 0, \tag{3.23}$$

where $\delta(r-1)$ is the Dirac delta distribution concentrated at $r=1$.

Proposition 3.5 *For any given* $\varepsilon > 0$*, there exists a positive integer* D_0 *such that*

$$\widetilde{E}_D(\tilde{\phi}_D) \le -\frac{1}{2} + \varepsilon, \text{ for any integer } D \ge D_0. \tag{3.24}$$

Proof Let $\varepsilon_0 > 0$ be given. By (3.22) and (3.23), we can take a small open neighborhood
$(1-\frac{\gamma}{2}, 1+\frac{\gamma}{2})$ of $r=1$ in $\mathbb{R}_+$ such that

$$\begin{aligned}\widetilde{E}_D(\tilde{\phi}_D) &= \int\limits_{\mathbb{R}_+} \left[\frac{1}{2}\left(\frac{2}{D-1}\tilde{\phi}'_D\right)^2 + \frac{2\Lambda(\Lambda+1)}{(D-1)^2}\frac{|\tilde{\phi}_D|^2}{r^2} - \frac{|\tilde{\phi}_D|^2}{r}\right] dr \\ &\le \int\limits_{1-\frac{\gamma}{2}}^{1+\frac{\gamma}{2}} \left[\frac{1}{2}\left(\frac{2}{D-1}\tilde{\phi}'_D\right)^2 + \frac{2\Lambda(\Lambda+1)}{(D-1)^2}\frac{|\tilde{\phi}_D|^2}{r^2} - \frac{|\tilde{\phi}_D|^2}{r}\right] dr + \varepsilon_0\end{aligned} \tag{3.25}$$

for all D sufficiently large. As $D\to\infty$, the RHS of (3.25) satisfies

$$\begin{aligned}&\lim_{D\to\infty} \int\limits_{1-\frac{\gamma}{2}}^{1+\frac{\gamma}{2}} \left[\frac{1}{2}\left(\frac{2}{D-1}\tilde{\phi}'_D\right)^2 + \frac{2\Lambda(\Lambda+1)}{(D-1)^2}\frac{|\tilde{\phi}_D|^2}{r^2} - \frac{|\tilde{\phi}_D|^2}{r}\right] dr + \varepsilon_0 \\ &= \lim_{D\to\infty} \int\limits_{1-\frac{\gamma}{2}}^{1+\frac{\gamma}{2}} \left[\frac{2\Lambda(\Lambda+1)}{(D-1)^2}\frac{|\tilde{\phi}_D|^2}{r^2} - \frac{|\tilde{\phi}_D|^2}{r}\right] dr + \varepsilon_0 \quad \text{(by (3.23))} \\ &= \lim_{D\to\infty} \left[\frac{2\Lambda(\Lambda+1)}{(D-1)^2} - 1\right] + \varepsilon_0 \quad \text{(by (3.22))} \\ &= -\frac{1}{2} + \varepsilon_0,\end{aligned}$$

implying that for D sufficiently large,

$$\int_{1-\frac{\gamma}{2}}^{1+\frac{\gamma}{2}} \left[\frac{1}{2} \left(\frac{2}{D-1} \tilde{\phi}_D' \right)^2 + \frac{2\Lambda(\Lambda+1)}{(D-1)^2} \frac{|\tilde{\phi}_D|^2}{r^2} - \frac{|\tilde{\phi}_D|^2}{r} \right] dr + \varepsilon_0$$
$$\leq -\frac{1}{2} + 2\varepsilon_0, \text{ for all } D \text{ sufficiently large.} \tag{3.26}$$

Combining (3.25) and (3.26), we have

$$\lim_{D\to\infty} \inf_{\substack{\phi\in\widetilde{F} \\ \|\phi\|_{L^2(\mathbb{R}_+)}=1}} \widetilde{E}_D(\phi) \leq \lim_{D\to\infty} \widetilde{E}_D(\tilde{\phi}_D) \leq -\frac{1}{2} + 2\varepsilon_0.$$

Since $\varepsilon_0 > 0$ is arbitrary, by choosing $\varepsilon = 2\varepsilon_0$, we have proved (3.24). □

Main Theorem *We have*

$$\lim_{D\to\infty} \inf_{\substack{\phi\in\widetilde{F} \\ \|\phi\|_{L^2(\mathbb{R}^+)=1}}} \widetilde{E}_D(\phi) = -1/2. \tag{3.27}$$

Proof This is an immediate consequence of Corollary 3.4 and Proposition 3.5, because $\varepsilon > 0$ in (3.24) is arbitrary. □

This value $-1/2$ is the ground state energy of the H-atom (in three-dimension).

Summary. We have rigorously proved in the Main Theorem that as the space dimension D tends to ∞, we have the limit of the "infinite dimensional variational problem" (3.27) equal to $-1/2$, the ground state energy of the three-dimensional hydrogen atom. In the process, we have also confirmed the rigor of Herschbach [7, Section II.A, p. 839] that the probability density $\tilde{\phi}_D^2(r)$, of the ground state wave function $\tilde{\phi}_D$, condenses into a delta function located at the (normalized) Bohr radius 1. This is consistent with the particle view of an electron held by the large chemistry community.

Our proofs in this paper are greatly simplified by the explicit knowledge of the D-dimensional ground state wave function (2.20).

The methods used herein obviously have difficulties to be extended to the helium atom, for example, because separation of variables does not work and no explicit solutions for the helium atom are known. More general methods need to be developed in order to tackle the helium case. In addition, there also exists some hope for a rigorous justification of the D-scaling method for the *excited states* of the H-atom as well as the *quantum harmonic* oscillator. We hope to study them in a sequel.

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Appendix A Proofs of two key Lemmas

A Proof of Lemma 3.2

We first prove that $f(r)r^{\frac{D+1}{2}}$ is continuous on $\mathbb{R}_+$. For any $r_1, r_2 \in \mathbb{R}_+, r_1 < r_2$, we have

$$f(r_2)r_2^{\frac{D+1}{2}} - f(r_1)r_1^{\frac{D+1}{2}} = \int_{r_1}^{r_2} \left[f'(r)r^{\frac{D+1}{2}} + \frac{D+1}{2} f(r)r^{\frac{D-1}{2}} \right] dr.$$

Thus

$$|f(r_2)r_2^{\frac{D+1}{2}} - f(r_1)r_1^{\frac{D-1}{2}}| \leq \int_{r_1}^{r_2} |f'(r)r^{\frac{D-1}{2}} r| dr + \frac{D+1}{2} \int_{r_1}^{r_2} |f(r)r^{\frac{D-1}{2}}| dr$$

$$\leq \left(\int_{r_1}^{r_2} |f'(r)r^{\frac{D-1}{2}}|^2 dr \right)^{1/2} \left(\int_{r_1}^{r_2} r^2\, dr \right)^{1/2} + \frac{D+1}{2} \left(\int_{r_1}^{r_2} |f(r)r^{\frac{D-1}{2}}|^2 dr \right)^{1/2} (r_2 - r_1)^{1/2}$$

$$\leq \left(\int_{\mathbb{R}_+} |f'(r)r^{\frac{D-1}{2}}|^2 dr \right)^{1/2} \left(\frac{r_2^3}{3} - \frac{r_1^3}{3} \right)^{1/2} + \frac{D+1}{2} \left(\int_0^{\infty} |f(r)r^{\frac{D-1}{2}}|^2 dr \right) (r_2 - r_1)^{1/2},$$

and $f(r)r^{\frac{D+1}{2}}$ is continuous on $\mathbb{R}_+$. Hence $f(\cdot)$ is continuous on $\mathbb{R}_+$, also $f(\cdot)r^{\frac{D-2}{2}}$ is continuous on $\mathbb{R}_+$.

Let $\varphi(r) = f'(r)r^{\frac{D-1}{2}}$. Then $\varphi \in L^2(\mathbb{R}_+)$, and

$$f'(r) = \varphi(r)r^{-\frac{D-1}{2}}.$$

For any $\mu_0 > 0, 0 < r < \mu_0 < 1$,

$$f(r) = f(\mu_0) - \int_r^{\mu_0} \varphi(s)s^{-\frac{D-1}{2}}\, ds,$$

$$|f(r)| \leq |f(\mu_0)| + \int_r^{\mu_0} |\varphi(s)|s^{-\frac{D-1}{2}} ds$$

$$\leq |f(\mu_0)| + \left(\int_r^{\mu_0} |\varphi(s)|^2 ds \right)^{1/2} \left(\int_r^{\mu_0} s^{-(D-1)} ds \right)^{1/2}$$

$$= |f(\mu_0)| + \left(\int_r^{\mu_0} |\varphi(s)|^2 ds \right)^{1/2} \left[\frac{1}{D-2} (r^{-(D-2)} - \mu_0^{-(D-2)}) \right]^{1/2}.$$

Since $D \geq 3, 0 < r < \mu_0$,

$$r^{-(D-2)} > \mu_0^{-(D-2)}.$$

Thus

$$|f(r)| \leq |f(\mu_0)| + \left(\int_r^{\mu_0} |\varphi(s)|^2 ds \right)^{1/2} \cdot \left(\frac{1}{D-2} \right)^{1/2} r^{-(\frac{D-2}{2})},$$

$$|f(r)| r^{\frac{D-1}{2}} \leq |f(\mu_0)| r^{\frac{D-1}{2}} + \left(\frac{1}{D-2} \right)^{1/2} \left(\int_r^{\mu_0} |\varphi(s)|^2 ds \right)^{1/2}.$$

Therefore

$$\lim_{r \to 0^+} |f(r)| r^{\frac{D-2}{2}} \leq \left(\frac{1}{D-2} \right)^{1/2} \left(\int_0^{\mu_0} |\varphi(s)|^2 ds \right)^{1/2}.$$

Since $\mu_0 > 0$ is arbitrary, let $\mu_0 \downarrow 0$; we have

$$\lim_{s \to 0^+} |f(r)| r^{\frac{D-2}{2}} = 0.$$

Now, we prove that

$$\lim_{r \to \infty} |f(r)| r^{\frac{D-2}{2}} = 0. \tag{A.1}$$

By assumptions $f(r) r^{\frac{D-1}{2}} \in L^2(\mathbb{R}_+)$, there exists a sequence $\{r_n\} \subseteq \mathbb{R}_+$ such that

$$\lim_{n \to \infty} r_n = \infty, \quad \text{and} \quad \lim_{n \to \infty} f(r_n) r_n^{\frac{D-1}{2}} = 0. \tag{A.2}$$

Thus, for any $\varepsilon > 0$, there exists an $N > 0$ such that

$$|f(r_n) r_n^{\frac{D-1}{2}}| \leq \varepsilon \quad \text{for all } n \geq N.$$

Also, since $f'(\cdot) r^{\frac{D-1}{2}} \in L^2(\mathbb{R}_+)$, there exists an $R_0 > 0$ such that

$$\int_R^{\infty} |f'(r) r^{\frac{D-1}{2}}|^2 dr \leq \varepsilon \quad \text{for any} \quad R > R_0.$$

For any $r \in \mathbb{R}_+, r \geq R_0, n_0 \geq N$, and $r_{n_0} > r$, we have

$$f(r_{n_0}) - f(r) = \int_r^{r_{n_0}} f'(s)ds = \int_r^{r_{n_0}} \varphi(s)s^{-\frac{D-1}{2}}ds,$$

$$\begin{aligned}|f(r)| &\leq |f(r_{n_0})| + \int_r^{r_{n_0}} |\varphi(s)|s^{-\frac{D-1}{2}}ds \\ &\leq |f(r_{n_0})| + \left[\int_r^{r_{n_0}} |\varphi(s)|^2 ds\right]^{1/2} \left[\frac{1}{D-2}(r^{-(D-2)} - r_{n_0}^{-(D-2)})\right]^{\frac{1}{2}} \\ &\leq |f(r_{n_0})| + \left[\int_r^{\infty} |\varphi(s)|^2 ds\right]^{1/2} \cdot \left[\frac{1}{D-2}r^{-(D-2)}\right]^{1/2}.\end{aligned}$$

Hence

$$\begin{aligned}|f(r)|r^{\frac{D-2}{2}} &\leq |f(r_{n_0})|r^{\frac{D-2}{2}} + (D-2)^{-1/2}\left[\int_r^{\infty} |\varphi(s)|^2 ds\right]^{1/2} \\ &\leq |f(r_{n_0})|r_{n_0}^{\frac{D-2}{2}} + (D-2)^{-1/2}\left[\int_r^{\infty} |\varphi(s)|^2 ds\right]^{1/2} \\ &\leq \varepsilon + \frac{\sqrt{\varepsilon}}{\sqrt{D-2}}, \quad \text{for all } r \geq R_0,\end{aligned}$$

and (A.1) is proved. □

Lemma A.1 *Let*

$$\tilde{\phi}_D(r) = \frac{(D-1)^{D/2}}{\sqrt{(D-1)!}} r^{\frac{D-1}{2}} e^{-\frac{D-1}{2}r}, \quad r \in \mathbb{R}_+. \tag{A.3}$$

Then we have, in the sense of distributions,

$$\lim_{D\to\infty} \tilde{\phi}_D^2(r) = \delta(r-1), \quad \lim_{D\to\infty}\left[\frac{2}{D-1}\tilde{\phi}'_D\right]^2 = 0, \tag{A.4}$$

where δ is the delta distribution.

Proof

$$\begin{aligned}&\int_{\mathbb{R}_+} \tilde{\phi}_D^2(r)dr = \frac{(D-1)^D}{(D-1)!}\int_{\mathbb{R}_+} r^{D-1}e^{-(D-1)r}dr\\ &\text{(change of variable } t=(D-1)r) \Rightarrow\\ &= \frac{1}{(D-1)!}\int_{\mathbb{R}_+} t^{D-1}e^{-t}\,dt = \frac{\Gamma(D)}{(D-1)!} = 1, \quad (\Gamma:\ \text{the gamma function}).\end{aligned} \tag{A.5}$$

Let

$$g(r) \equiv \tilde{\phi}_D^2(r) = \frac{(D-1)^D}{(D-1)!}r^{D-1}e^{-(D-1)r}.$$

Then $g(0)=0$,

$$\lim_{r\to\infty} g(r) = 0, \quad g(r) \geq 0 \text{ on } \mathbb{R}_+, \tag{A.6}$$

and

$$\begin{aligned}g'(r) &= \frac{(D-1)^D}{(D-1)!}[(D-1)r^{D-2}e^{-(D-1)r} - (D-1)r^{D-1}e^{-(D-1)r}]\\ &= -\frac{(D-1)^D}{(D-1)!}(D-1)(r-1)r^{D-2}e^{-(D-1)r}.\end{aligned} \tag{A.7}$$

So $g'(r)$ has only one zero at $r=1$, and $g(1)$ is a global maximum on $\mathbb{R}_+$ at $r=1$.

By Stirling's formula,

$$n! \approx e^{-n}n^n\sqrt{2\pi n} \quad \text{as} n \to \infty.$$

Thus

$$\begin{aligned}\lim_{D\to\infty} g(1) &= \lim_{D\to\infty} \frac{(D-1)^D e^{-(D-1)}}{e^{-(D-1)}(D-1)^{D-1}\sqrt{2\pi(D-1)}}\\ &= \lim_{D\to\infty}\sqrt{\frac{D-1}{2\pi}} = \infty.\end{aligned} \tag{A.8}$$

From (A.5), (A.6) and (A.8), it is now routine to establish that for any test function $\tau(\cdot) \in C_c^\infty(\overline{\mathbb{R}}_+)$, we have

$$\lim_{D\to\infty}\int_{\mathbb{R}_+} \tau(r)\phi_D^2(r)dr = \tau(1).$$

Hence

$$\lim_{D\to\infty} g(r) = \lim_{D\to\infty} \tilde{\phi}_D^2(r) = \delta(r-1).$$

So the first limit in (A.4) has been proven. To prove the second limit in (A.4), we note from (A.3) that

$$\tilde{\phi}'_D(r) = \frac{D-1}{2}(r-1)\cdot\frac{(D-1)^{D/2}}{\sqrt{(D-1)!}}r^{\frac{D-3}{2}}e^{-\frac{D-1}{2}r},$$

$$r\phi'_D(r) = \left[\left(\frac{D-1}{2}\right)\cdot(r-1)\right]\cdot\frac{(D-1)^{D/2}}{\sqrt{(D-1)!}}r^{\frac{D-1}{2}}e^{-\frac{D-1}{2}r} \tag{A.9}$$

$$\frac{2}{D-1}\phi'_D(r) = \left(\frac{r-1}{r}\right)\cdot\frac{(D-1)^{D/2}}{\sqrt{(D-1)!}}r^{\frac{D-1}{2}}e^{-\frac{D-1}{2}r}, \quad r\neq 0. \tag{A.10}$$

Since $D \geq 3$, the RHS of (A.10) can be extended as a continuous function at $r = 0$, where it takes a finite value $\frac{2}{D-1}\tilde{\phi}'_D(0)$. Therefore,

$$\frac{2}{D-1}\tilde{\phi}'_D(r) = \frac{r-1}{r}\tilde{\phi}_D(r), \quad r \in \overline{\mathbb{R}}_+.$$

Hence, in the sense of distributions,

$$\begin{aligned}\lim_{D\to\infty}\left[\frac{2}{D-1}\tilde{\phi}'_D(r)\right]^2 &= \lim_{D\to 0}\left[\left(\frac{r-1}{r}\right)^2\tilde{\phi}_D^2(r)\right]\\ &= \left(\frac{r-1}{r}\right)^2\cdot\lim_{D\to\infty}\tilde{\phi}_D^2(r) = \left(\frac{r-1}{r}\right)^2\delta(r-1) = 0\\ &= 0.\end{aligned}$$

The proof is complete. □

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