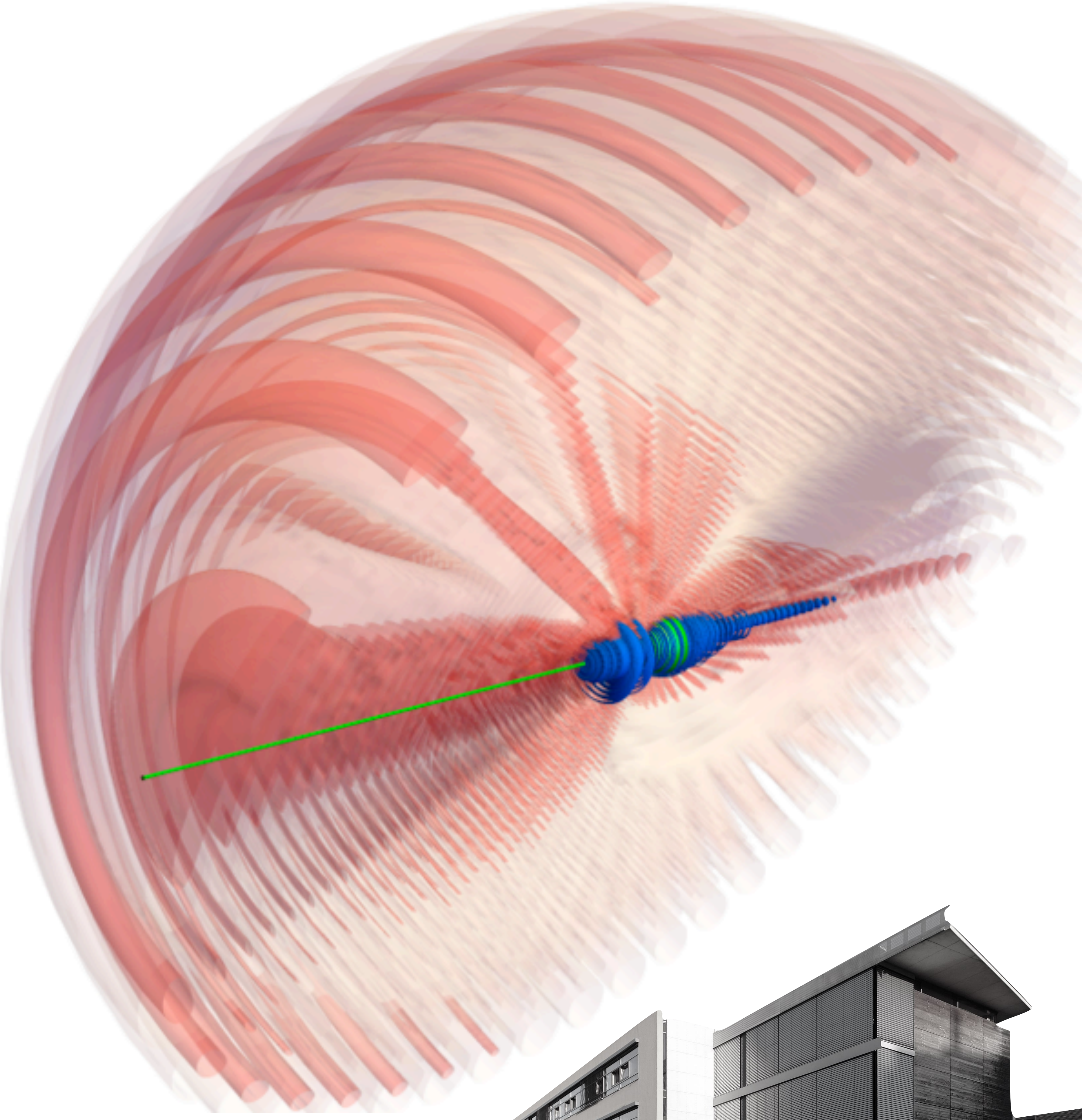
Quantum simulation from first principles

Matt Eiles - MPI-PKS - IMPRS Summer School 2022 - August 28-31

What this is:

- The second of two lectures on quantum simulation from **first principles** - in other words, from a few-body perspective.
- A time to ask plenty of **questions** … and **discuss**!
- A lot of equations, but for ¿good? reason!



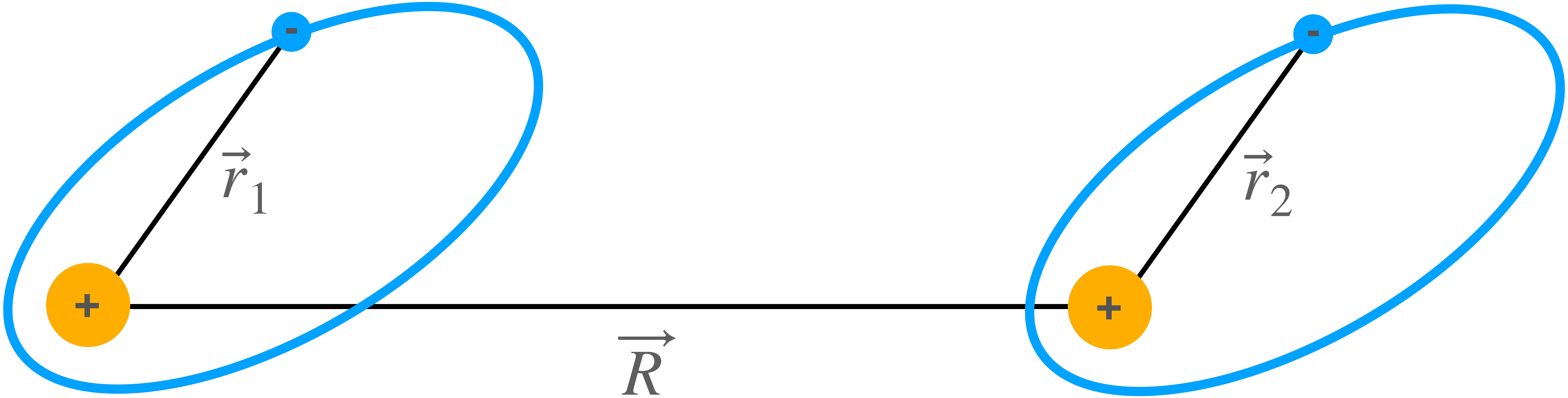
Rough outline:

- **Review!**
- Finish Rydberg atoms
- Return to our "quantum Rydberg atom simulator"

MAX PLANCK INSTITUTE
FOR THE PHYSICS OF COMPLEX SYSTEMS

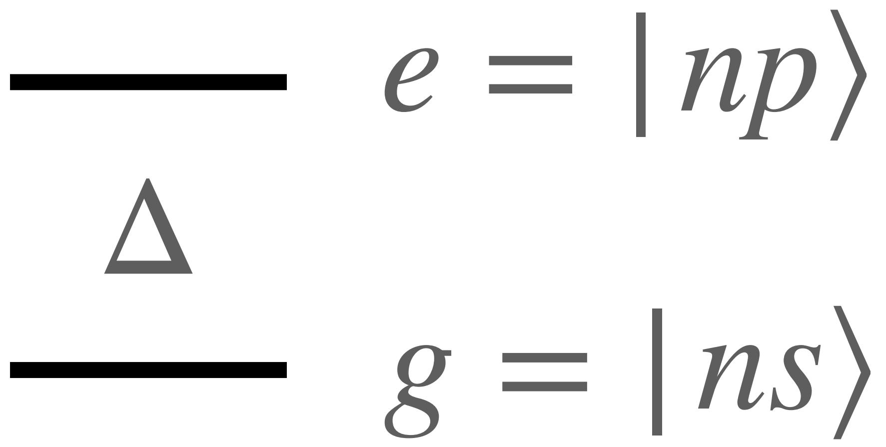
Review: How do two atoms interact at a distance?

$$H = \frac{-\nabla_1^2}{2} - \frac{1}{r_1} + \frac{-\nabla_2^2}{2} - \frac{1}{r_2} + \frac{1}{R} + \frac{1}{|\vec{R} - \vec{r}_1 + \vec{r}_2|} - \frac{1}{|-\vec{R} + \vec{r}_1|} - \frac{1}{|\vec{R} + \vec{r}_2|}$$



$$H \approx \frac{-\nabla_1^2}{2} - \frac{1}{r_1} + \frac{-\nabla_2^2}{2} - \frac{1}{r_2} + \frac{\vec{r}_1 \cdot \vec{r}_2 - 3(\vec{r}_1 \cdot \hat{z})(\vec{r}_2 \cdot \hat{z})}{R^3}$$

Review: How do two atoms interact at a distance?



We take two levels per atom

$$d = \langle ns | r | np \rangle$$

$$0 = \langle ns | r | ns \rangle = \langle ns | r | ns \rangle$$

$$\Longrightarrow \quad \langle ge | r_1 r_2 | eg \rangle = \langle g | r_1 | e \rangle \langle e | r_2 | g \rangle$$

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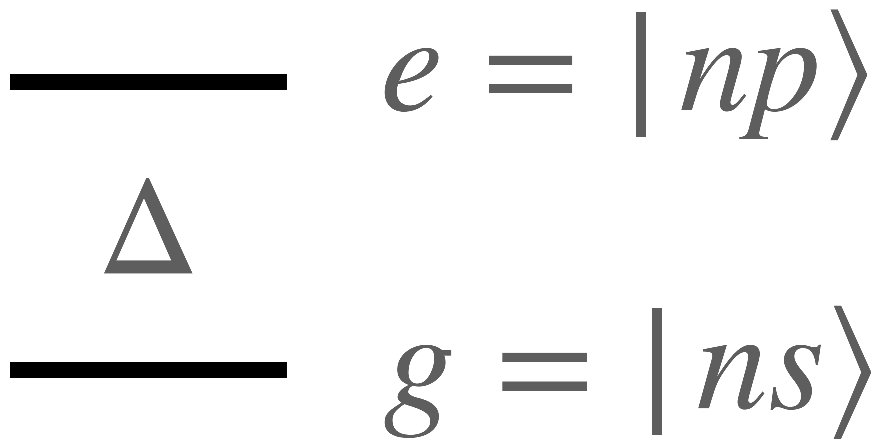

$$e = |np\rangle$$

$$\Delta$$

$$g = |ns\rangle$$

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To form the interaction matrix:

$$\begin{array}{cc} & \begin{array}{cccc} |ee\rangle, & |gg\rangle, & |eg\rangle, & |ge\rangle \end{array} \\ \underline{V}(R) = & \begin{pmatrix} 0 & \frac{d_1 d_2}{R^3} & 0 & 0 \\ \frac{d_1 d_2}{R^3} & 2\Delta & 0 & 0 \\ 0 & 0 & \Delta & \frac{d_1 d_2}{R^3} \\ 0 & 0 & \frac{d_1 d_2}{R^3} & \Delta \end{pmatrix} \end{array}$$

Two regimes:

Upper block: induced vdW interaction:

$$E_+(R) \approx 2\Delta + \frac{(d_1 d_2)^2/(2\Delta)}{R^6}, \quad E_-(R) \approx -\frac{(d_1 d_2)^2/(2\Delta)}{R^6}.$$

Lower block: resonant dipole-dipole interaction:

$$E_+(R) = \Delta + \frac{(d_1 d_2)}{R^3}, \qquad E_-(R) = \Delta - \frac{(d_1 d_2)}{R^3},$$

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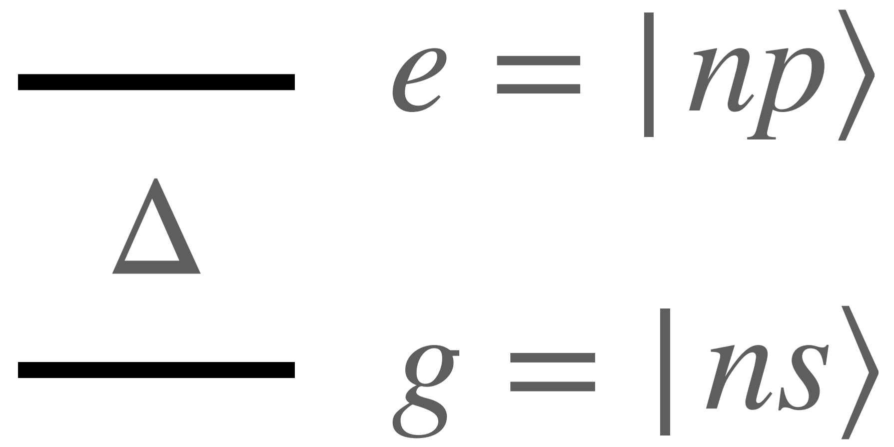

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$$\underline{V}(R) = \begin{array}{c} \begin{matrix} |ee\rangle, & |gg\rangle, & |eg\rangle, & |ge\rangle \end{matrix} \\ \begin{pmatrix} 0 & \frac{d_1 d_2}{R^3} & 0 & 0 \\ \frac{d_1 d_2}{R^3} & 2\Delta & 0 & 0 \\ 0 & 0 & \Delta & \frac{d_1 d_2}{R^3} \\ 0 & 0 & \frac{d_1 d_2}{R^3} & \Delta \end{pmatrix} \end{array}$$

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$$E_+(R) = \Delta + \frac{(d_1 d_2)}{R^3}, \qquad E_-(R) = \Delta - \frac{(d_1 d_2)}{R^3},$$

These interactions tell us how alkali atoms interact at "long range" (before electron clouds overlap)

$$V_{vdW}(n, R) = -\frac{C_6(gs) \cdot n^{11}}{R^6}$$

Quasi-review: Quantum simulator exhibit C

A QS is an experimental system that mimics a **simple model, or a family of simple models** of condensed matter (or high-energy physics, quantum chemistry, etc). A QS should fulfill the following four requirements:

(a) **Relevance**: the simulated models should be of some relevance for applications and/or our understanding of challenges in the areas of physics mentioned above.

(b) **Controllability**: a QS should allow for broad control of the parameters of the simulated model, and for control of preparation, initialization, manipulation, evolution and detection of the relevant observables of the system.

(c) **Reliability**: within some prescribed error, one should be ensured that the observed physics of the QS corresponds faithfully to that of the ideal model whose properties we seek to understand.

(d) **Efficiency**: the QS should solve problems more efficiently than is practically possible on a classical computer.

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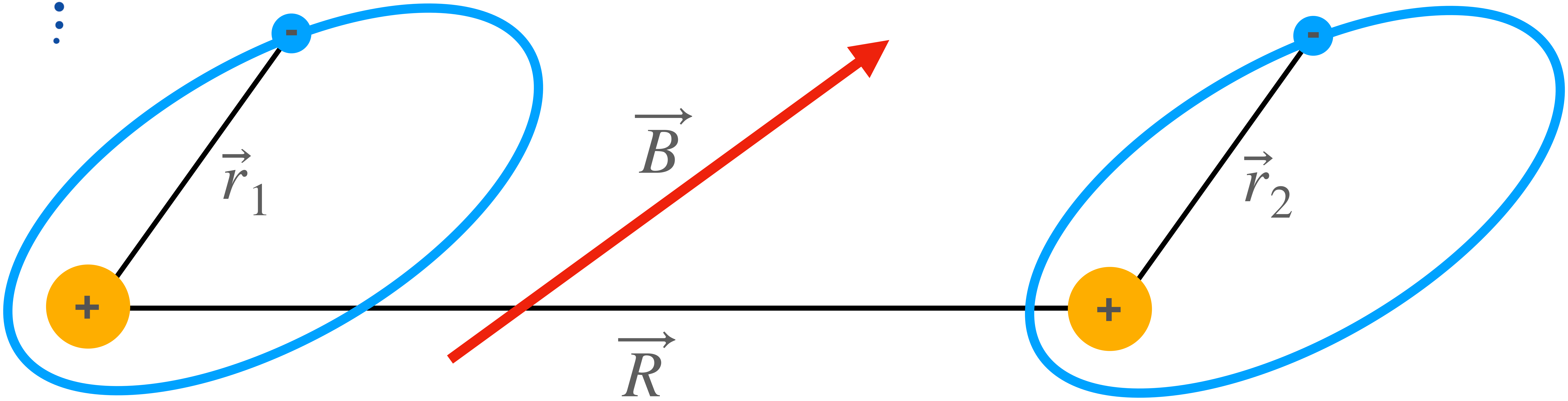
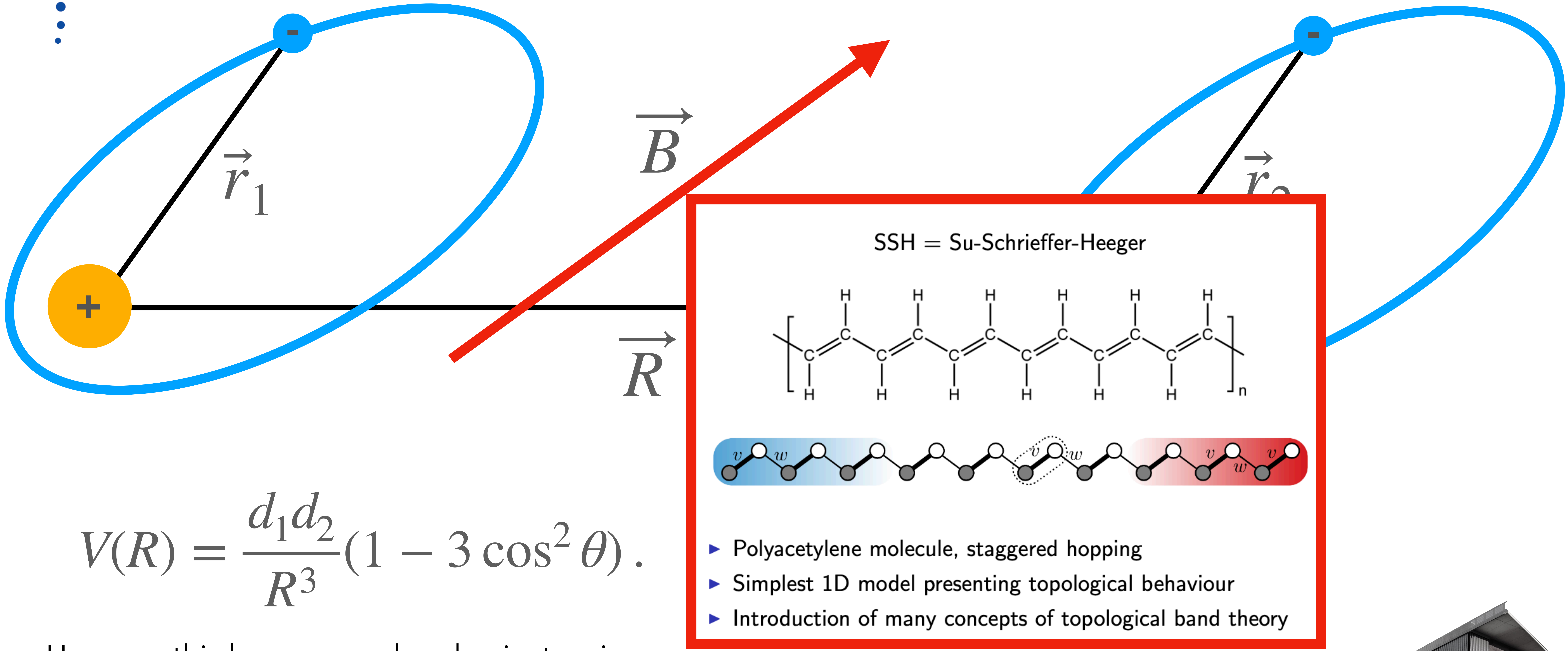


$$V(R) = \frac{d_1 d_2}{R^3}(1 - 3\cos^2\theta)\,.$$

How can this long-ranged and anisotropic interaction be used for quantum simulation?

Quasi-review: Quantum simulator exhibit C



SSH = Su-Schrieffer-Heeger

- Polyacetylene molecule, staggered hopping
- Simplest 1D model presenting topological behaviour
- Introduction of many concepts of topological band theory

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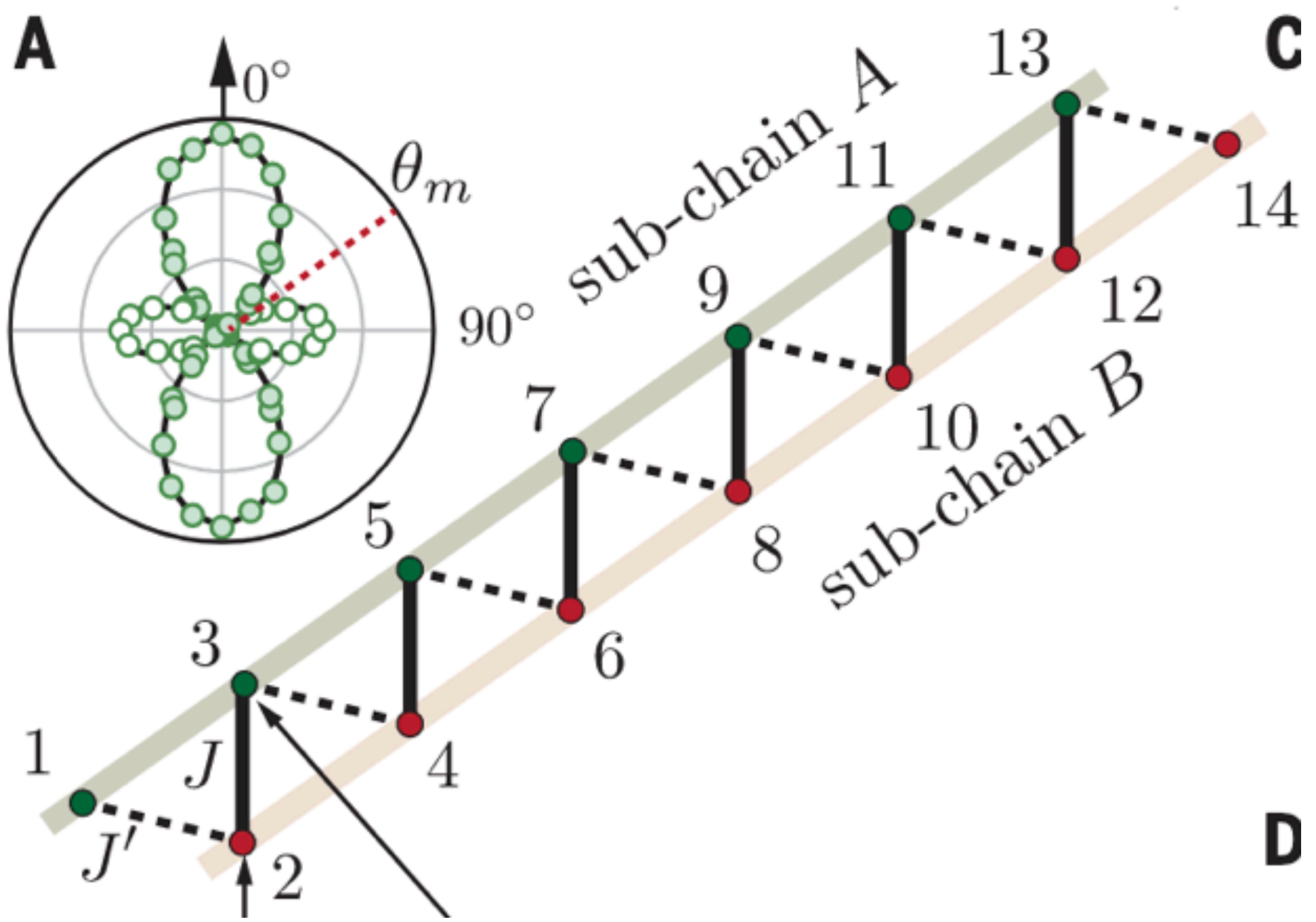

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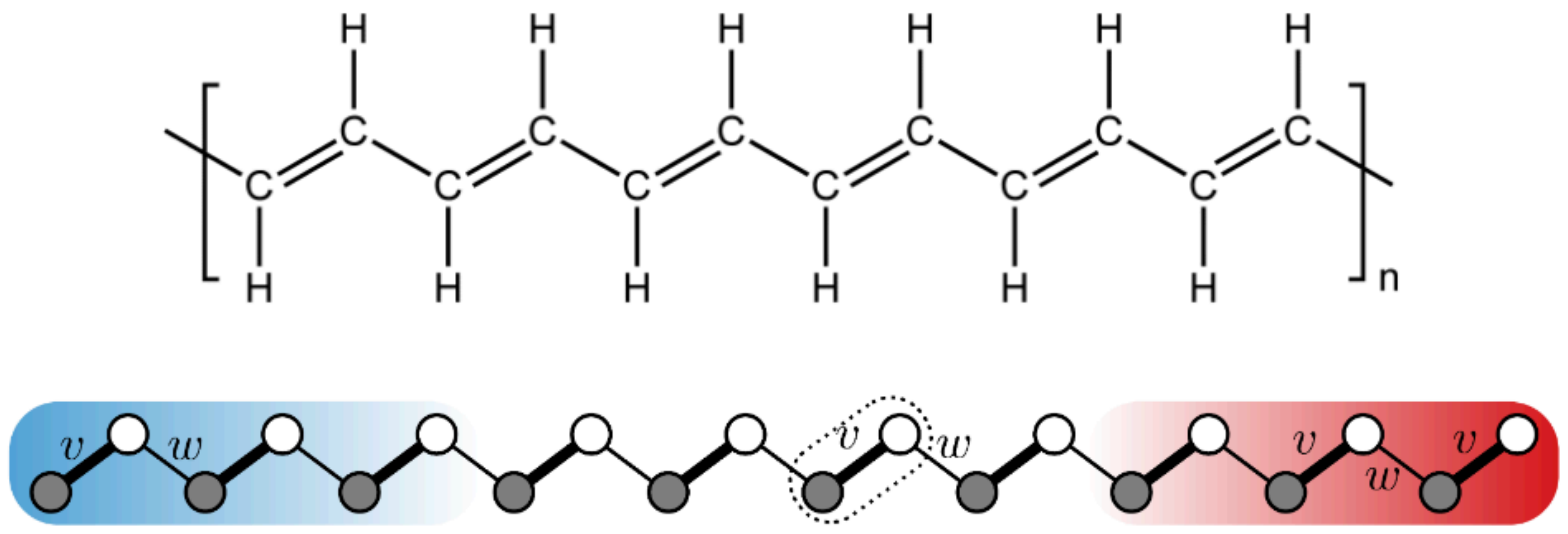

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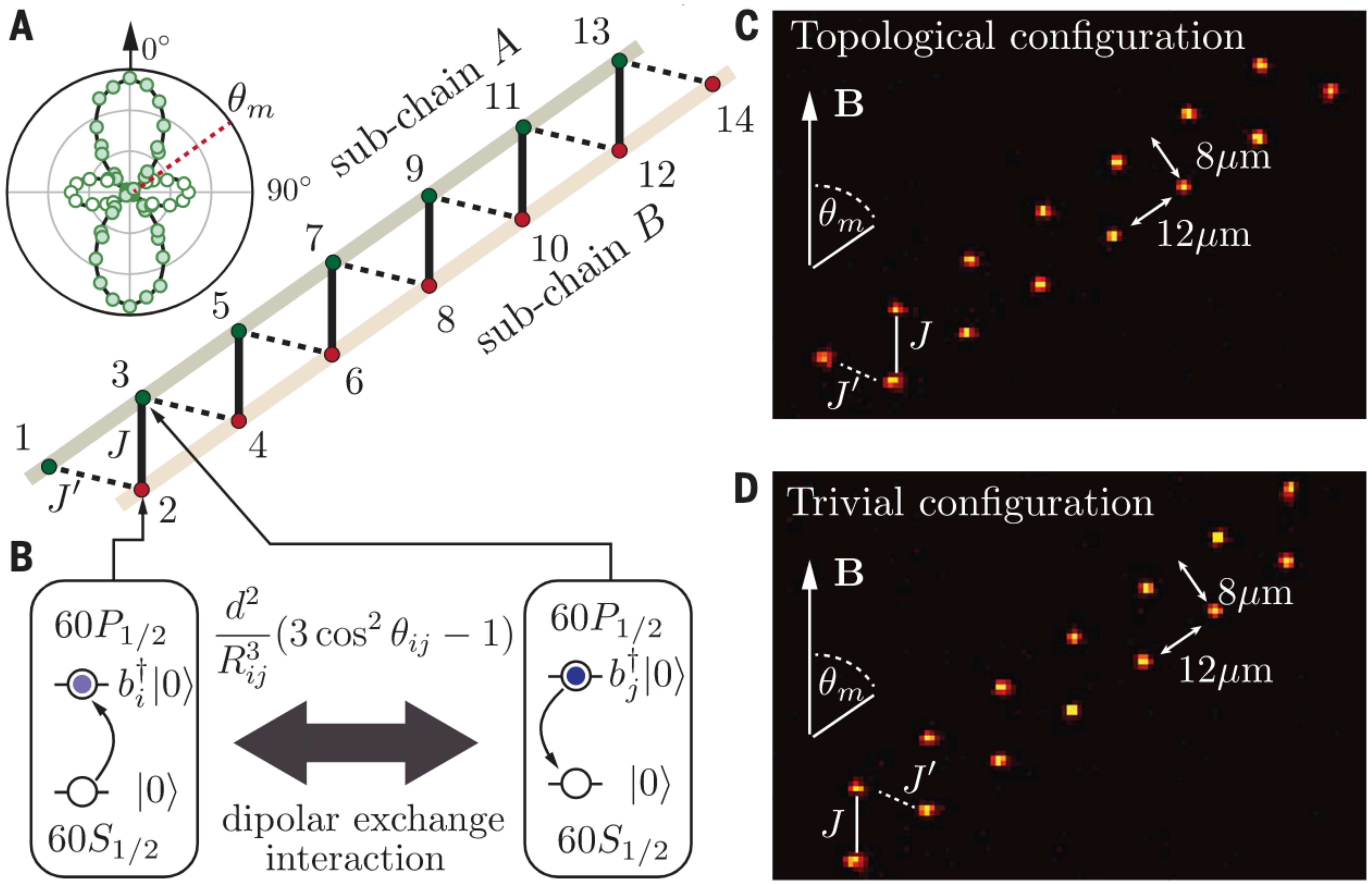

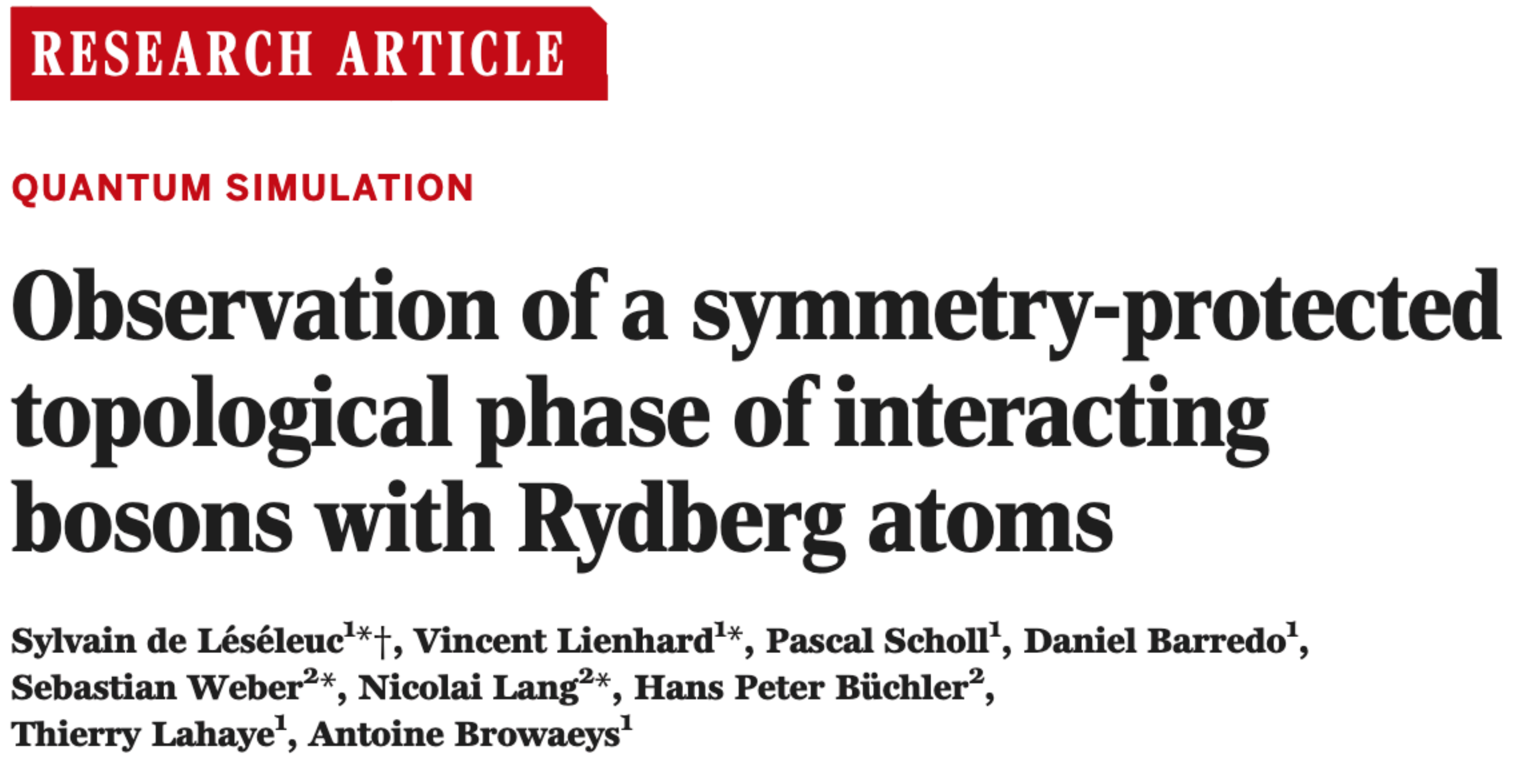
RESEARCH ARTICLE

QUANTUM SIMULATION

Observation of a symmetry-protected topological phase of interacting bosons with Rydberg atoms

Sylvain de Léséleuc[1]*†, Vincent Lienhard[1]*, Pascal Scholl[1], Daniel Barredo[1], Sebastian Weber[2]*, Nicolai Lang[2]*, Hans Peter Büchler[2], Thierry Lahaye[1], Antoine Browaeys[1]

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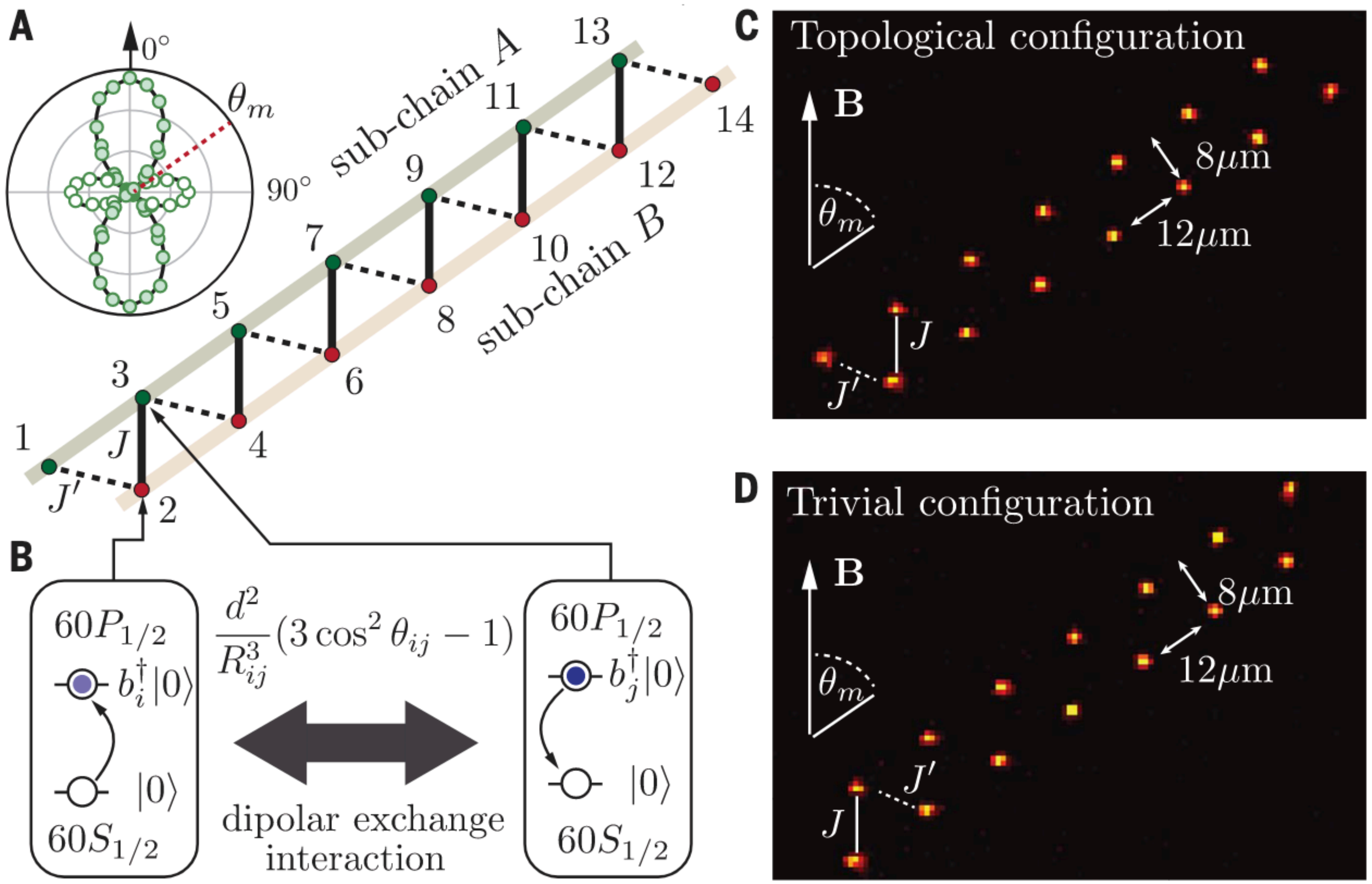

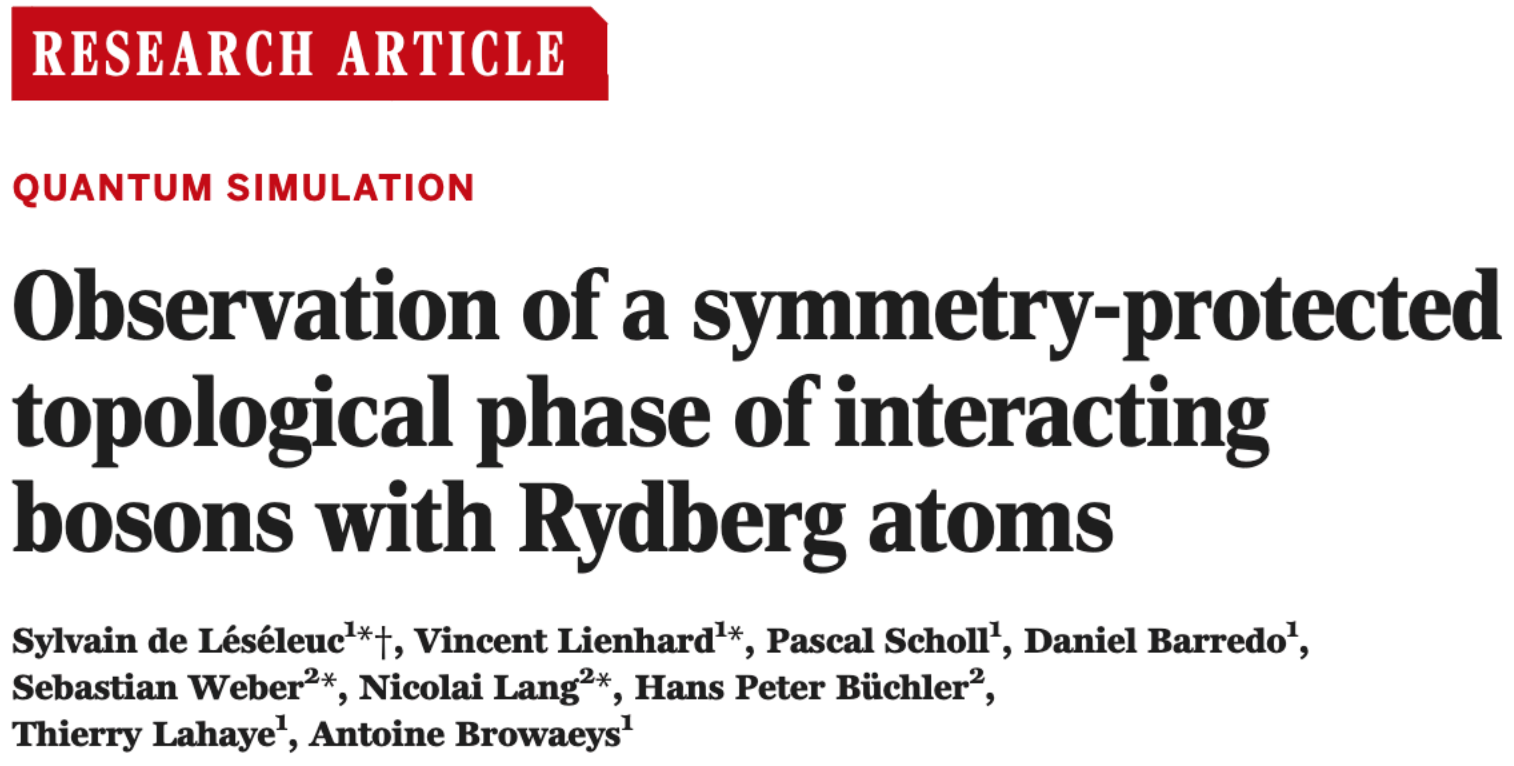

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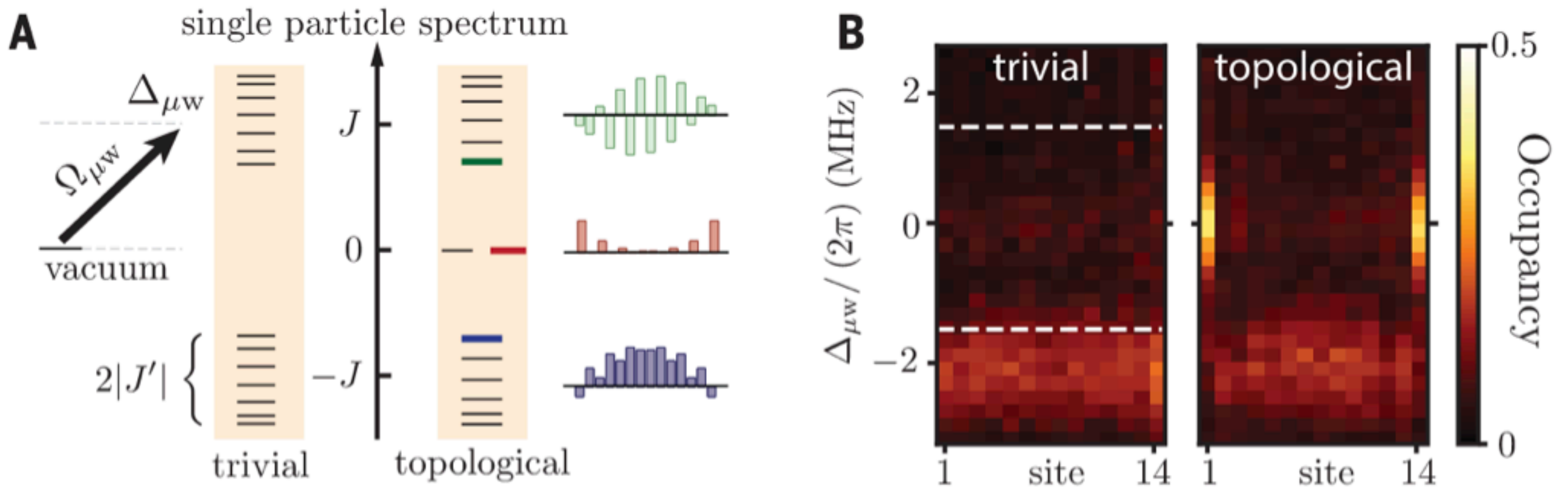


Review: hydrogen atom

We solved this radial SE

$$0 = -\frac{1}{2}u''_{\nu l}(r) + \left(\frac{l(l+1)}{2r^2} - \frac{1}{r} + \frac{1}{2\nu^2}\right)u_{\nu l}(r)$$

By superimposing its two linearly independent solutions

$$u_{\nu l}(r) \sim f_{\nu l}(r) - \tan\delta_{\nu l}g_{\nu l}(r)$$

And using asymptotic forms of these solutions to apply boundary conditions

small r

$$f_{\nu,l}(r) \propto r^{l+1}, \;\; g_{\nu,l}(r) \propto r^{-l}$$

large r

$$f_{\nu,l}(r) \to Ar^{-\nu}e^{r/\nu}\sin\pi(\nu - l) - Br^{\nu}e^{-r/\nu}\cos\pi(\nu - l)$$

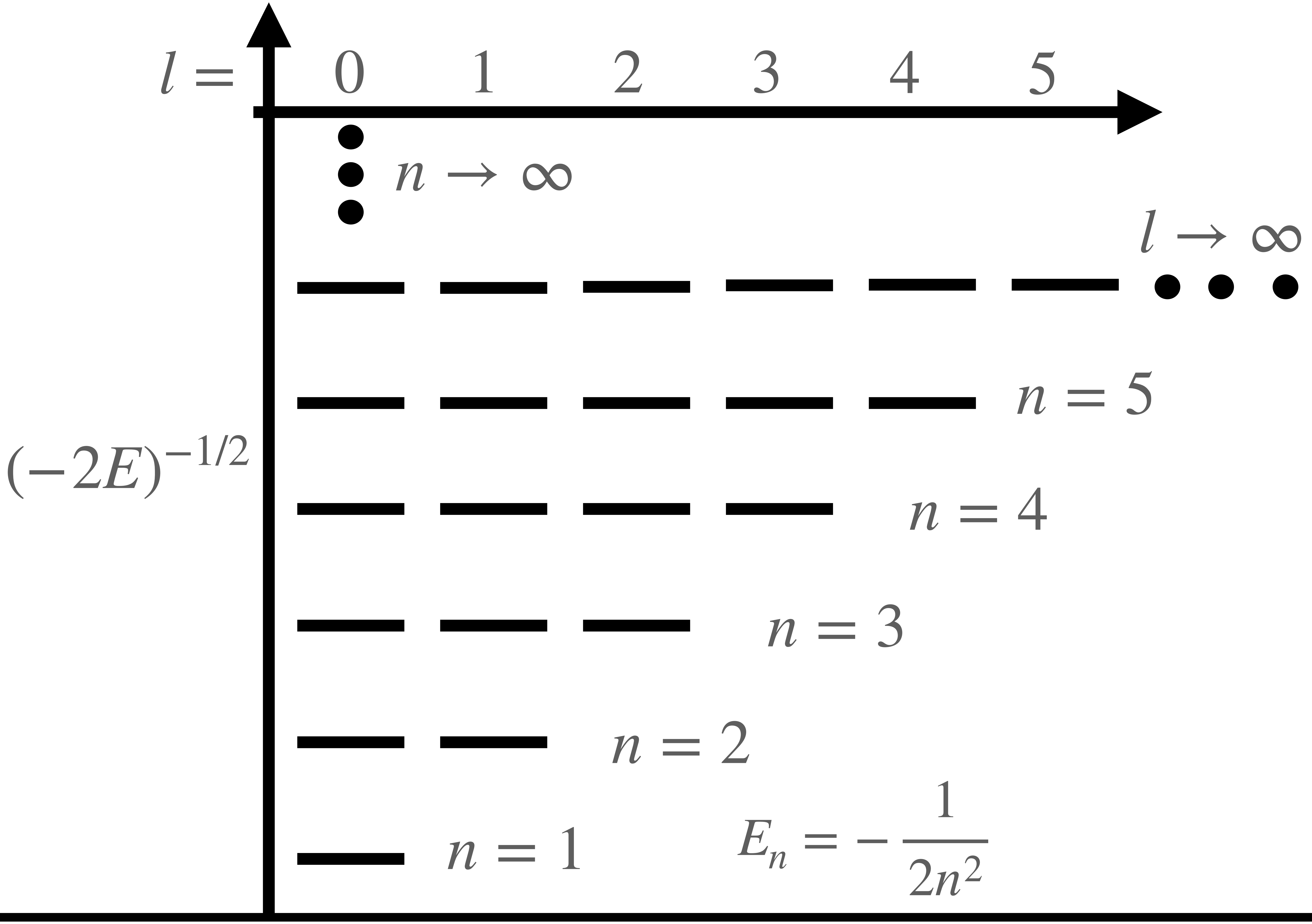
Concluding that:

$$\delta_{\nu l} = 0, \; \nu = n$$

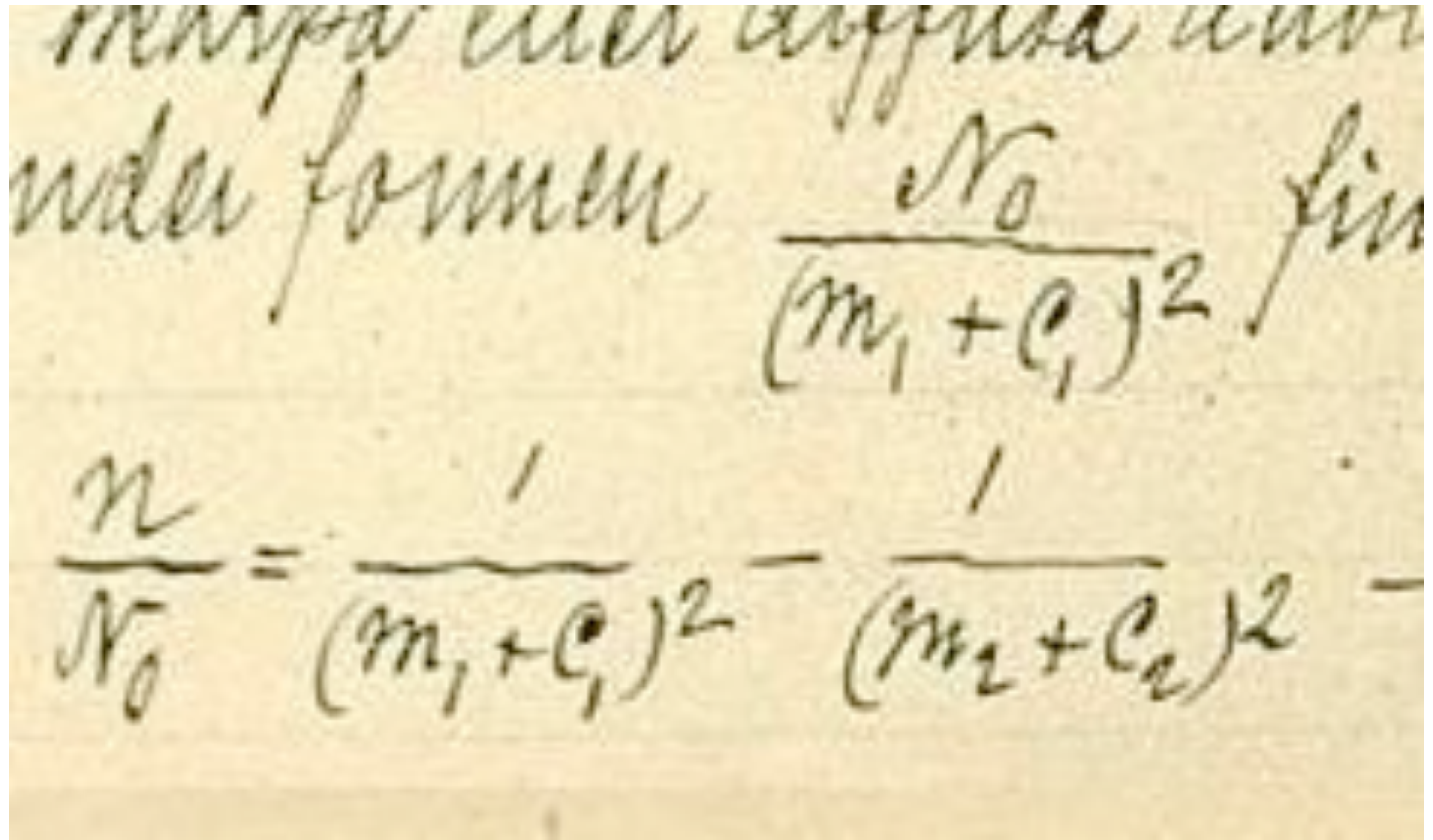
The hydrogen wave function is composed of only the regular solution, and is normalizable only at quantized energy levels…

A quick survey of atomic structure: hydrogen

For hydrogen: an infinite series of highly degenerate bound states



$$E_n = -\frac{1}{2n^2}$$



formen $\frac{N_0}{(m_1+c_1)^2}$

$$\frac{n}{N_0} = \frac{1}{(m_1+c_1)^2} - \frac{1}{(m_2+c_2)^2} -$$

1888: Johannes Rydberg synthesizes empirical results to obtain this formula!

A quick survey of atomic structure: not-hydrogen

Here we will go through a quick overview of the structure of alkali atoms: Li, Na, K, Rb, and Cs, which all have a single valence electron.

Schrödinger equation:

$$0 = \left(-\frac{\nabla^2}{2} - \frac{1}{r} + V_{sr}(r) - E \right) \psi(\vec{r})\,. \quad (R11)$$

The other electrons are tightly confined to a small region around the atom's nucleus: the influence of these electrons can typically be modeled by

$$V_{sr}(r) = -\frac{(Z-1)e^{-a_1 r}}{r} - \frac{\alpha_c}{2r^4}\left(1 - e^{-(r/r_c)^3}\right)^2$$

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These screening and polarization terms fall off rapidly as a function of r, vanishing once r>r0.

Our new radial equation is:

$$0 = -\frac{1}{2}u''_{\nu l}(r) + \left(\frac{l(l+1)}{2r^2} - \frac{1}{r} + V_{sr}(r) - \left(-\frac{1}{2\nu^2} \right) \right) u_{\nu l}(r) \,. \quad (R12)$$

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This is a second-order differential equation, so it has two linearly independent solutions, and u must be a linear combination of these FOR LARGE r!.

$$u_{\nu l}(r) \sim f_{\nu l}(r) - \tan\delta_{\nu l} g_{\nu l}(r), \quad r \geq r_0 . \qquad (R13)$$

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Making sure the wave function and its derivative are continuous functions gives:

$$\left.\frac{F'(r)}{F(r)}\right|_{r=r_0} = \left.\frac{f'_{\nu l}(r) - g'_{\nu l}(r)\tan\delta_{\nu l}}{f_{\nu l}(r) - g_{\nu l}(r)\tan\delta_{\nu l}}\right|_{r=r_0}$$

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$$= \left.\frac{W(f_{\nu l}(r), F(R))}{W(g_{\nu l}(r), F(r))}\right|_{r=r_0}$$

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At a given energy: we have found the phase shift characterizing the “non-Coulomb” parts of our atom. In fact, this phase shift barely changes as a function of energy: all Rydberg states can be characterized by this one number!

Next step: we just have to prevent an explosion in $u_{\nu l}(r) \sim f_{\nu l}(r) - \tan\delta_{\nu l} g_{\nu l}(r), \;\; r \geq r_0\,.$

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$$r \to \infty : \qquad f_{\nu,l}(r) \to A r^{-\nu} e^{r/\nu} \sin \pi(\nu - l) - B r^{\nu} e^{-r/\nu} \cos \pi(\nu - l) \quad (R6)$$

$$g_{\nu,l}(r) \to -A r^{-\nu} e^{r/\nu} \cos \pi(\nu - l) - B r^{\nu} e^{-r/\nu} \sin \pi(\nu - l) \quad (R7)$$

$$u_{\nu,l}(r) \to A r^{-\nu} e^{r/\nu} \sin \pi(\nu - l) \cos \delta_{\nu l} + A r^{-\nu} e^{r/\nu} \cos \pi(\nu - l) \sin \delta_{\nu l} + \text{decaying terms}$$

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$$u_{\nu,l}(r) \to A r^{-\nu} e^{r/\nu} \sin[\pi(\nu - l) + \delta_{\nu l}]$$

$$\implies \nu - l + \frac{\delta_{\nu l}}{\pi} = n_r + 1$$

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Here we will go through a quick overview of the structure of alkali atoms: Li, Na, K, Rb, and Cs, which all have a single valence electron.

And finally:

$$E_{nl} = \frac{-1}{2(n - \mu_l(E))^2}, \quad \mu_l = \delta_l/\pi \, .$$

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Where the quantum defect is (nearly) independent of energy!

We can insert this quantum defect into any of our previously-derived scaling laws!

J. Phys. B: At. Mol. Opt. Phys. **42** (2009) 165004 (6pp)
doi:10.1088/0953-4075/42/16/165004

Precision measurements of quantum defects in the $n\mathrm{P}_{3/2}$ Rydberg states of ^{85}Rb

B Sanguinetti, H O Majeed, M L Jones and B T H Varcoe

School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT, UK

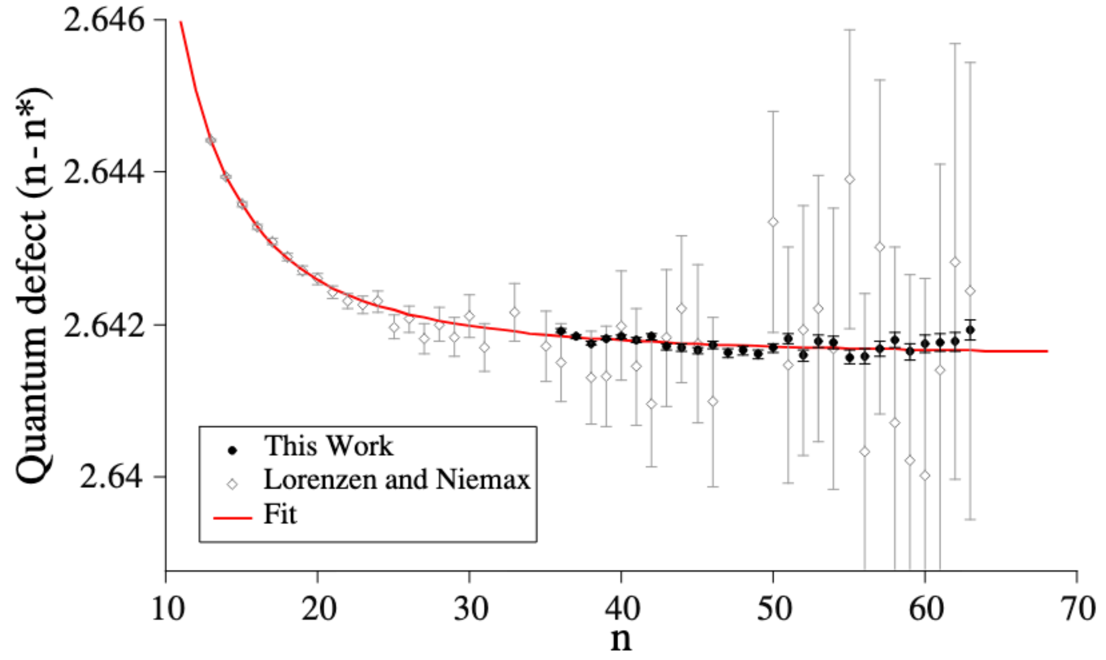


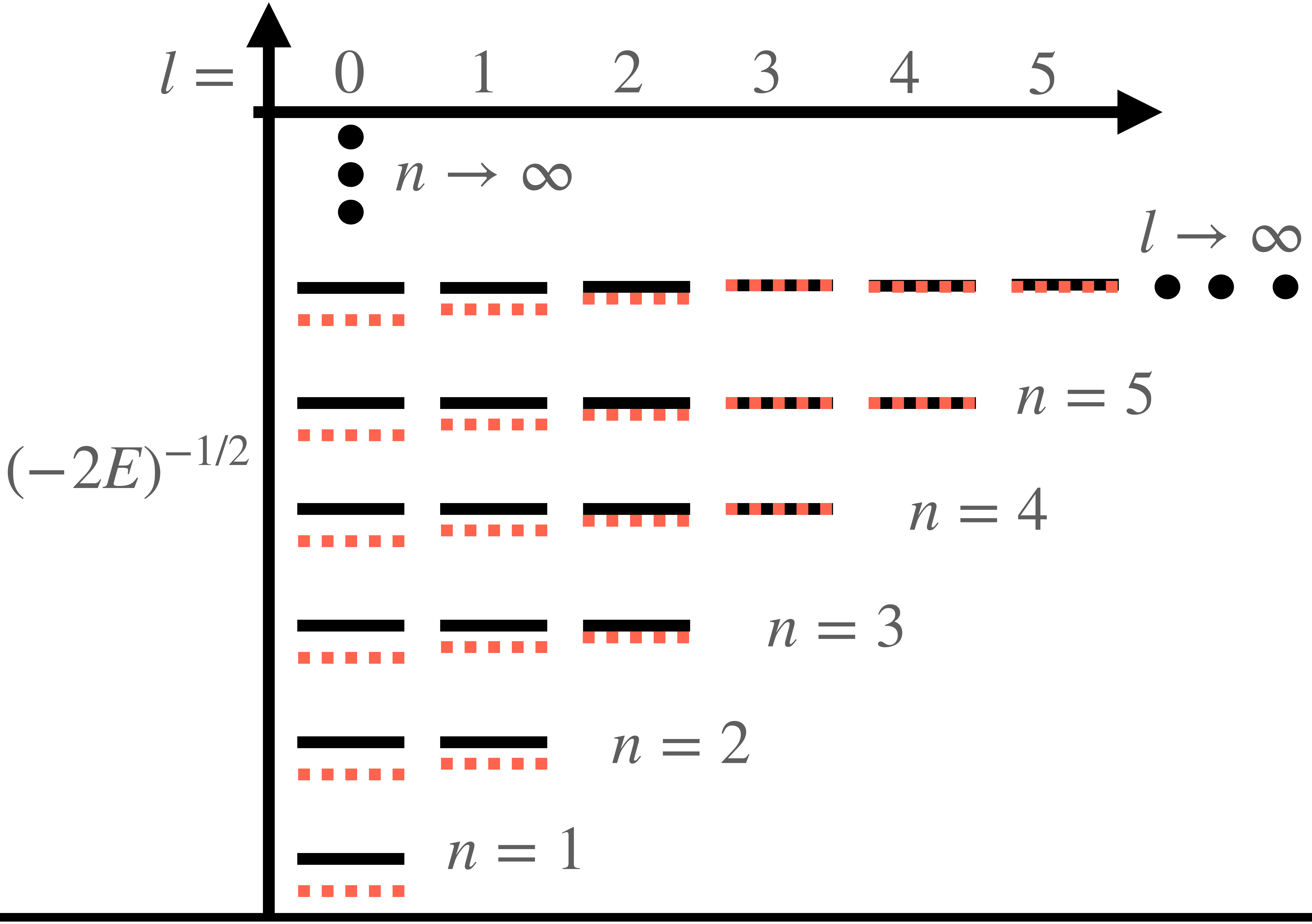
Figure 6. Quantum defects from the three different fitting methods. Data points for $n = 5$ and $n = 6$ were included in the calculations but are not shown, as their quantum defects are off the scale: 2.707 178 and 2.670 358, respectively.

Table 2. Measured frequencies for the $n\mathrm{P}_{3/2}$ states and respective quantum defects. E_n is measured from the centre of mass of the lower and upper states and contains a small correction to the wavemeter calibration. The third step data are reported exactly as measured.

n	Third step (MHz)	E_n (MHz)	δ	δ Error ($\times 10^{-5}$)
36	236 496 706	1007 068 254	2.641 87	2.3
37	236 666 310	1007 237 858	2.641 79	2.5
38	236 821 728	1007 393 277	2.641 70	2.7
39	236 964 479	1007 536 027	2.641 75	2.9
40	237 095 926	1007 667 475	2.641 77	3.2
41	237 217 235	1007 788 783	2.641 73	3.4
42	237 329 406	1007 900 954	2.641 76	3.7
43	237 433 360	1008 004 909	2.641 62	4.0
44	237 529 853	1008 101 402	2.641 60	4.3
45	237 619 595	1008 191 144	2.641 56	4.6
46	237 703 191	1008 274 740	2.641 63	5.0
47	237 781 211	1008 352 760	2.641 51	5.3
48	237 854 117	1008 425 666	2.641 54	5.7
49	237 922 362	1008 493 911	2.641 48	6.1
50	237 986 322	1008 557 870	2.641 55	6.5
51	238 046 352	1008 617 901	2.641 67	6.9
52	238 102 791	1008 674 339	2.641 44	7.3
53	238 155 879	1008 727 427	2.641 61	7.8
54	238 205 906	1008 777 455	2.641 59	8.2
55	238 253 103	1008 824 651	2.641 39	8.7
56	238 297 662	1008 869 210	2.641 39	9.2
57	238 339 780	1008 911 329	2.641 48	9.8
58	238 379 637	1008 951 185	2.641 58	10.3
59	238 417 400	1008 988 949	2.641 41	10.9
60	238 453 197	1009 024 746	2.641 51	11.5
61	238 487 172	1009 058 721	2.641 51	12.1
62	238 519 445	1009 090 994	2.641 51	12.7
63	238 550 123	1009 121 672	2.641 65	13.4

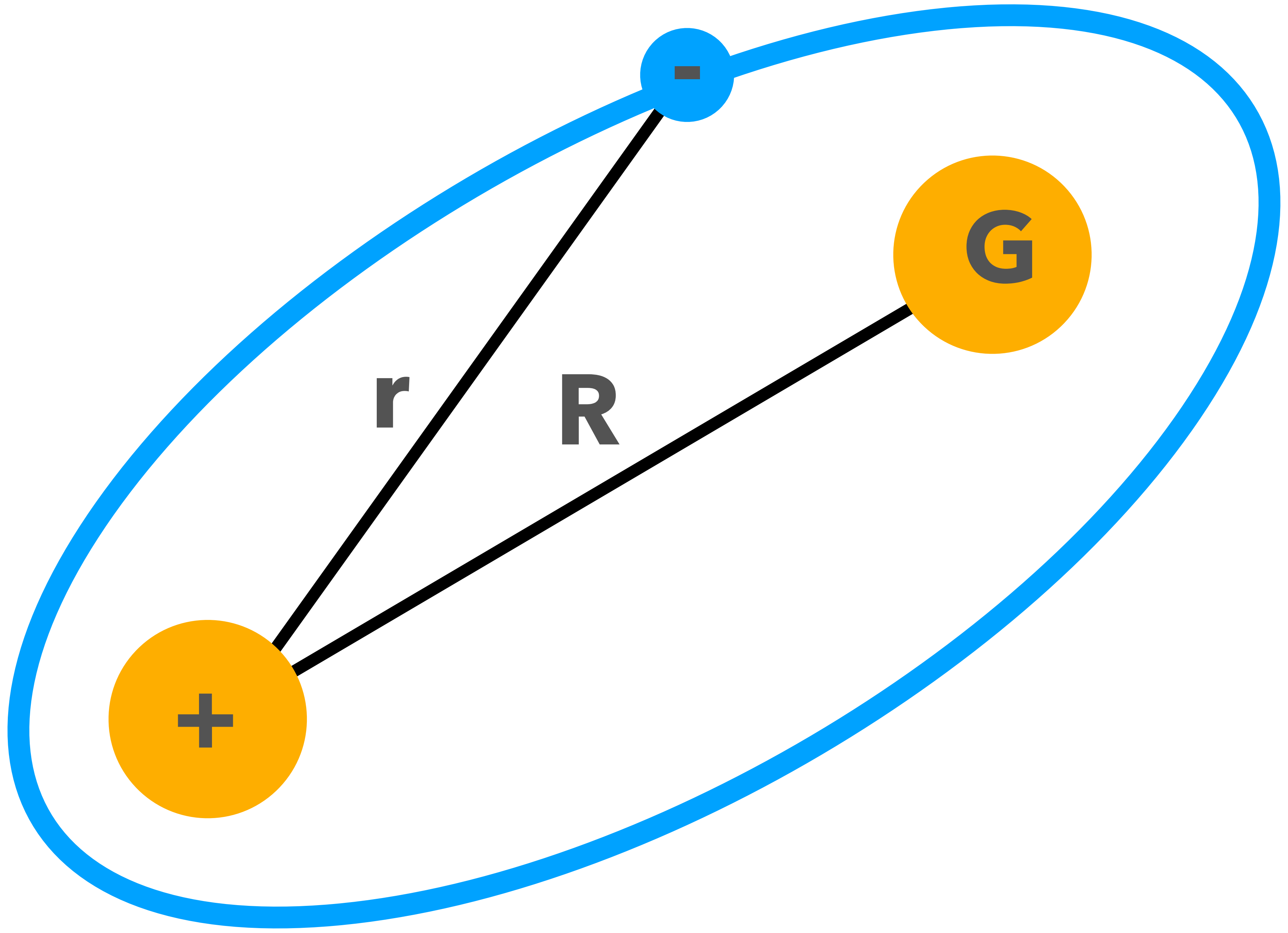
A quick survey of atomic structure

Energy spectrum of hydrogen and an alkali atom.



Building a quantum simulator of a Rydberg atom

Using a Rydberg atom bound to a ground state molecule to form an *ultralong-range Rydberg molecule*, we want to simulate…a Rydberg atom.



The target Hamiltonian:

$$H_{\text{sim}} = -\frac{\nabla_R^2}{2M} - \frac{Z}{R} + V_{sr}(R)$$

Keep in mind:

- Many equations to come: but it will be worth it!!!!
- At the end: you tell me if this is a quantum simulator (even though it is ridiculous!)

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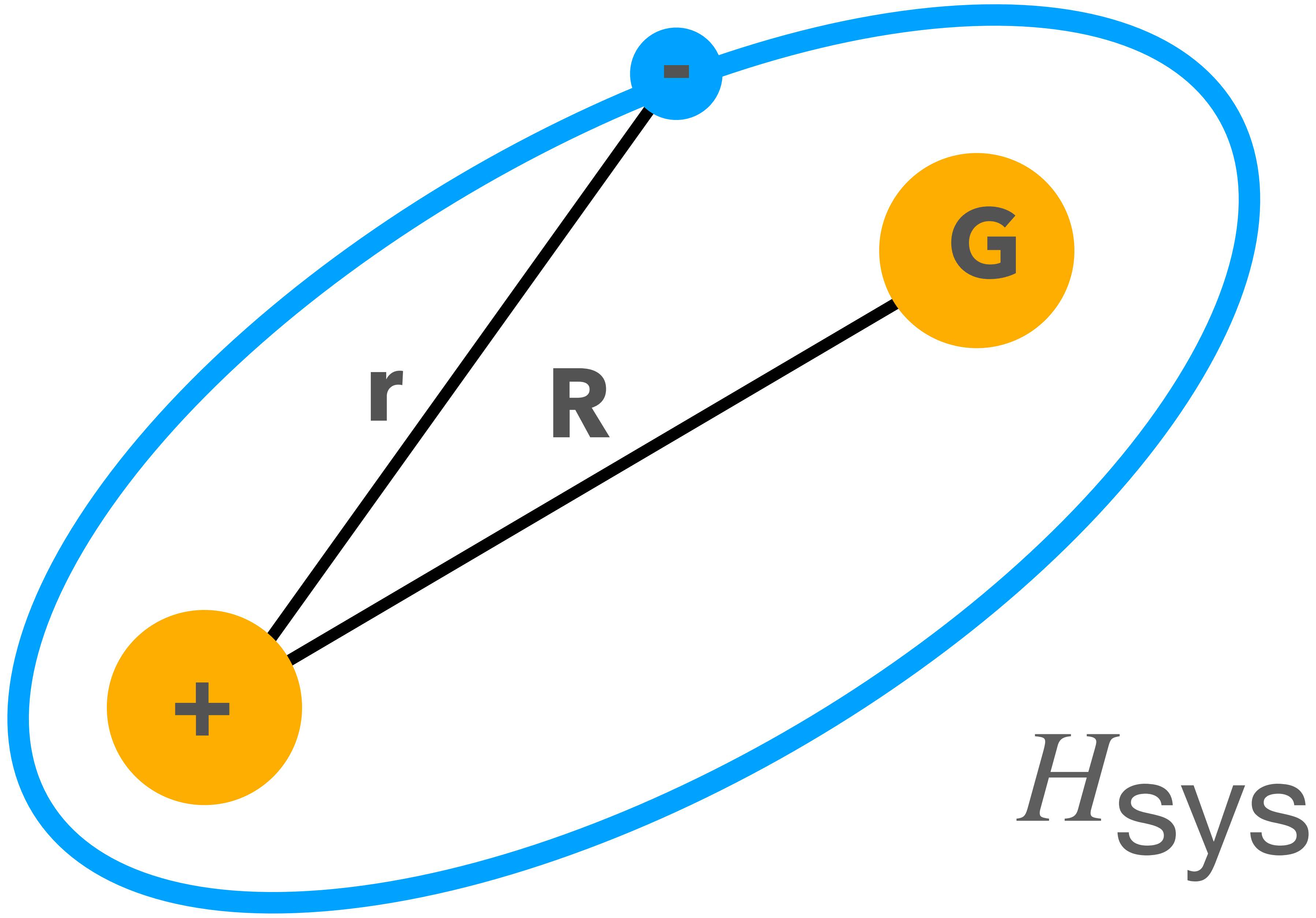

The target Hamiltonian:

$$H_{\text{sim}} = -\frac{\nabla_R^2}{2M} - \frac{Z}{R} + V_{sr}(R)$$

The actual Hamiltonian:

$$H_{\text{sys}} = -\frac{\nabla_R^2}{2M} - \frac{\nabla^2}{2} - \frac{1}{r} + V_{sr}(r) + U(\vec{r} - \vec{R})\,.$$

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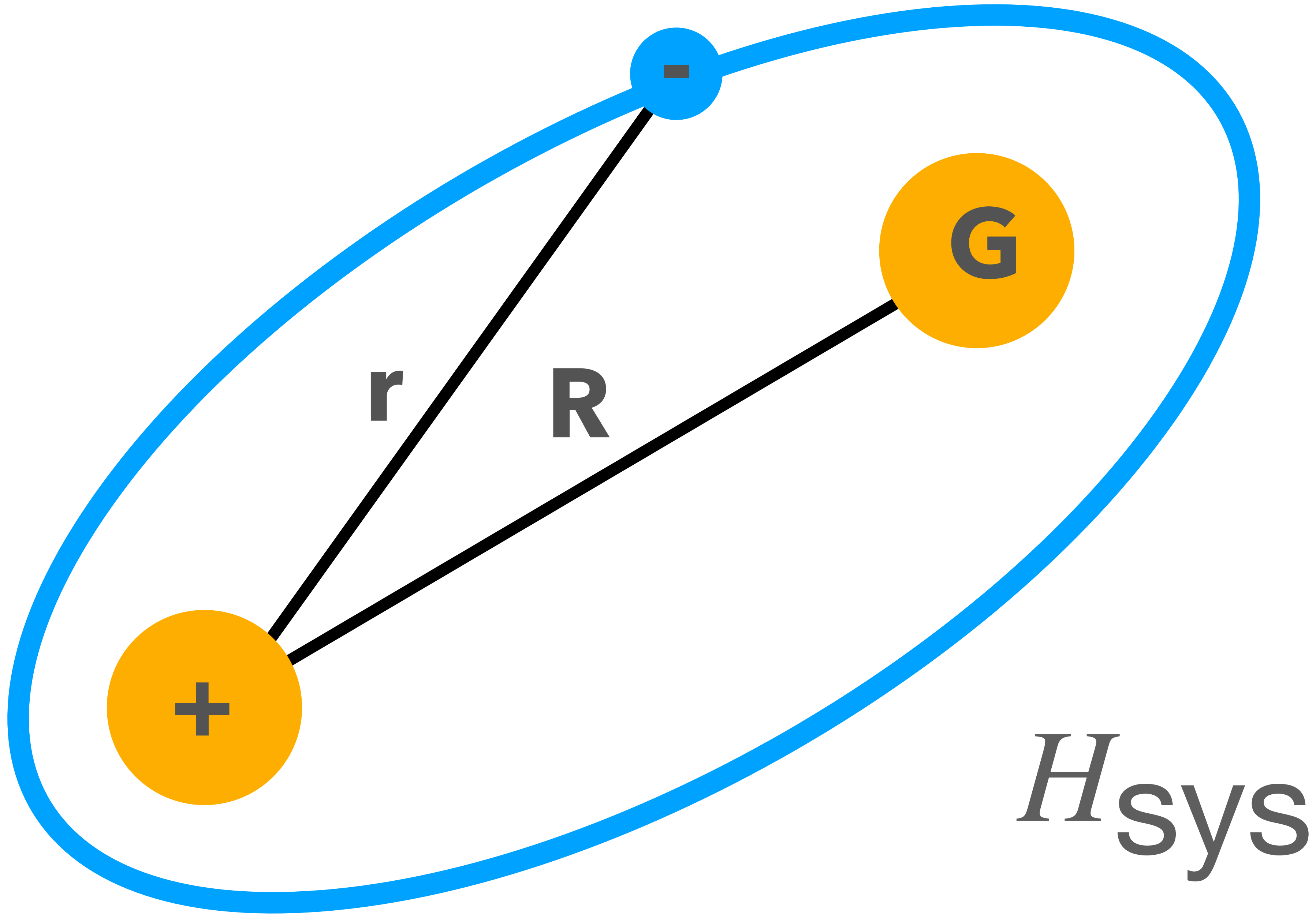

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(first approximation: we assume a wave function in the Born-Oppenheimer approximation and take a single Rydberg manifold):

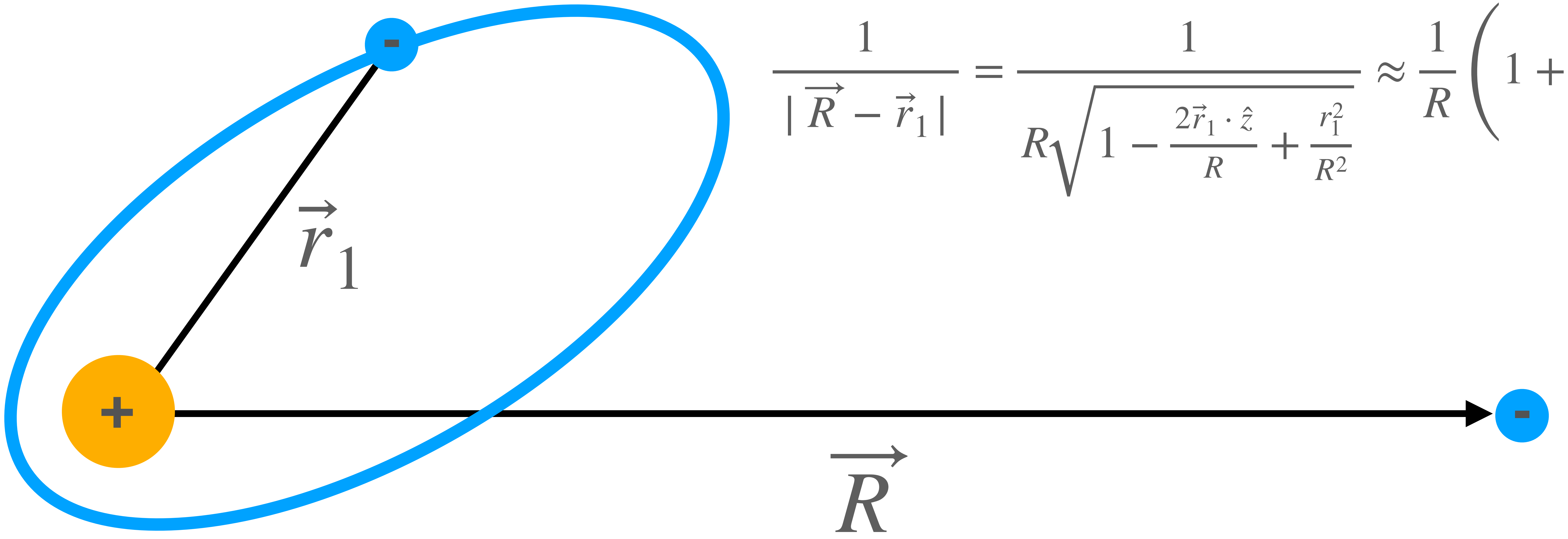
$$\Psi(\overrightarrow{R}, \vec{r}) = \chi_{EJ}(R) Y_{JM}(\theta_R, \phi_R) \sum_{l=0}^{n-1} c_l \Psi_{nlm}(\vec{r}) .$$

(this assumes adiabatic potential energy curves will be well-separated and weak compared to Rydberg level spacing…check this!)

Interlude: How does an electron interact with an atom?

$$H = \frac{-\nabla_1^2}{2} - \frac{1}{r_1} - \frac{1}{R} + \frac{1}{|\vec{r}_1 - \vec{R}\,|}$$

$$\frac{1}{|\vec{R} - \vec{r}_1|} = \frac{1}{R\sqrt{1 - \frac{2\vec{r}_1 \cdot \hat{z}}{R} + \frac{r_1^2}{R^2}}} \approx \frac{1}{R}\left(1 + \frac{\vec{r}_1 \cdot \hat{z}}{R}\right)$$



As the electron comes in from a large distance (Rydberg orbits, remember!) R will be much larger than the typical distances of the ground state atom's valence electron.
A great opportunity to do a Taylor expansion!

Interlude: How does an electron interact with an atom?

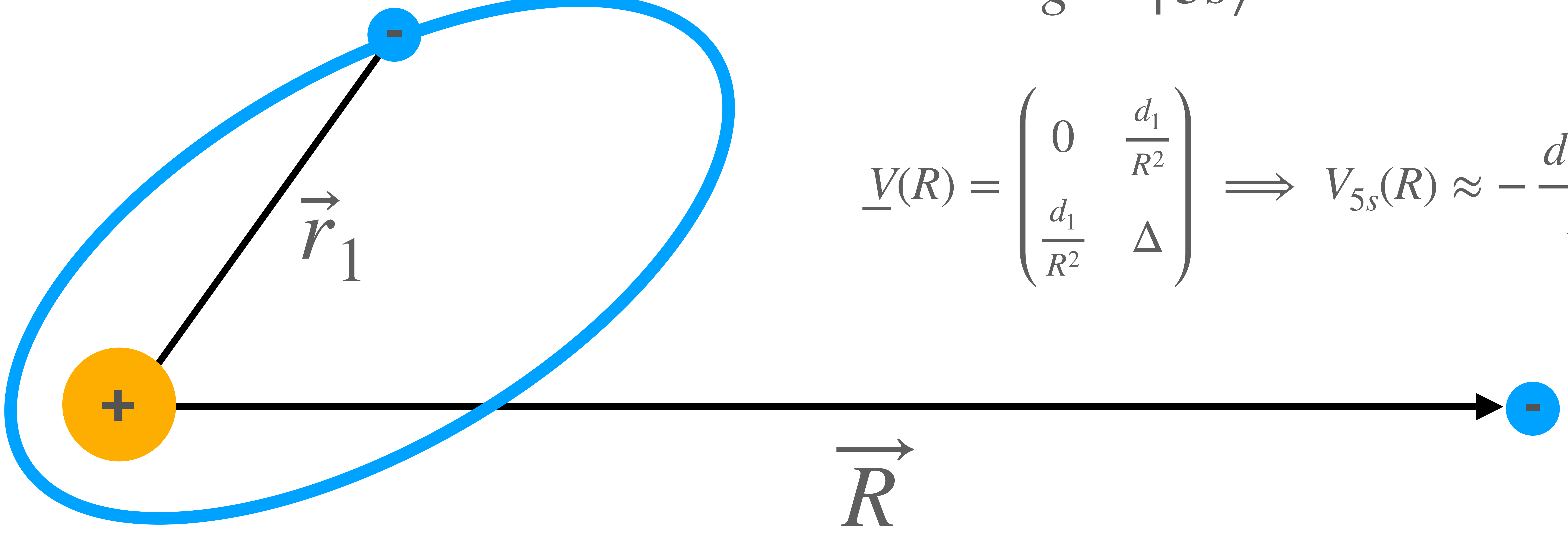
$$H = \frac{-\nabla_1^2}{2} - \frac{1}{r_1} + \frac{\vec{r}_1 \cdot \hat{z}}{R}$$

$e = |5p\rangle$

Δ

$g = |5s\rangle$

$$\underline{V}(R) = \begin{pmatrix} 0 & \frac{d_1}{R^2} \\ \frac{d_1}{R^2} & \Delta \end{pmatrix} \Longrightarrow V_{5s}(R) \approx -\frac{d_1^2/\Delta}{R^4} = -\frac{\alpha}{2R^4}.$$



At large distances (outside the range where the electrons overlap), the incoming electron sees a polarization potential!

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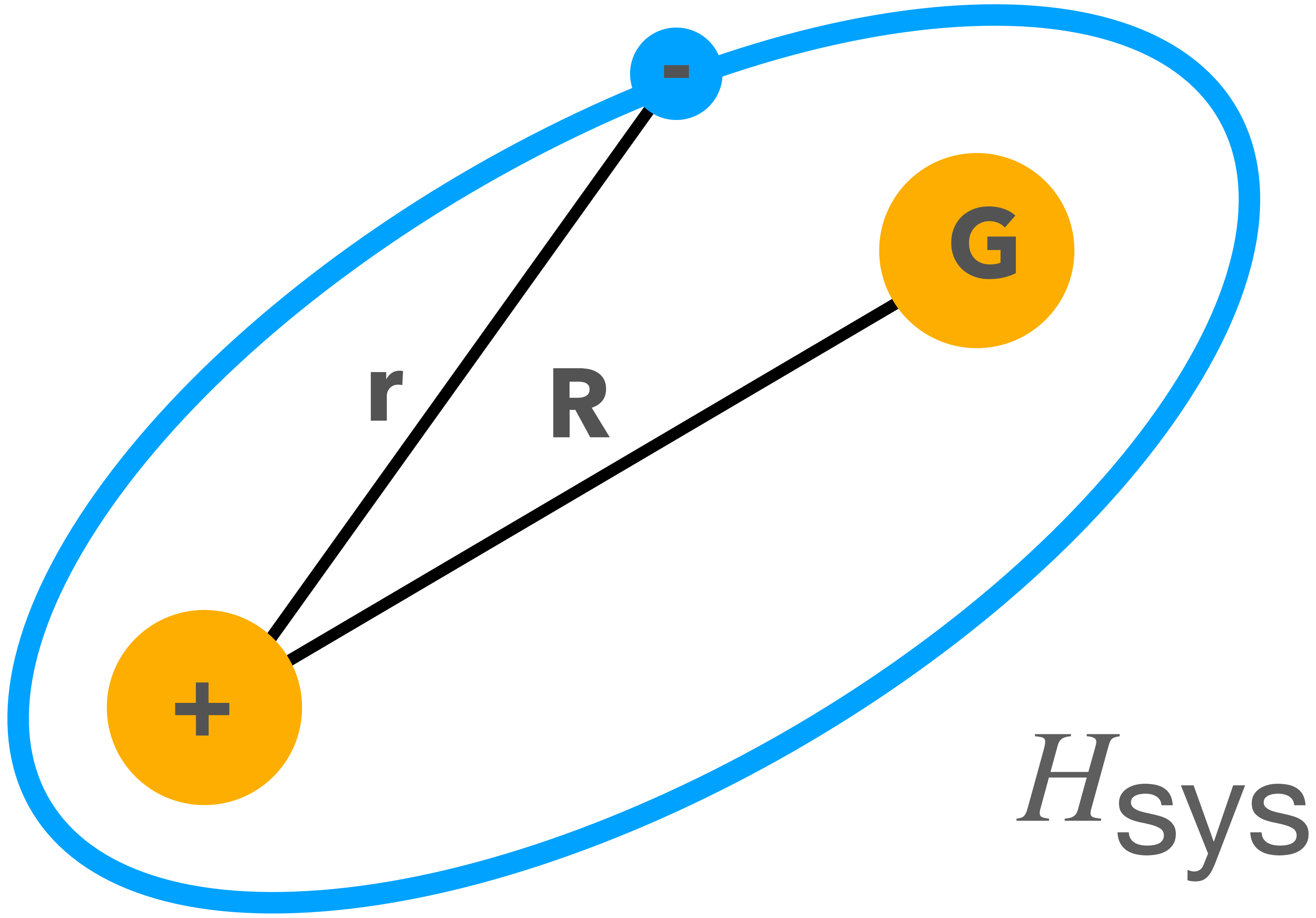

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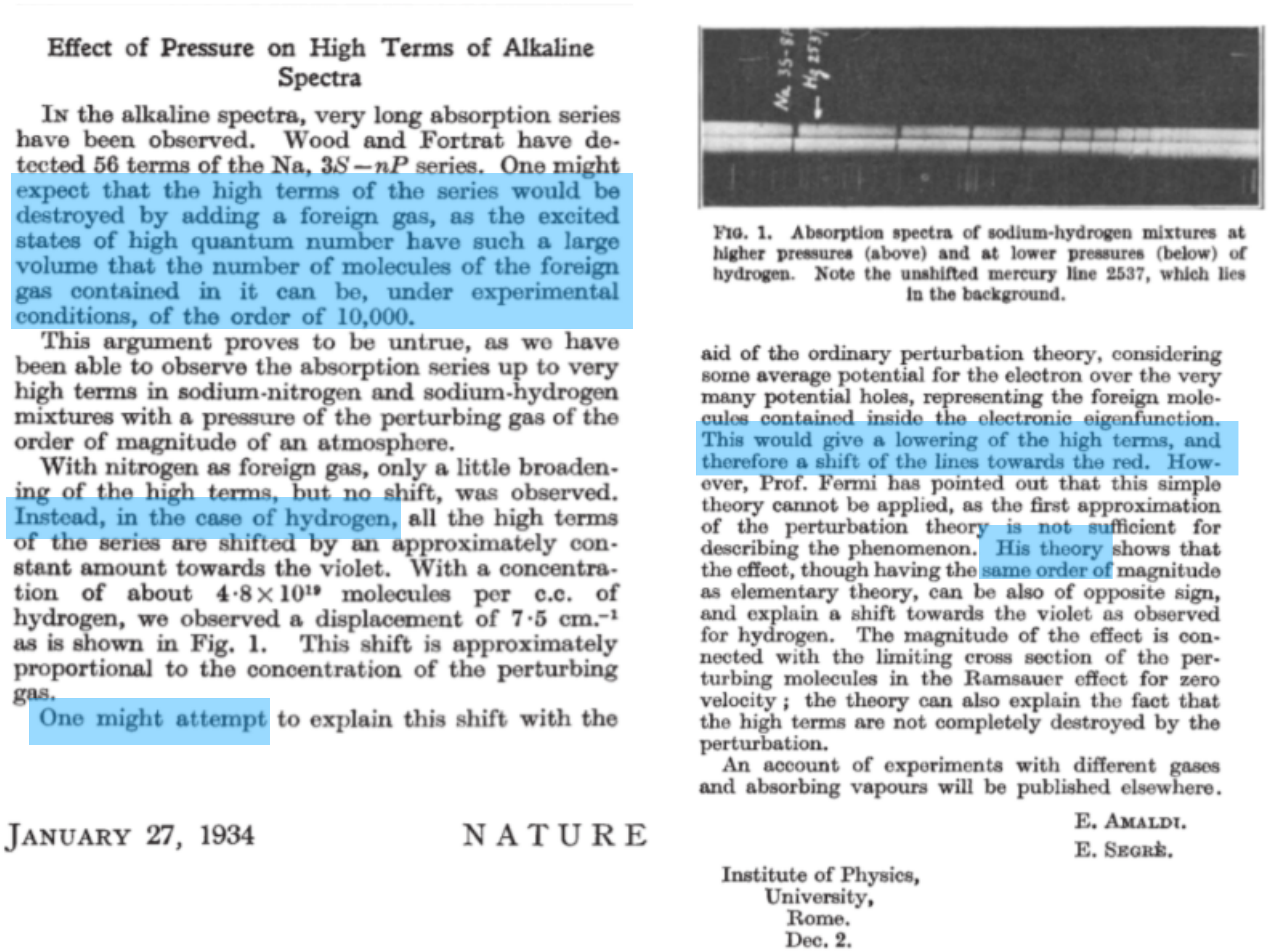
$$U(\vec{r} - \vec{R}) = -\frac{\alpha}{2|\vec{r} - \vec{R}|^4}?$$

Building a quantum simulator of a Rydberg atom



JANUARY 27, 1934 NATURE

Effect of Pressure on High Terms of Alkaline Spectra

In the alkaline spectra, very long absorption series have been observed. Wood and Fortrat have detected 56 terms of the Na, $3S-nP$ series. One might expect that the high terms of the series would be destroyed by adding a foreign gas, as the excited states of high quantum number have such a large volume that the number of molecules of the foreign gas contained in it can be, under experimental conditions, of the order of 10,000.

This argument proves to be untrue, as we have been able to observe the absorption series up to very high terms in sodium-nitrogen and sodium-hydrogen mixtures with a pressure of the perturbing gas of the order of magnitude of an atmosphere.

With nitrogen as foreign gas, only a little broadening of the high terms, but no shift, was observed. Instead, in the case of hydrogen, all the high terms of the series are shifted by an approximately constant amount towards the violet. With a concentration of about $4 \cdot 8 \times 10^{19}$ molecules per c.c. of hydrogen, we observed a displacement of $7 \cdot 5$ cm.$^{-1}$ as is shown in Fig. 1. This shift is approximately proportional to the concentration of the perturbing gas.

One might attempt to explain this shift with the aid of the ordinary perturbation theory, considering some average potential for the electron over the very many potential holes, representing the foreign molecules contained inside the electronic eigenfunction. This would give a lowering of the high terms, and therefore a shift of the lines towards the red. However, Prof. Fermi has pointed out that this simple theory cannot be applied, as the first approximation of the perturbation theory is not sufficient for describing the phenomenon. His theory shows that the effect, though having the same order of magnitude as elementary theory, can be also of opposite sign, and explain a shift towards the violet as observed for hydrogen. The magnitude of the effect is connected with the limiting cross section of the perturbing molecules in the Ramsauer effect for zero velocity; the theory can also explain the fact that the high terms are not completely destroyed by the perturbation.

An account of experiments with different gases and absorbing vapours will be published elsewhere.

FIG. 1. Absorption spectra of sodium-hydrogen mixtures at higher pressures (above) and at lower pressures (below) of hydrogen. Note the unshifted mercury line 2537, which lies in the background.

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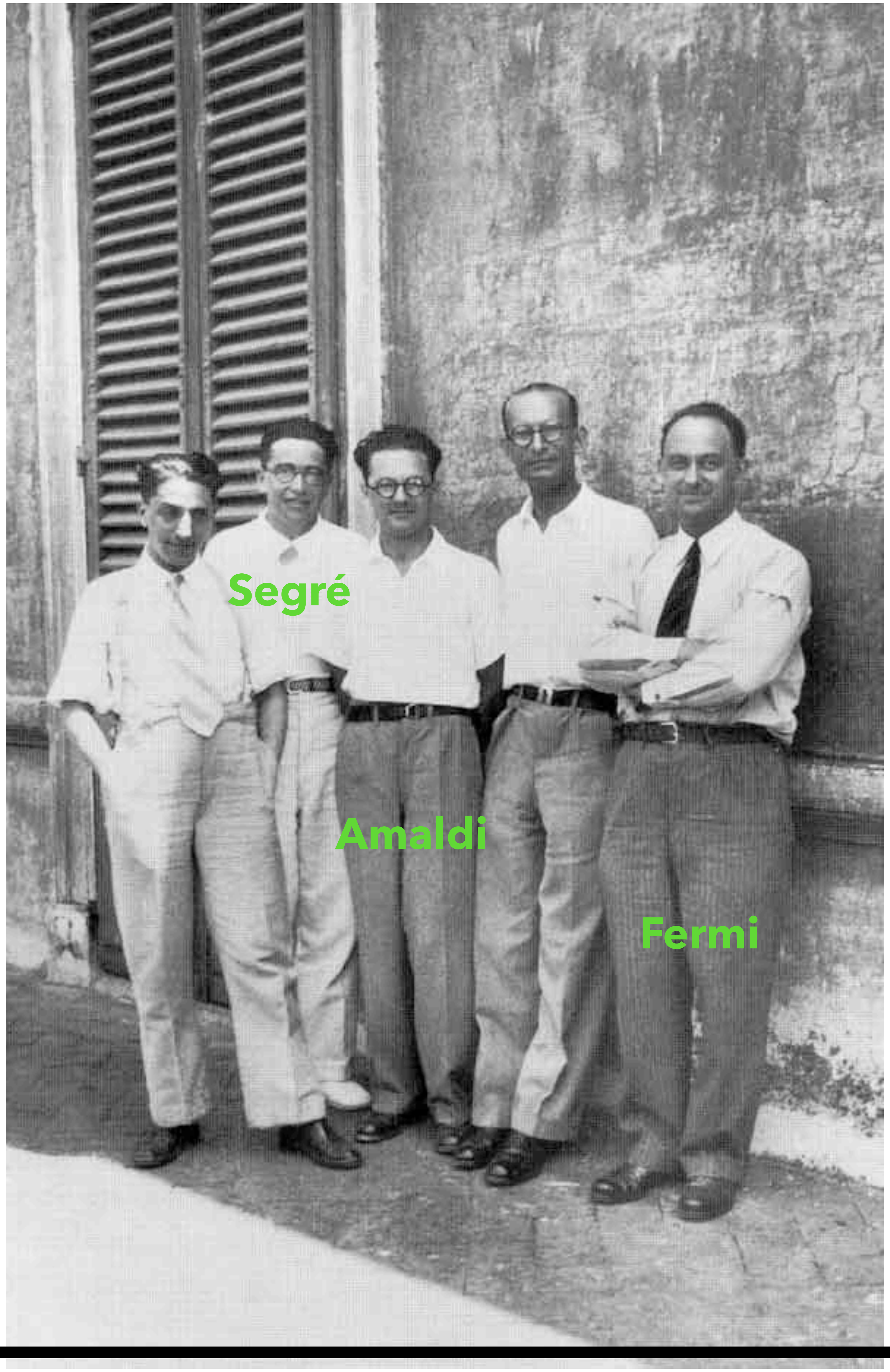
Dec. 2.

"I ragazzi di Via Panisperna" - the Via Panisperna Boys



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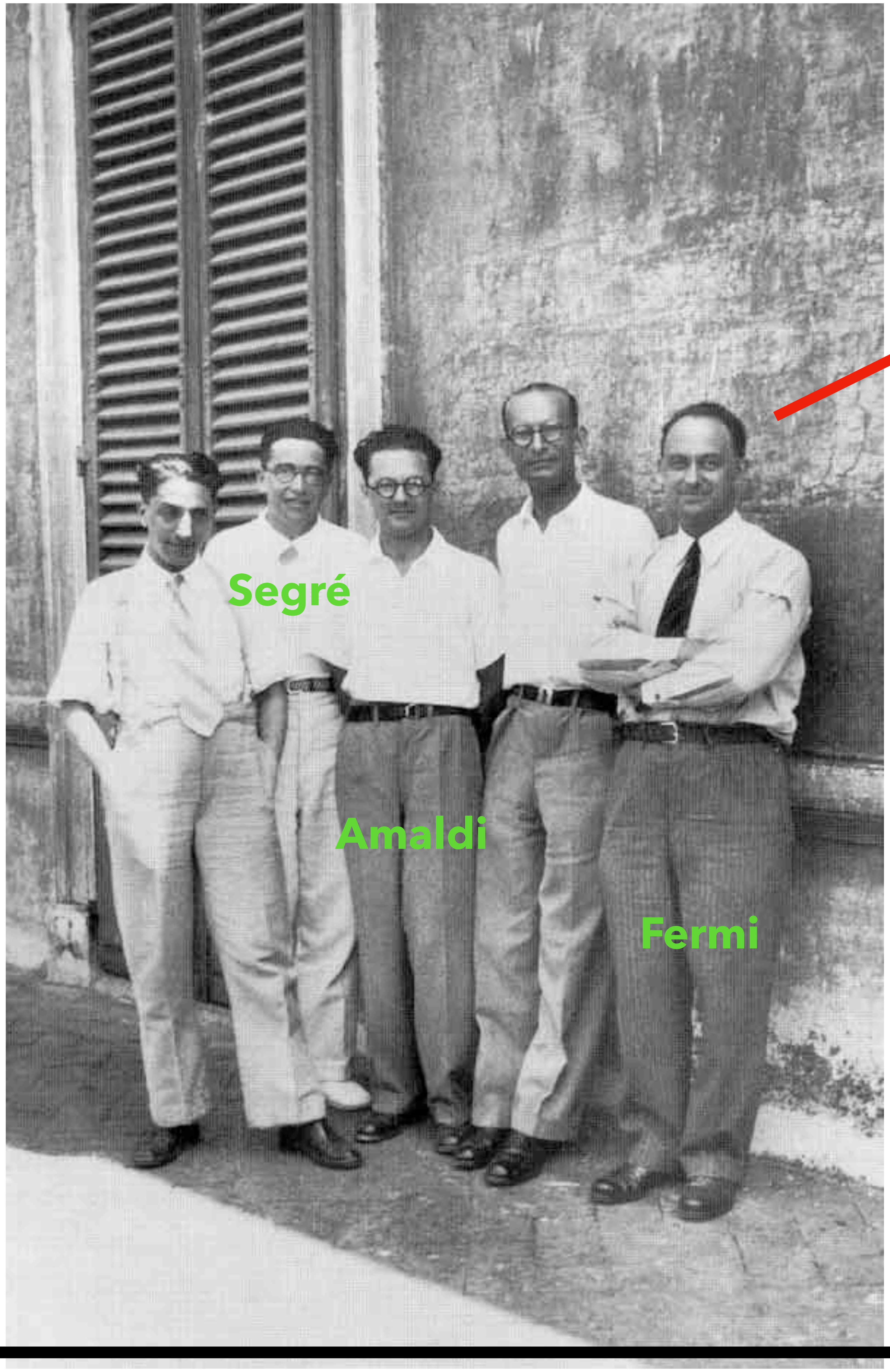

Fano

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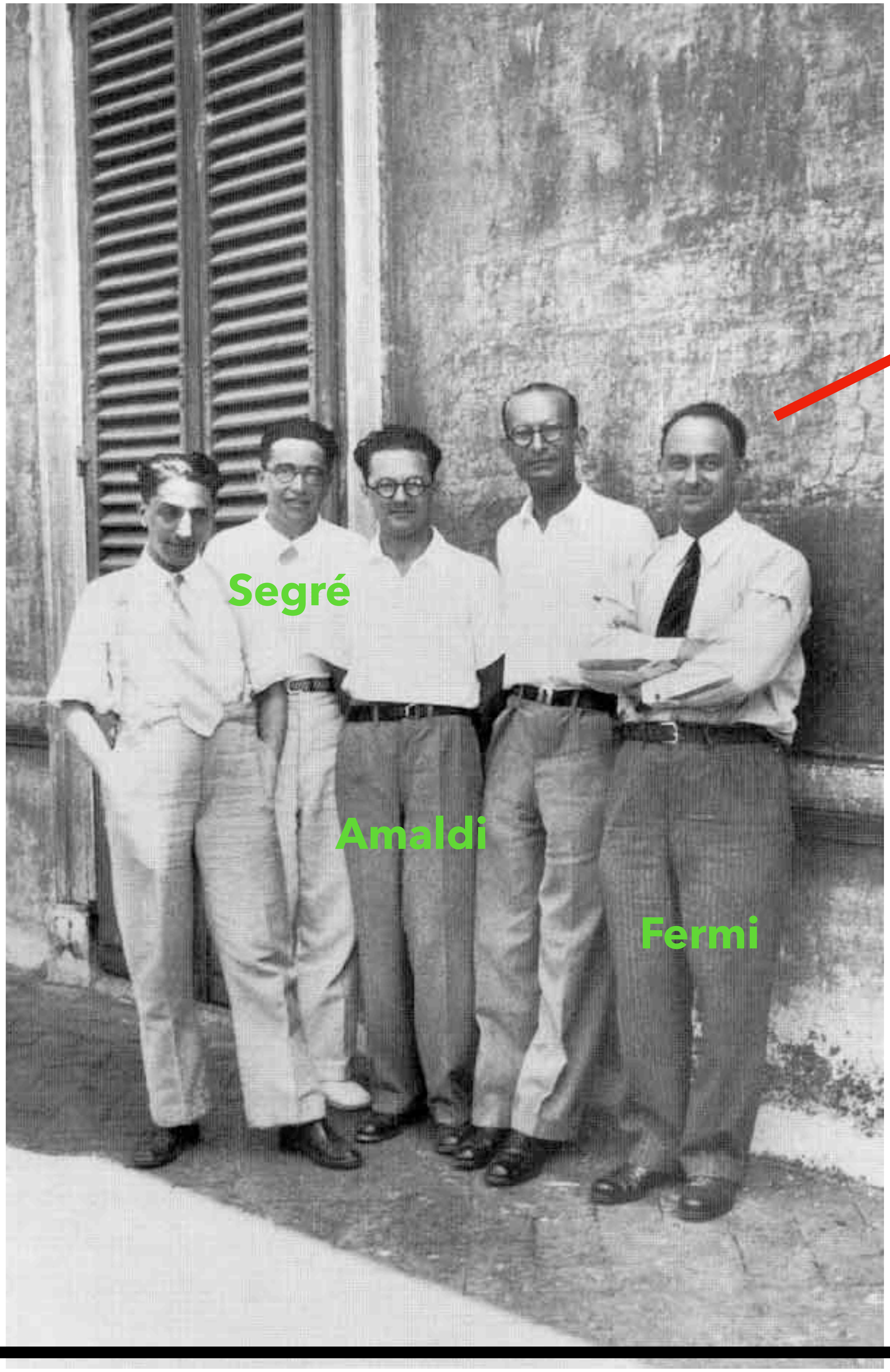

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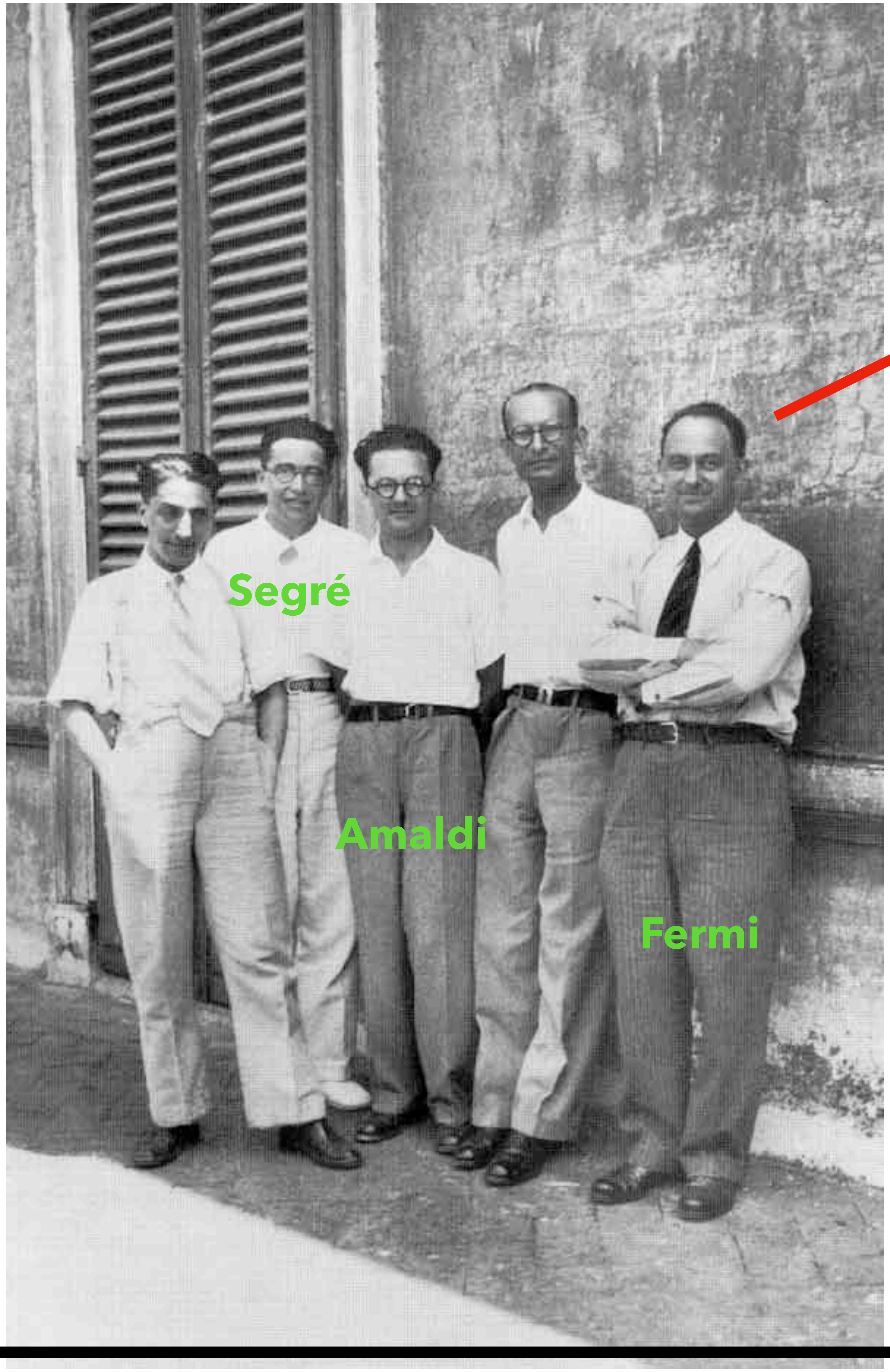


Fano


Greene

What happens to the electron?

Here we will go through a quick overview of the structure of alkali atoms: Li, Na, K, Rb, and Cs, which all have a single valence electron.

This is a second-order differential equation, so it has two linearly independent solutions, and u must be a linear combination of these FOR LARGE r!.

$$u_{\nu l}(r) \sim f_{\nu l}(r) - \tan\delta_{\nu l} g_{\nu l}(r), \quad r \geq r_0 \,. \qquad (R13)$$

For small r, we can solve the S. E. numerically (in principle) for the wave function inside: $F(r)$

Making sure the wave function and its derivative are continuous functions gives:

$$\left.\frac{F'(r)}{F(r)}\right|_{r=r_0} = \left.\frac{f'_{\nu l}(r) - g'_{\nu l}(r)\tan\delta_{\nu l}}{f_{\nu l}(r) - g_{\nu l}(r)\tan\delta_{\nu l}}\right|_{r=r_0} \implies \tan\delta_{\nu l} = \left.\frac{F'(r)f_{\nu l}(r) - F(r)f'_{\nu l}(r)}{F'(r)g_{\nu l}(r) - F(r)g'_{\nu l}(r)}\right|_{r=r_0}$$

$$= \left.\frac{W(f_{\nu l}(r), F(R))}{W(g_{\nu l}(r), F(r))}\right|_{r=r_0}$$

What really happens to the electron?

The polarization potential falls off so fast that (as long as the polarization is not too large - see effective range corrections by O'Malley and coworkers in the 60s, also Watanabe and Greene in the 80s…) that it “vanishes” at sufficiently large r

This is a second-order differential equation, so it has two linearly independent solutions, and u must be a linear combination of these FOR LARGE r!.

$$u_{El}(r) \sim f_{El}(r) - \tan\delta_{El} g_{El}(r), \quad r \geq r_0 \,.$$

f and g are now just spherical Bessel functions, much friendlier!

For small r, we can solve the S. E. numerically (in principle) for the wave function inside: $F(r)$

Making sure the wave function and its derivative are continuous functions gives:

$$\left.\frac{F'(r)}{F(r)}\right|_{r=r_0} = -\, b_l(E) = \left.\frac{f'_{El}(r) - g'_{El}(r)\tan\delta_{El}}{f_{El}(r) - g_{El}(r)\tan\delta_{El}}\right|_{r=r_0}$$

$$\Longrightarrow \quad \tan\delta_l(E) = \left.\frac{f'_{El}(r) + b_l(E) f_{El}(r)}{g'_{El}(r) + b_l(E) g_{El}(r)}\right|_{r=r_0}$$

What really happens to the electron?

This expression for the phase shift shows that (plugging in expansions for f and g…)

$\tan \delta_l(k^2/2) \to -k^{2l+1}a_l(1+\ldots)$ at low energies!

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So the s-wave phase shift is:

$$\delta_s(k) \rightarrow -k a_s$$

And likewise, the zero-energy scattering length is:

$$a_s = - \left. \frac{\tan \delta_s(k)}{k} \right|_{k \rightarrow 0}$$

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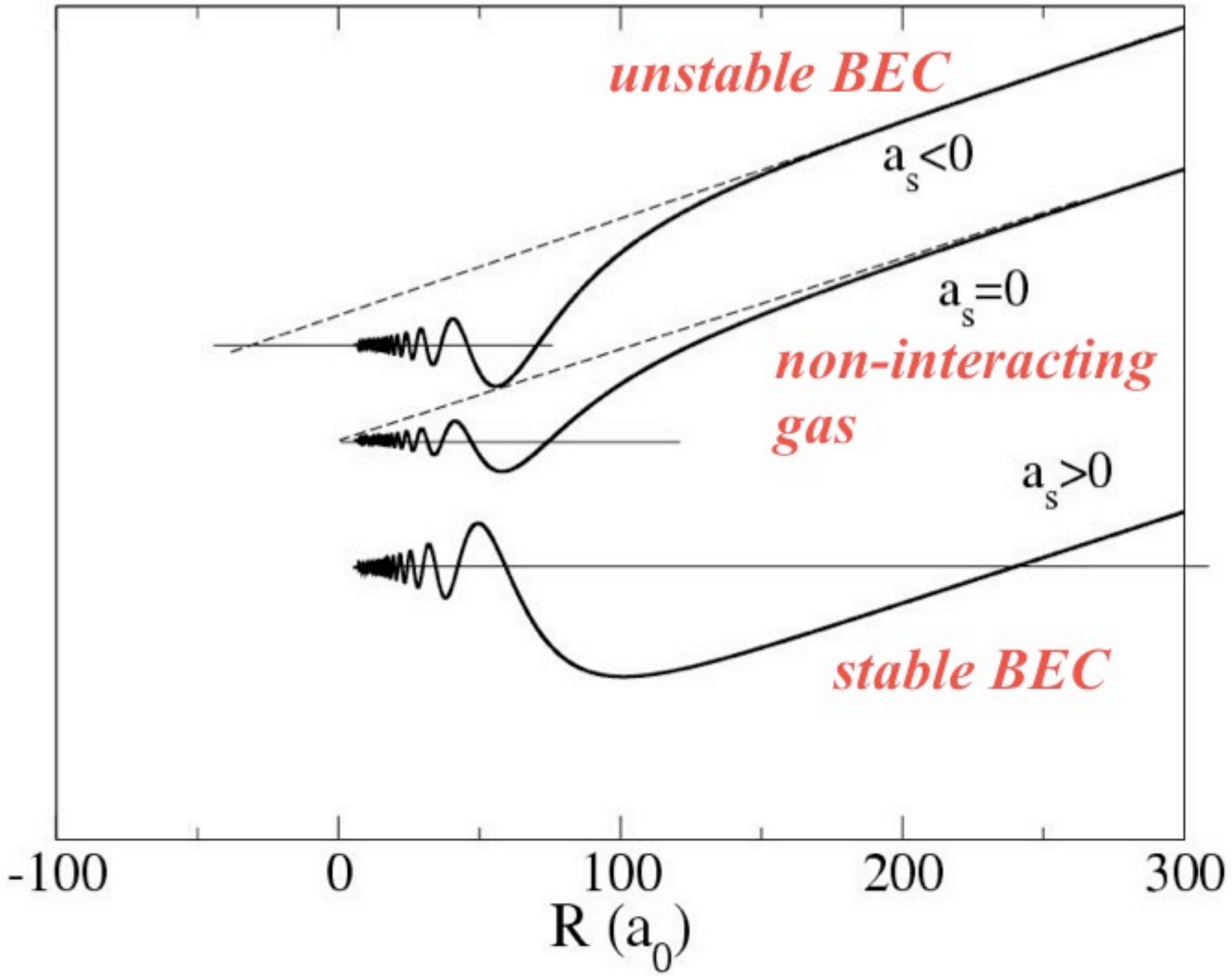

(Robin Cote)

$$u(r) \approx \frac{\sin[kr + \delta(k)]}{k}$$

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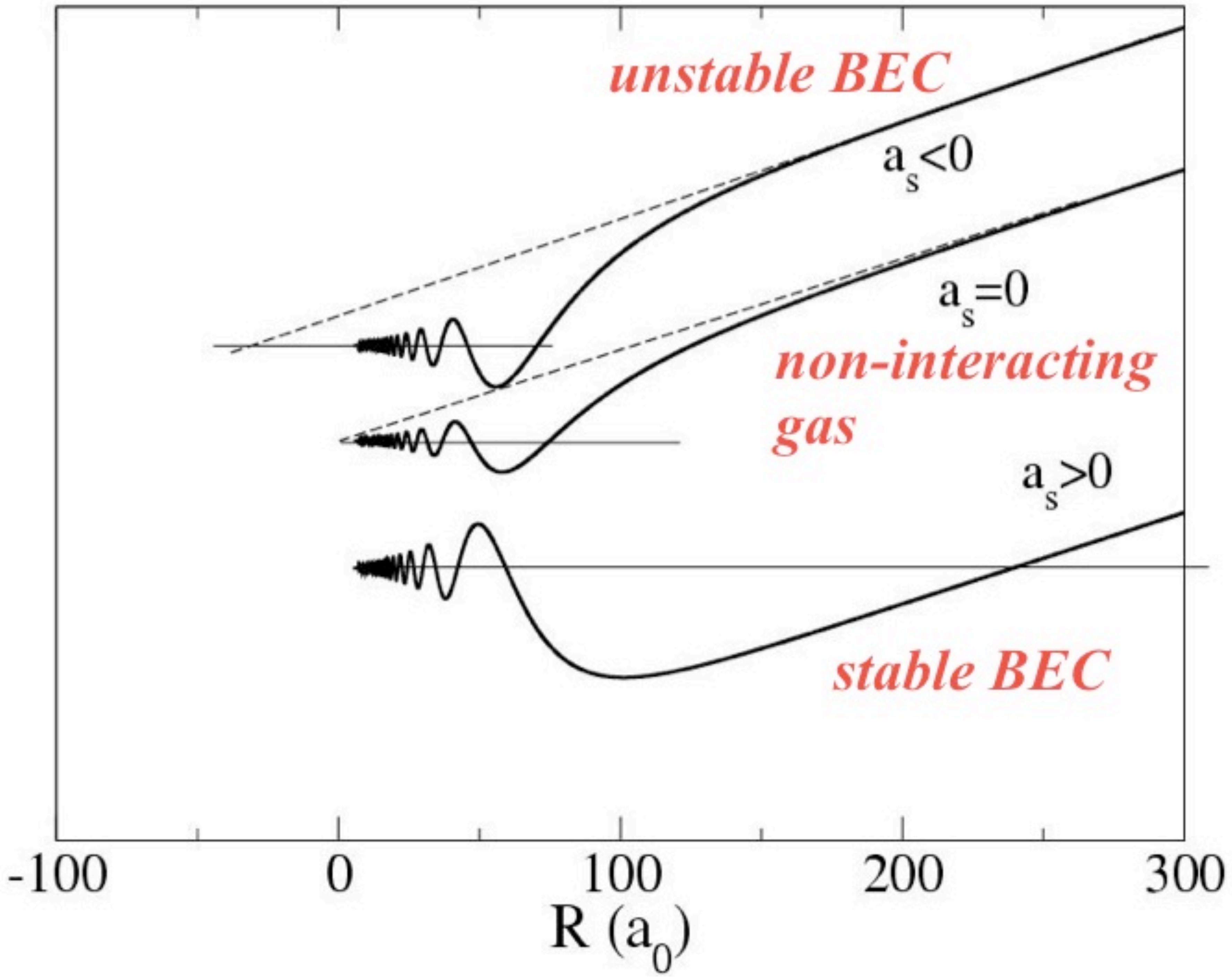
And crucially! The **Fermi Pseudopotential is**

$$U(\vec{r}, \vec{R}) = 2\pi a_s(k) \delta^3(\vec{r} - \vec{R}) \, .$$



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$$= -\pi\left(\frac{2}{\pi k}\right)\int_0^\infty (kr)^2[j_l(kr)]^2\left(-\frac{\alpha}{2r^N}\right)dr$$

$$= 2\alpha k^{N-2}\int_0^\infty \frac{j_l^2(x)}{x^{N-2}}dx$$

$$= 2\alpha k^{N-2}\frac{\sqrt{\pi}}{4}\frac{\Gamma(3/2+l-N/2)\Gamma(N/2-1/2)}{\Gamma(1/2+l+N/2)\Gamma(N/2)}$$

IF! $2l-(N-2) > -1$

$$j_l(x) \approx \frac{x^l}{1\cdot 3\cdot 5\ldots(2l+1)}$$

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$$\delta_L(k) = \overline{\alpha_L} k^2$$

$$\overline{\alpha_L} = \frac{\alpha}{(4L^2-1)(2L+3)}$$

$$\tan \delta_l(k) = -\pi \int_0^\infty f_{kl}(r) V(r) f_{kl}(r) dr$$

$$= -\pi \left(\frac{2}{\pi k}\right) \int_0^\infty (kr)^2 [j_l(kr)]^2 \left(-\frac{\alpha}{2r^N}\right) dr$$

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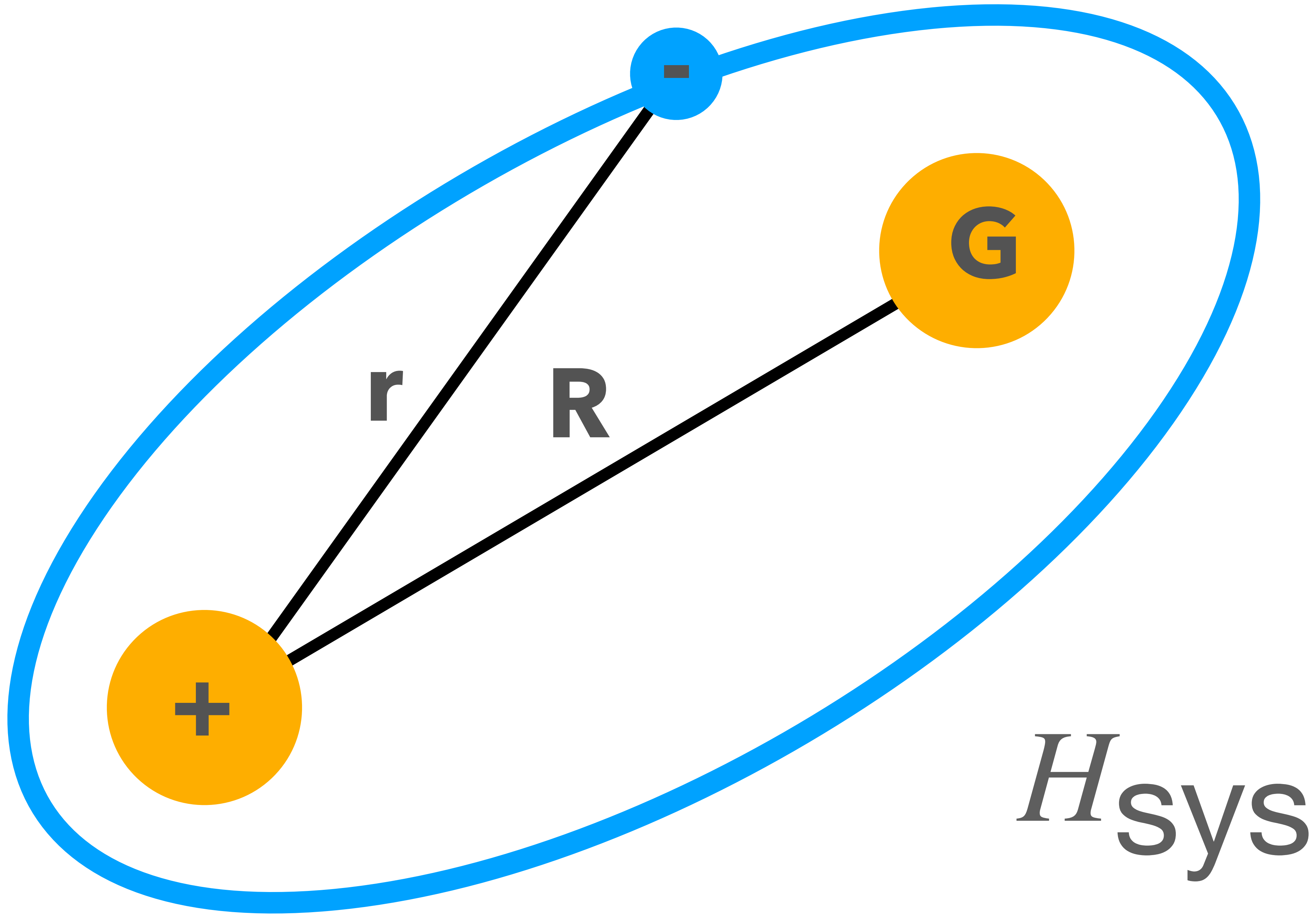

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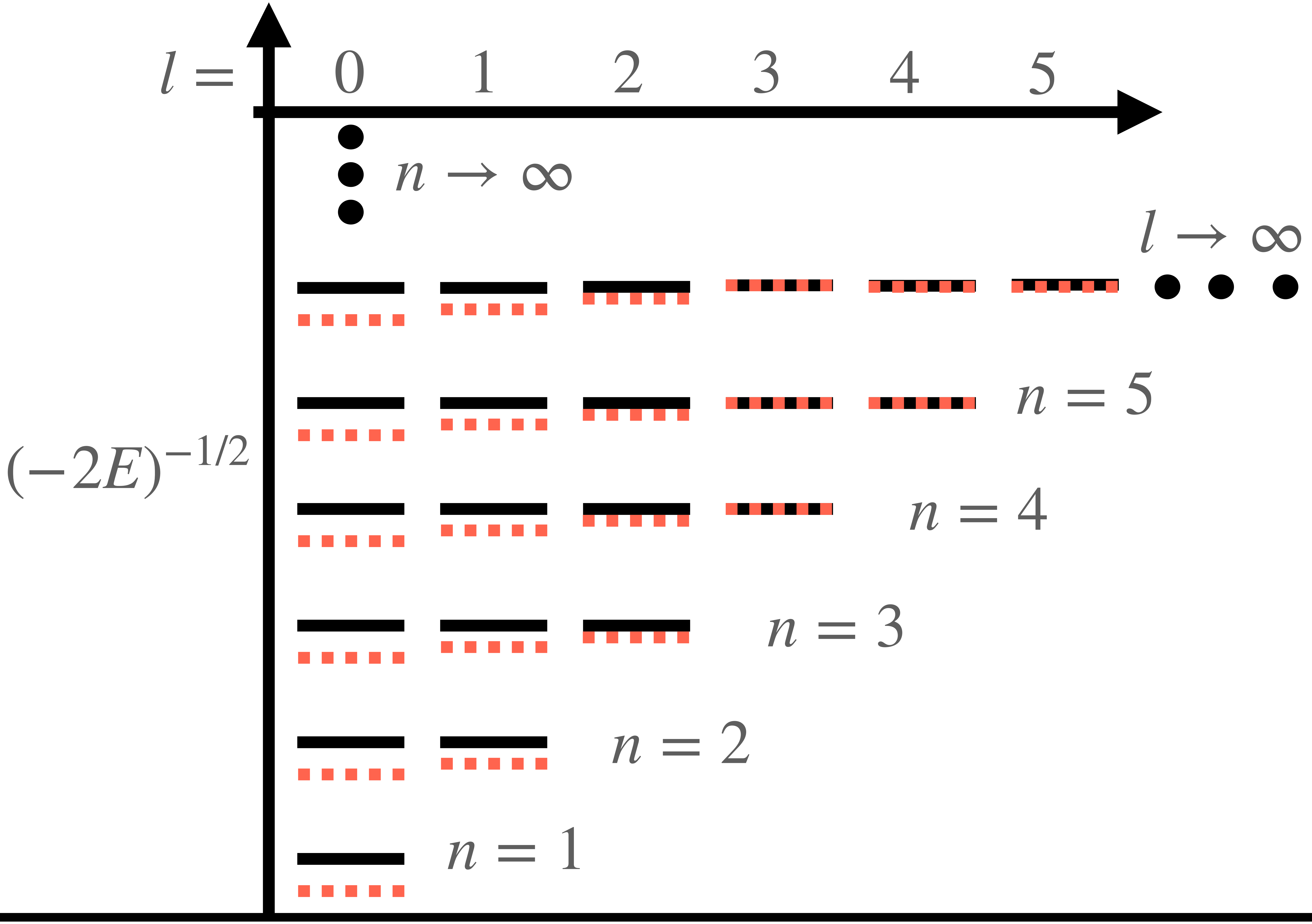
A quick survey of atomic structure

Energy spectrum of hydrogen and an alkali atom.



Non-degenerate quantum defect case

To a good approximation, the molecular potential curve associated with one of these states is just the diagonal matrix element of

$$V(\overrightarrow{R}, \vec{r}) = H_{\text{electron}} + 2\pi a_s \delta^3(\vec{r} - \overrightarrow{R})$$

"in other words"

$$U(R) = \langle nlm \,|\, V(R, r) \,|\, nlm \rangle = -\frac{1}{2(n-\mu_l)^2} + 2\pi a_s \,|\, \Psi_{nlm}(R) \,|^2$$

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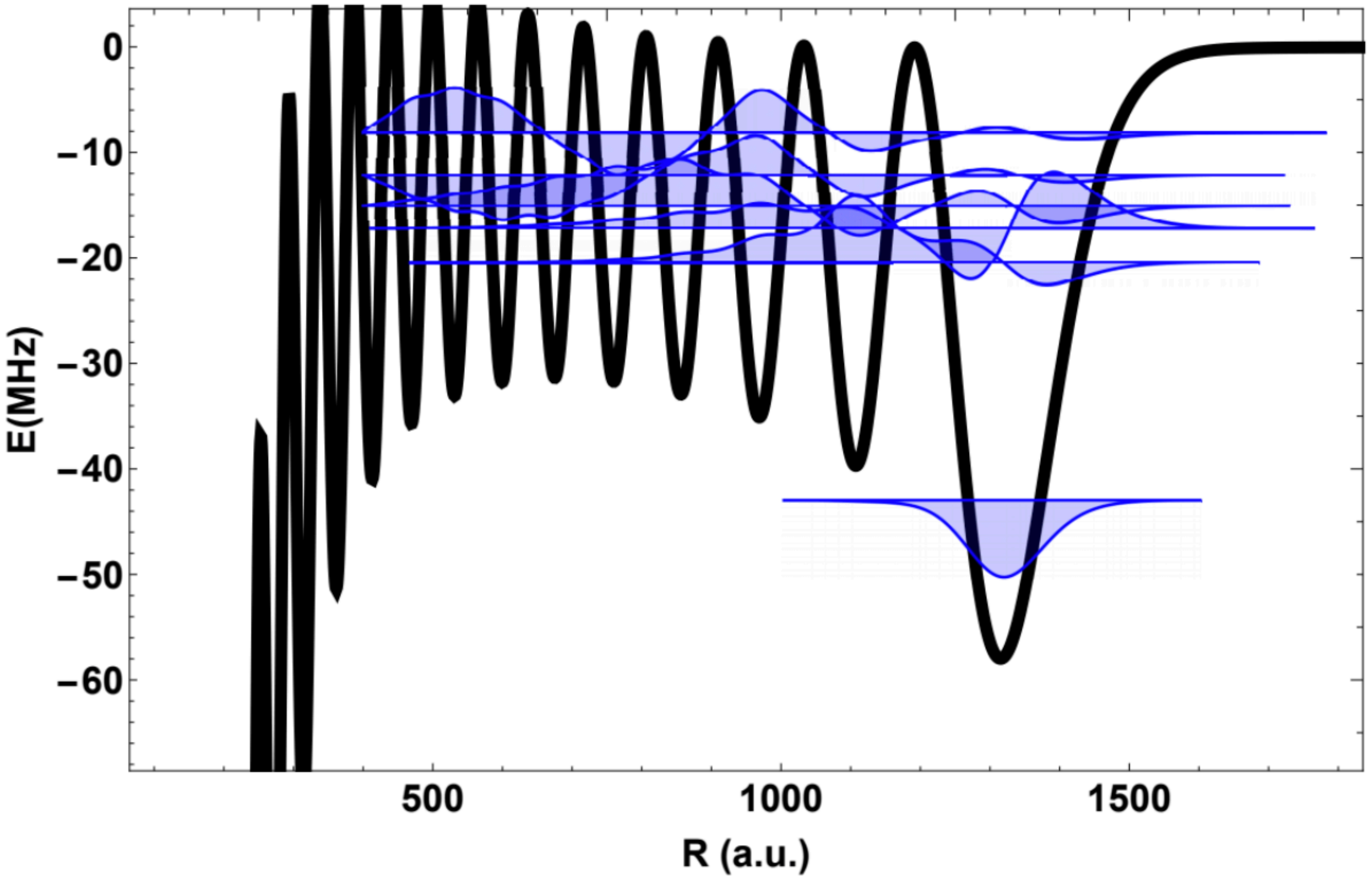

The molecular potential energy curves are oscillatory! wacky! But not Coulomb!

Degenerate non-quantum-defect case

Now we diagonalize

$$V(\overrightarrow{R}, \vec{r}) = H_{\text{electron}} + 2\pi a_s \delta^3(\vec{r} - \overrightarrow{R})$$

in just the basis of degenerate states.

Diagonalize: $\langle nlm \,|\, V(R, r) \,|\, nl'm' \rangle = 2\pi a_s \Psi^*_{nlm}(R)\Psi_{nl'm'}(R)$

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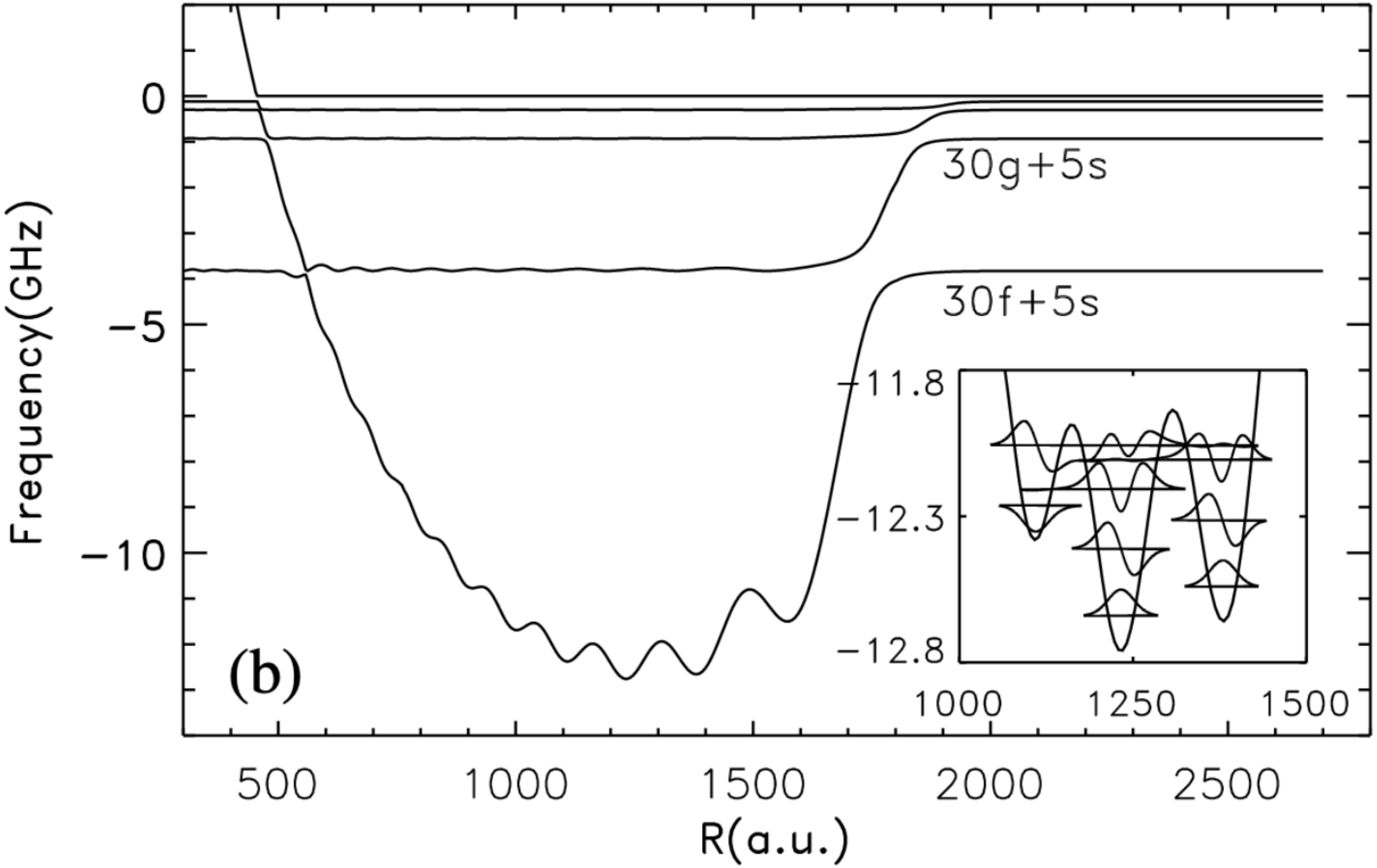
$$2\pi a_s \left(\overrightarrow{\Psi} \cdot \overrightarrow{\Psi}^\dagger\right) \overrightarrow{C} = E\overrightarrow{C}$$

$$\implies 2\pi a_s \left(\overrightarrow{\Psi}^\dagger \cdot \overrightarrow{\Psi}\right)\left(\overrightarrow{\Psi}^\dagger \cdot \overrightarrow{C}\right) = E\left(\overrightarrow{\Psi}^\dagger \cdot \overrightarrow{C}\right)$$

$$\implies E = 2\pi a_s \left(\overrightarrow{\Psi}^\dagger \cdot \overrightarrow{\Psi}\right) \implies U(R) = 2\pi a_s \sum_{l \geq l_0}^{n-1} \left| \psi_{nlm}(\overrightarrow{R}) \right|^2 .$$

The trilobite emerges!

Rydberg molecule potential energy curves are even wackier but still not Coulombier!



C. H. Greene, A. S. Dickinson, and H. R. Sadeghpour. PRL. **85,** 2458 (2000)

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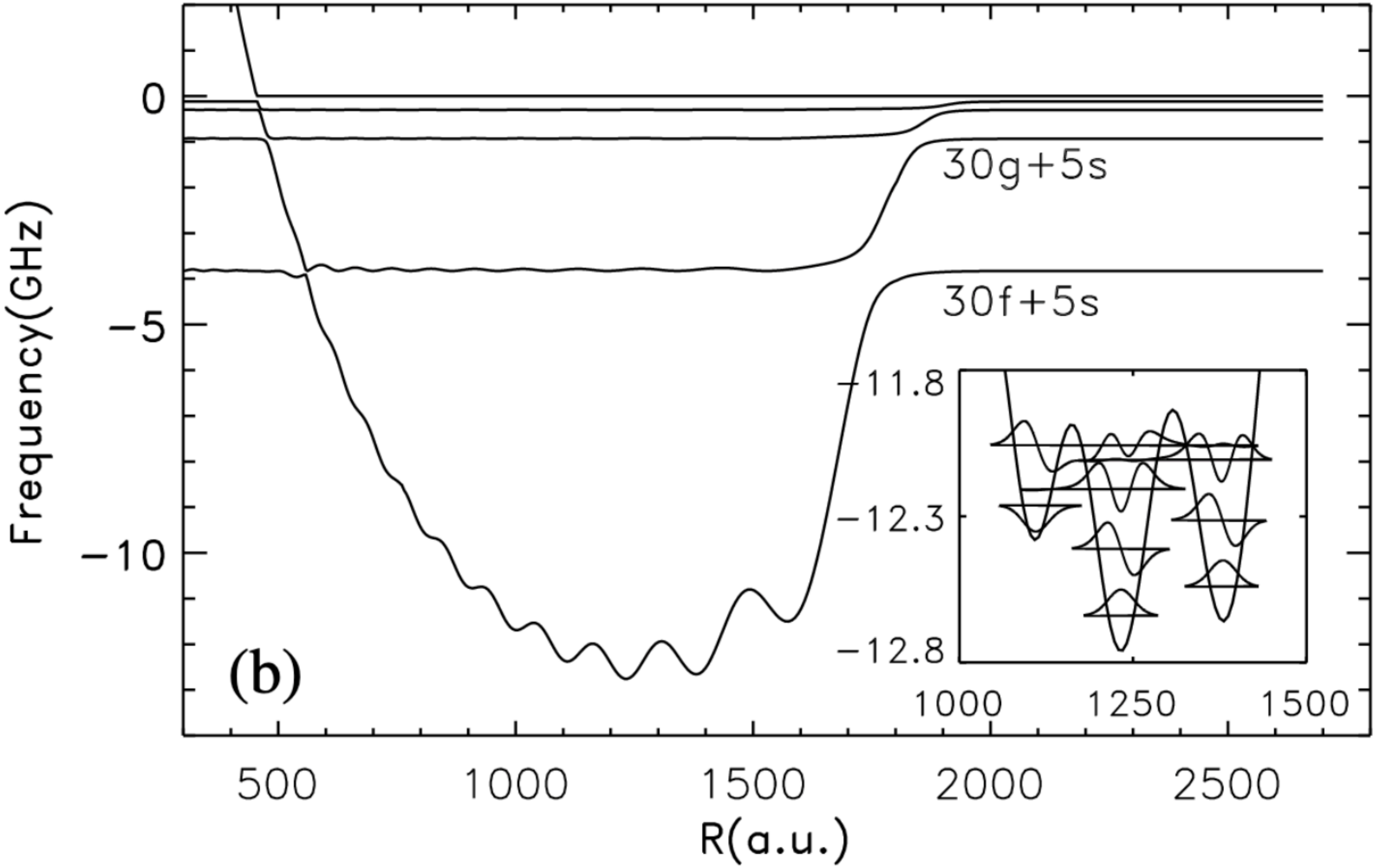
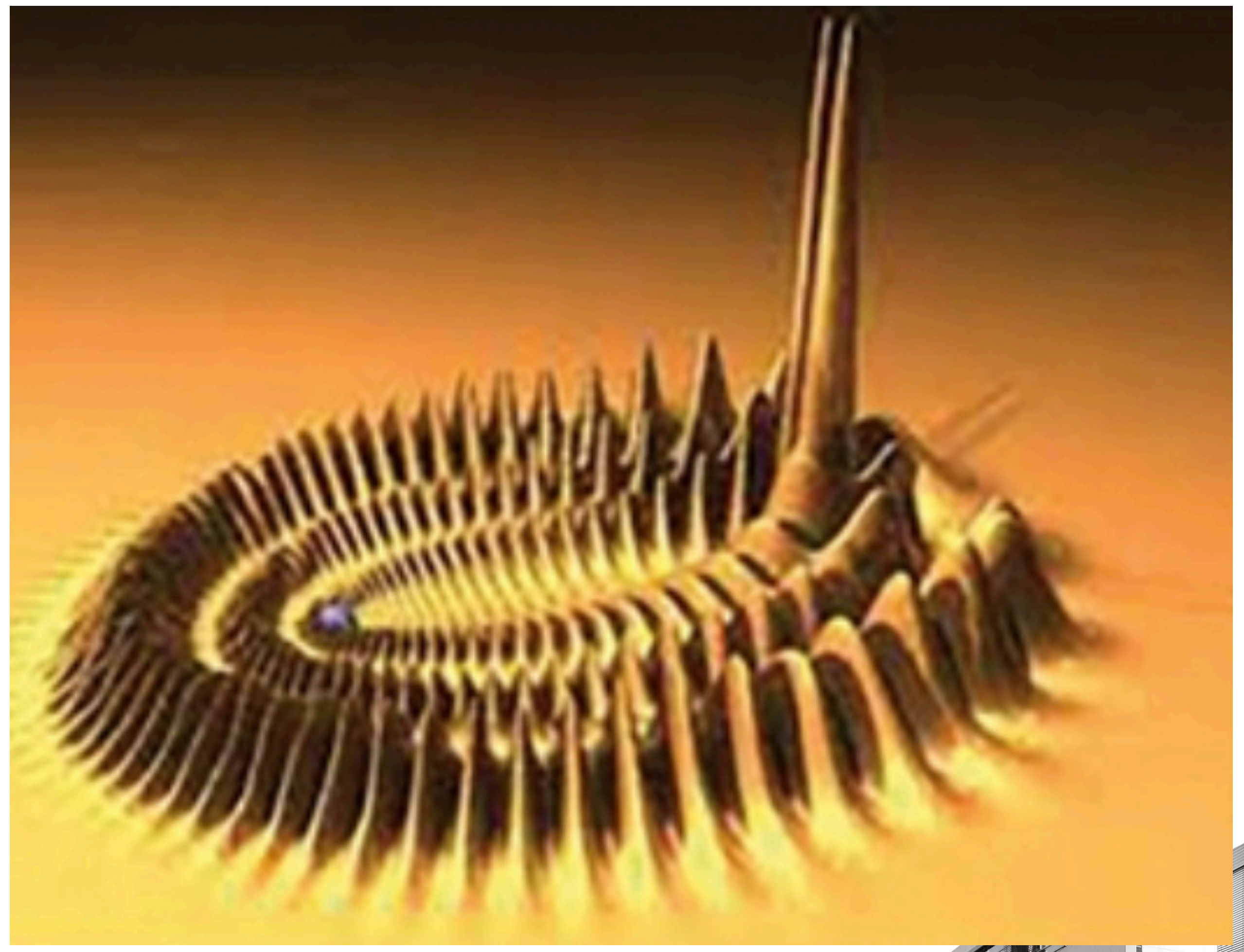




C. H. Greene, A. S. Dickinson, and H. R. Sadeghpour. PRL. **85,** 2458 (2000)

Degenerate non-quantum-defect case

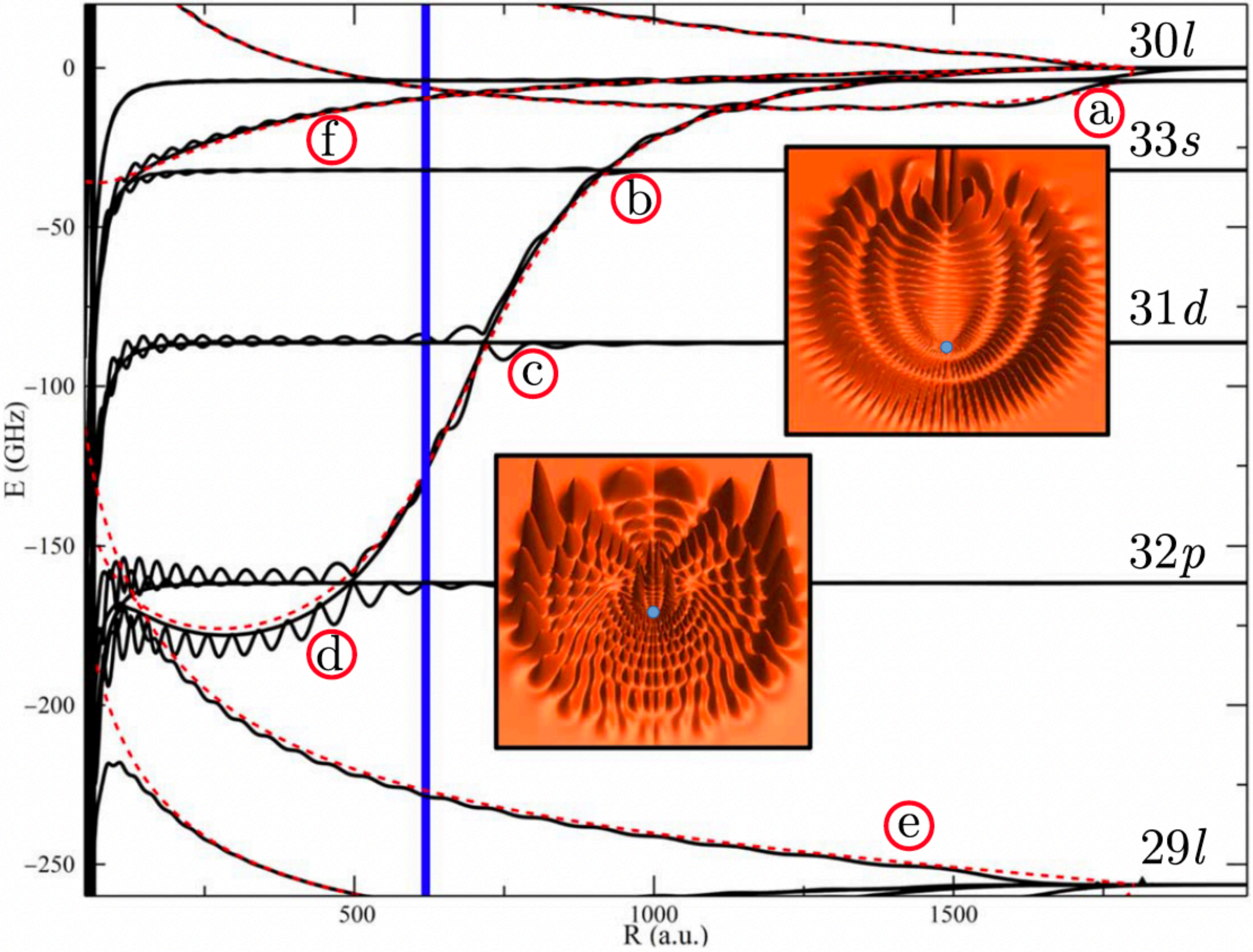
Now we get desperate and start looking at higher-order scattering…

$$V(\overrightarrow{R},\vec{r}) = H_{\text{electron}} + 6\pi a_p^3 \nabla \delta^3(\vec{r} - \overrightarrow{R}) \nabla$$

(and repeat the same procedure, knowing that alkali atoms have p-wave shape resonances and this term should be large…)

$$\implies U(R) = 6\pi a_p^3 \sum_{l\geq l_0}^{n-1} \left|\psi'_{nlm}(\overrightarrow{R})\right|^2 .$$

Trilobites and butterflies



Full picture:

1) degenerate and non-degenerate levels
2) butterfly state from p-wave interaction
3) phase shifts determine strengths: compare singlet and triplet phases
4) STILL NO COULOMB

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Degenerate non-quantum-defect case

Now we get really desperate and start looking at even higher-order scattering…

…and diagonalize a D-wave pseudopotential, with matrix elements

$$V^{\mathrm{D}}_{\alpha\alpha'} = 5\pi a_d^5[k(R)]\,\langle nlm|\left(3\left(\overleftarrow{\nabla}\cdot\overrightarrow{\nabla}\right)^2 - \overleftarrow{\nabla}^2\overrightarrow{\nabla}^2\right)|n'l'm'\rangle\,.$$

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These “simplify” to

$$V^{\mathrm{D},M=0}_{\alpha\alpha'} = -\frac{5a_d^5}{8R^6}\left(f_{nl}(R)u_{nl}(R) - 6Ru'_{nl}(R)\right)\left(f_{nl'}(R)u_{nl'}(R) - 6Ru'_{nl'}(R)\right)\sqrt{(2l+1)(2l'+1)}$$

$$f_{nl}(R) = 6 + 3l(l+1) - 4R + 2(R/n)^2$$

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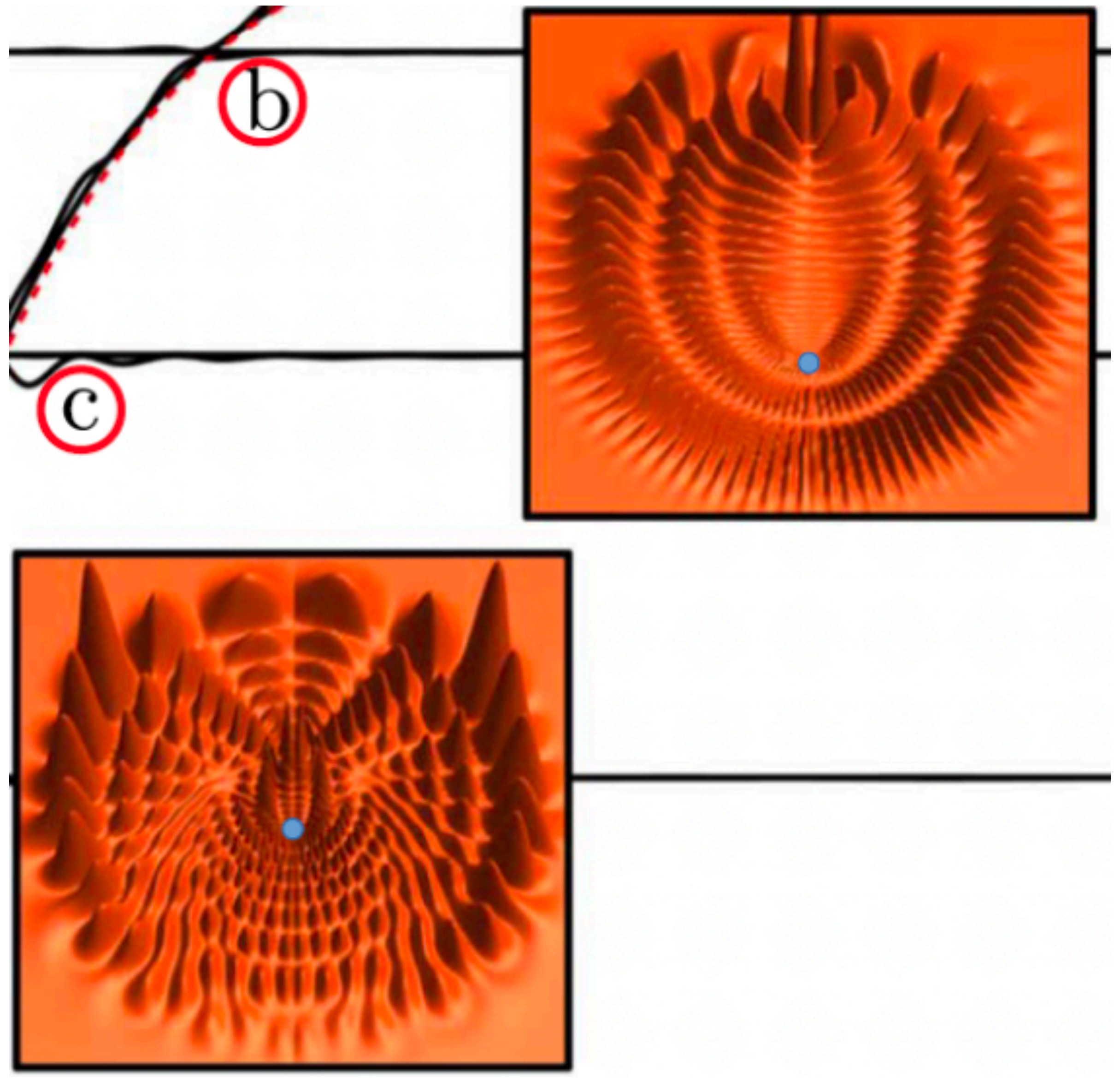
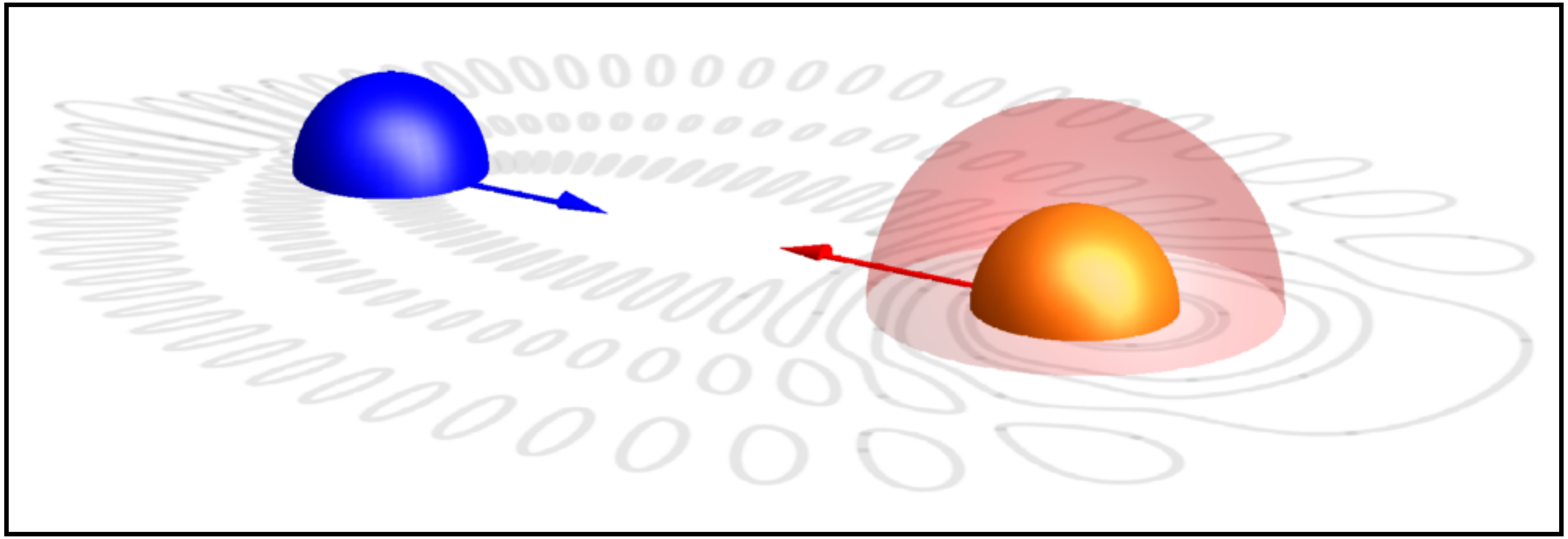
$$f_{nl}(R) = 6 + 3l(l+1) - 4R + 2(R/n)^2$$



Can the neutral atom be “dressed” by some charge?

Since the electron localizes near the ground state atom, we can calculate the “effective excess charge” sitting there…



This way we can try to get simpler expressions and make it look as Coulombic as possible!

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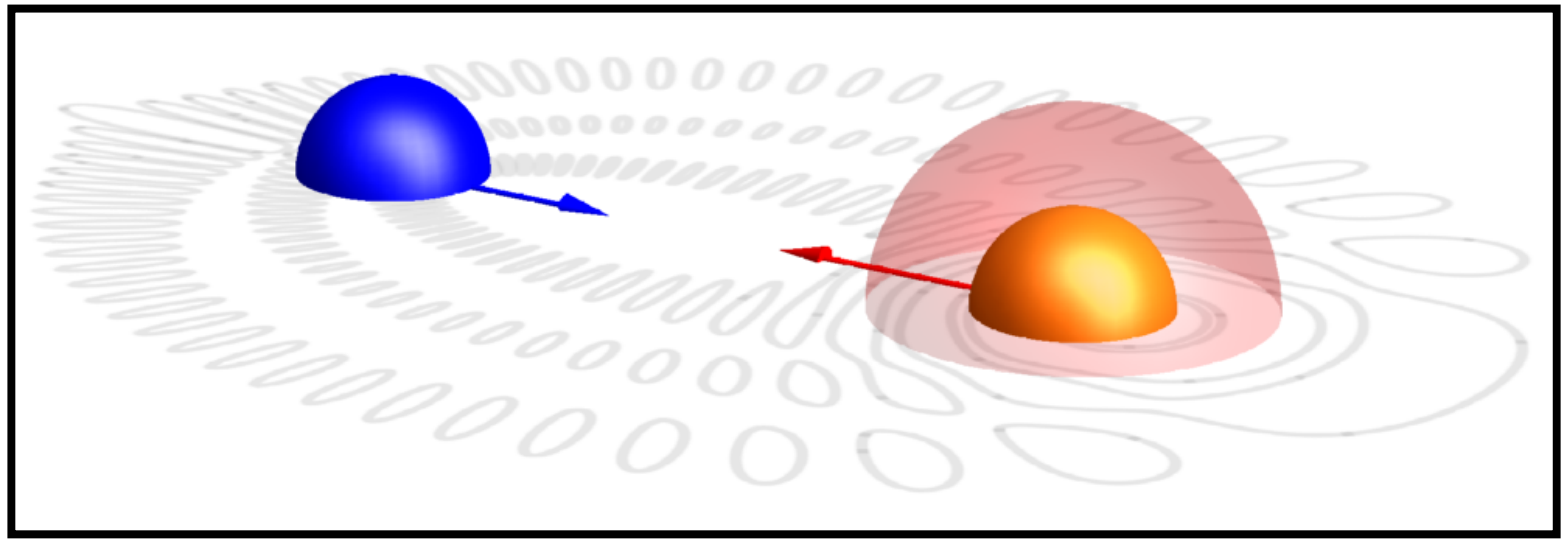

$$Q_L(\xi_0, R) = -\int_{\xi \le \xi_0} \left(|\Phi_L(\boldsymbol{\xi})|^2 - |\Phi_L^0(\boldsymbol{\xi})|^2\right) \mathrm{d}\boldsymbol{\xi},$$

$$\Phi_L(\boldsymbol{\xi}_0) \to A\sqrt{\frac{2}{\pi k}} \sin[k\xi_0 - L\pi/2 - \delta_L(k)] Y_{LM}(\hat{\xi}_0),$$

$$Q_L(\xi_0, R) = -\left(\frac{d\nu}{dE}\right)^{-1} \left(\frac{\delta_L'(k)}{\pi k} - \frac{\cos(2k\xi_0 - L\pi - \delta_L(k)) \sin \delta_L(k)}{\pi k^2}\right)$$

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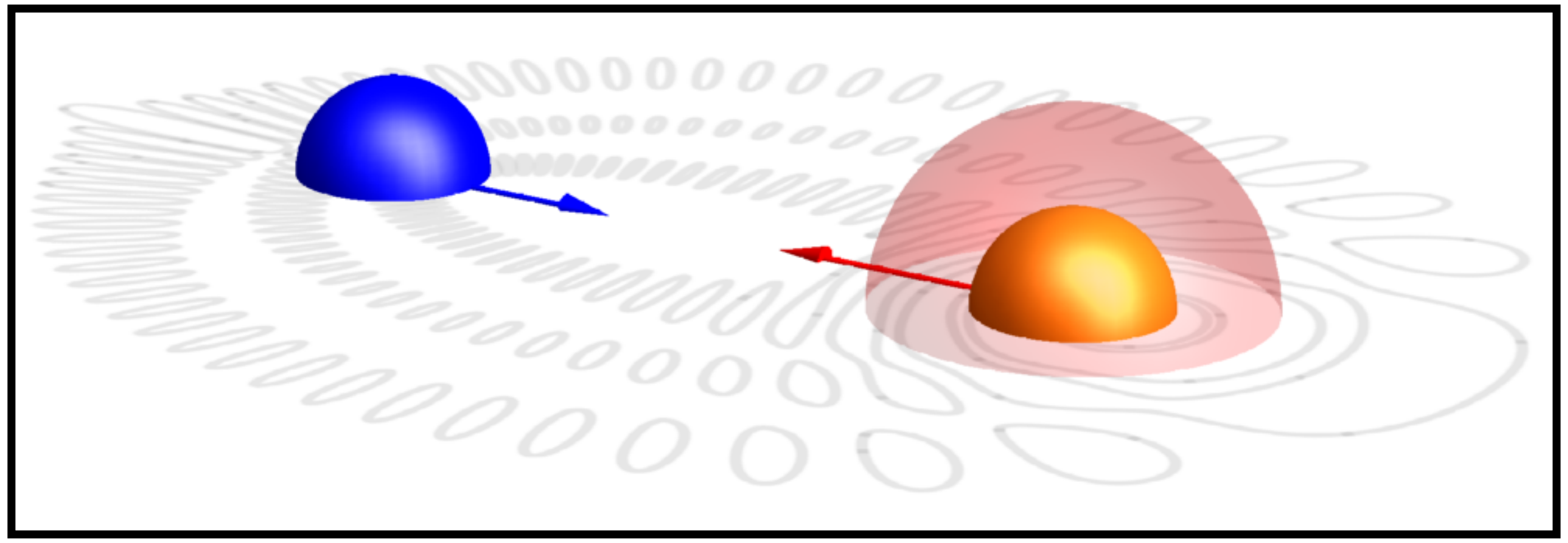

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$$\langle Q_L(R)\rangle = -\frac{1}{2n^3}\left(\frac{2}{\pi k}\frac{d\delta_L(k)}{dk}\right)$$

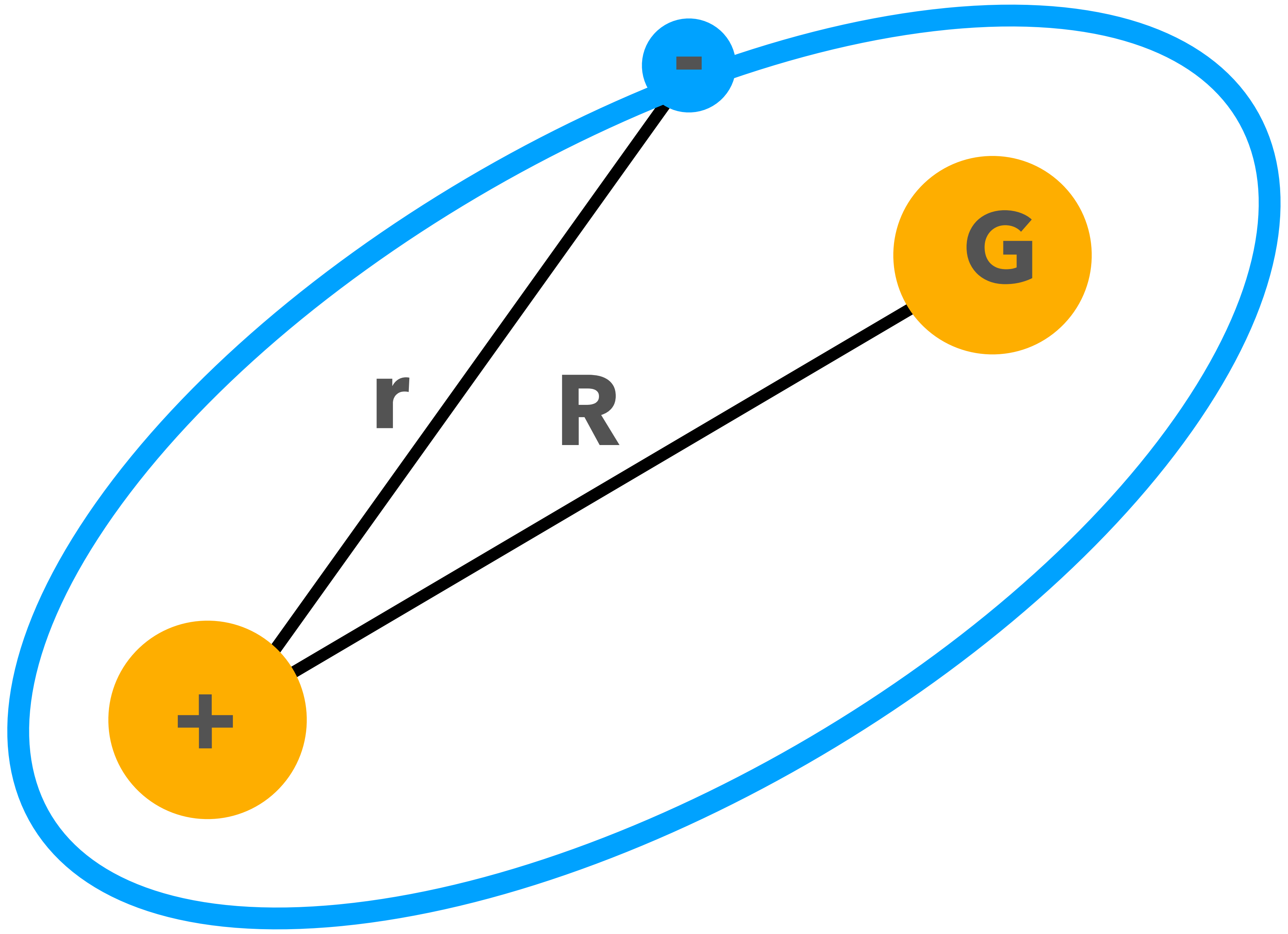
intuition: the charge is proportional to the *time delay.*
—if scattering causes the electron to lag behind a free electron, it 'spends more time' by the perturber and negative charge accumulates.
—and vice versa

This implies a Coulomb force!

$$F_L(R) = \frac{\langle Q_L(R) \rangle}{R^2} \qquad U_L(R) = -\int F_L(R)\mathrm{dR}$$

After doing the integral…

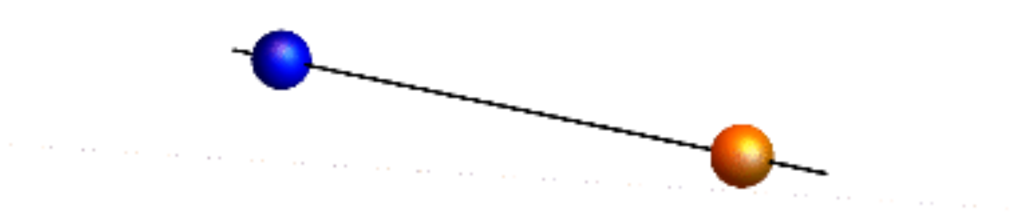
$$U_L(R) = \frac{1}{2n^2} - \frac{1}{2\left(n - \frac{\delta_L(k)}{\pi}\right)^2}$$

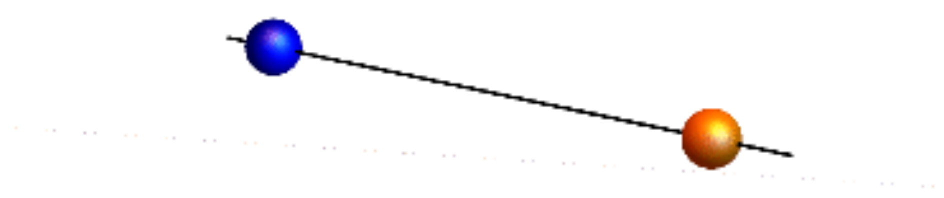


Dressed ion-pairs?

trilobite **butterfly**

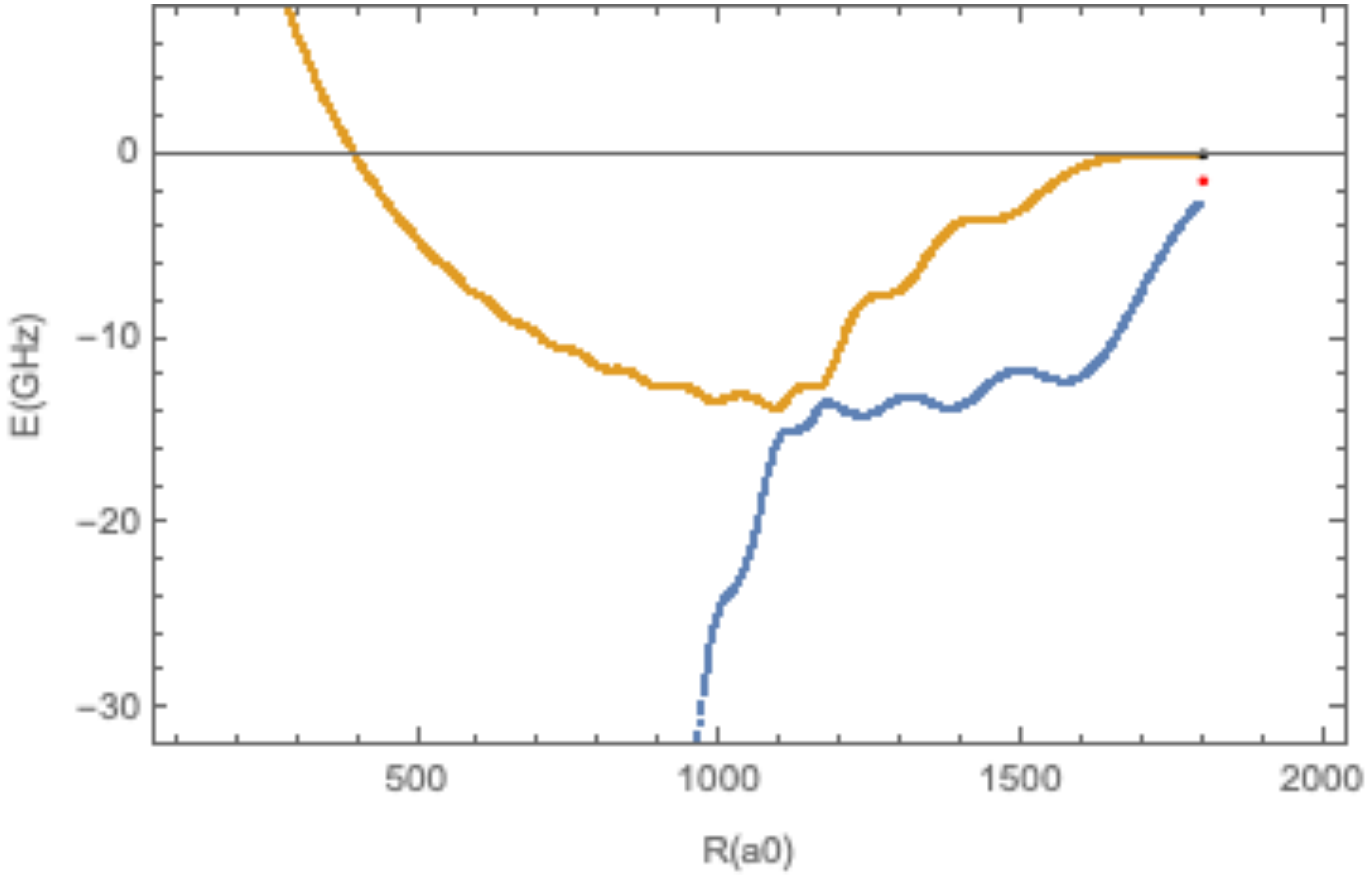
charges: red = negative / green = positive





potential energy curves

black / red are the semiclassical result



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PUT THE PIECES TOGETHER

Let’s take our charge…

$$\langle Q_L(R)\rangle = -\frac{1}{2n^3}\left(\frac{2}{\pi k}\frac{d\delta_L(k)}{dk}\right)$$

and the phase shifts for L>1 calculated earlier…

$$\delta_L(k) = \overline{\alpha_L}k^2$$

$$\overline{\alpha_L} = \frac{\alpha}{(4L^2-1)(2L+3)}$$

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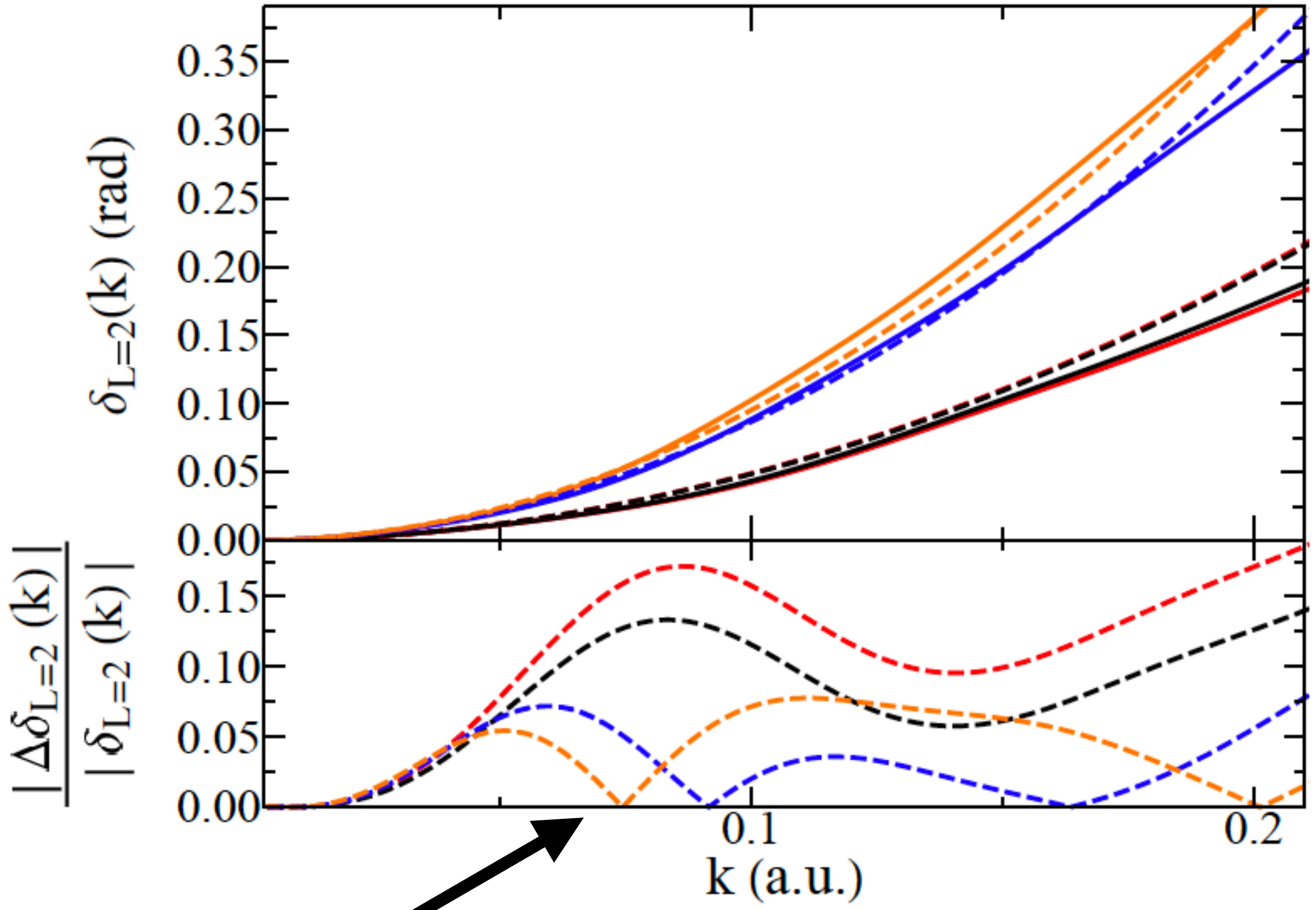
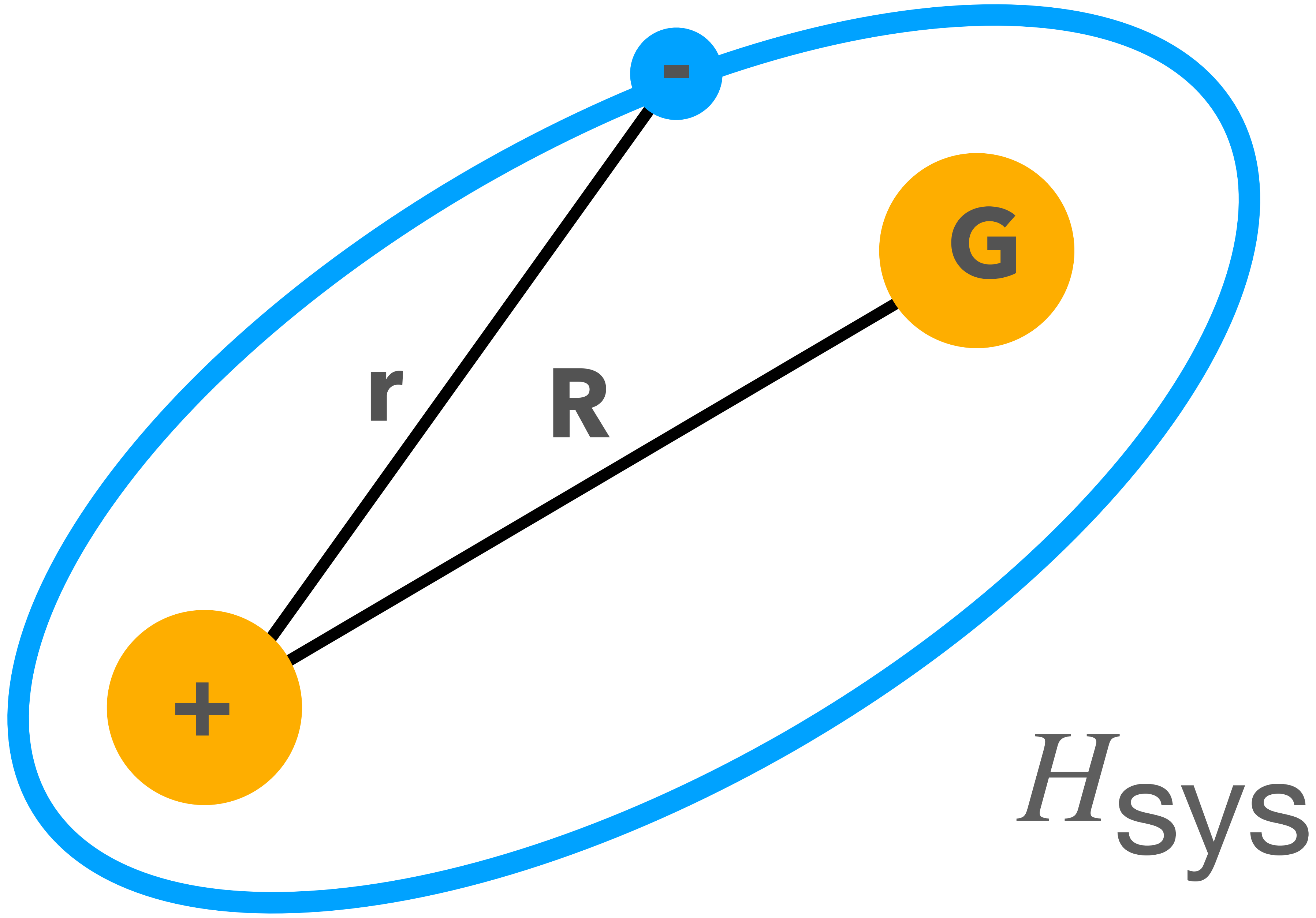


Born vs real phase shifts

Building a quantum simulator of a Rydberg atom

Using a Rydberg atom bound to a ground state molecule to form an *ultralong-range Rydberg molecule*, we want to simulate…a Rydberg atom.



The target Hamiltonian:

$$H_{\text{sim}} = -\frac{\nabla_R^2}{2M} - \frac{Z}{R} + V_{sr}(R)$$

The actual Hamiltonian:

$$H_{\text{sys}} = -\frac{\nabla_R^2}{2M} - \frac{\nabla^2}{2} - \frac{1}{r} + V_{sr}(r) + U(\vec{r} - \vec{R}) \, .$$

$$H_{\text{sys}} = -\frac{\nabla_R^2}{2M} + \frac{1}{2n^2} - \frac{1}{2(n - \delta_L(k)/\pi)^2}$$

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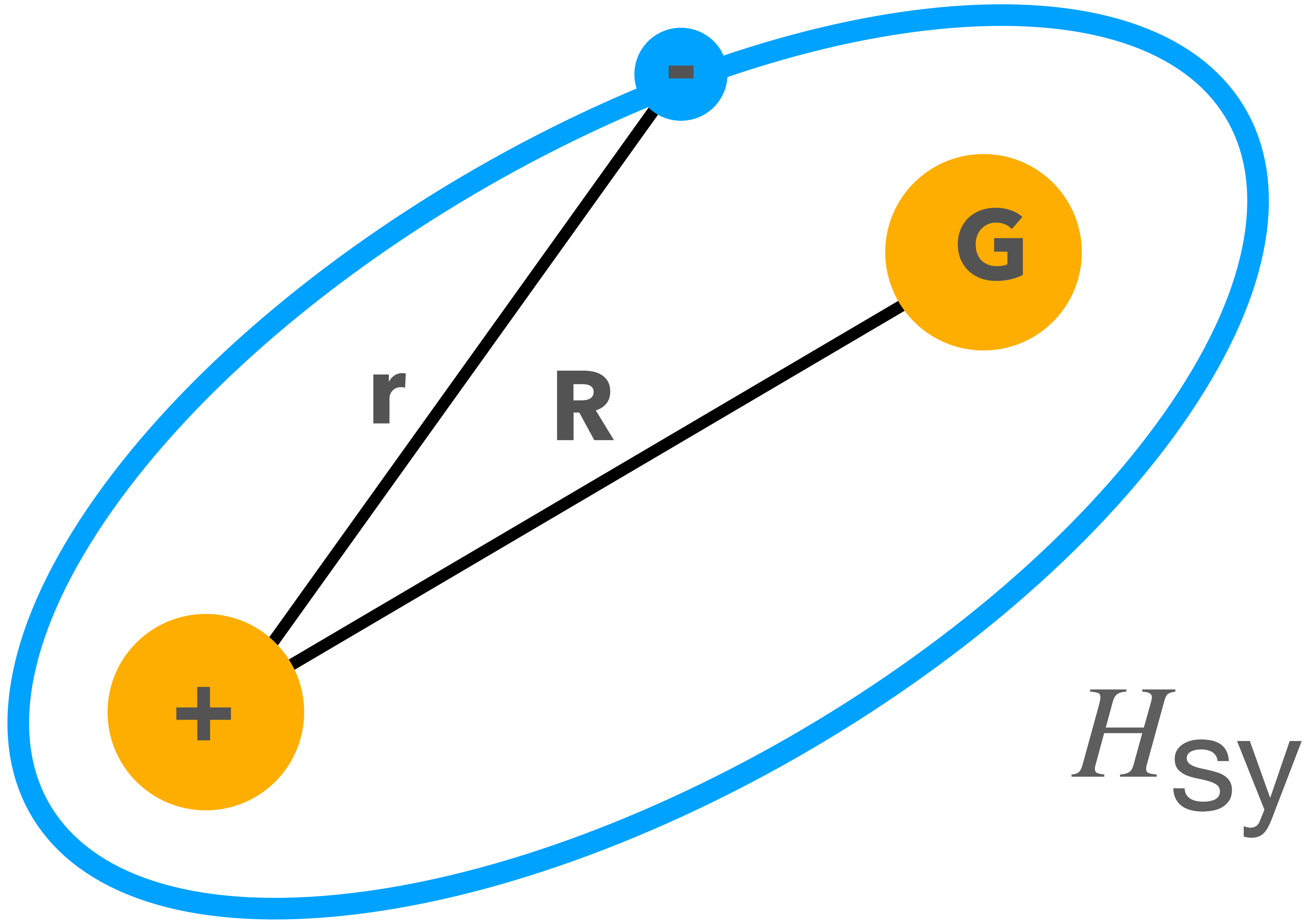

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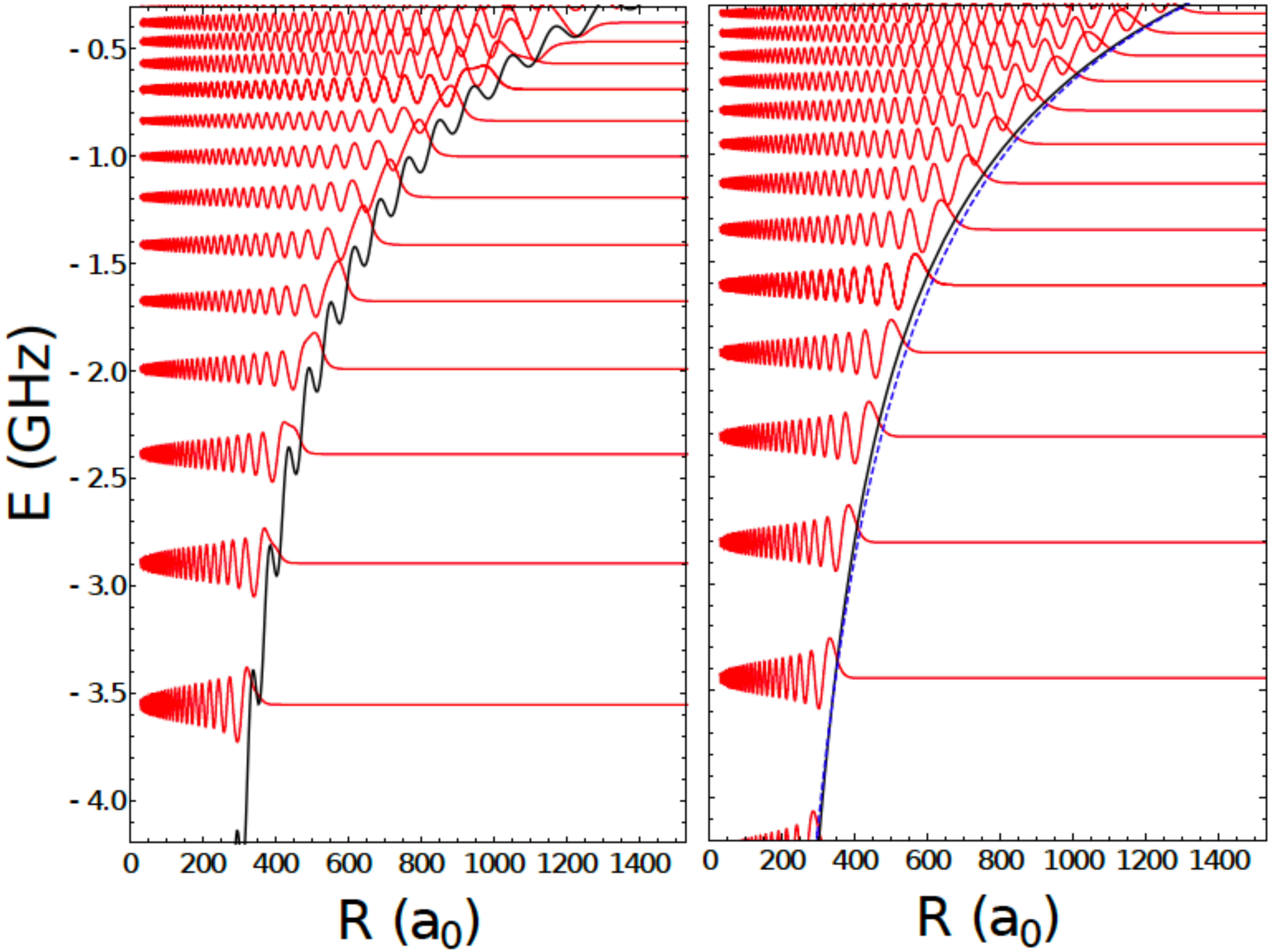
$$H_{\mathrm{sys}} = -\frac{\nabla_R^2}{2M} - \frac{2\overline{\alpha}_L/n^3}{R} + \dots$$

A Rydberg molecule simulator of a Rydberg atom



(every fourth bound state is plotted)

$$E_N^{nL} = -\frac{R'_{nL}}{(N-\mu)^2}$$

$$R'_{nL} = \frac{2M\overline{\alpha_L}}{m_e n^6}$$

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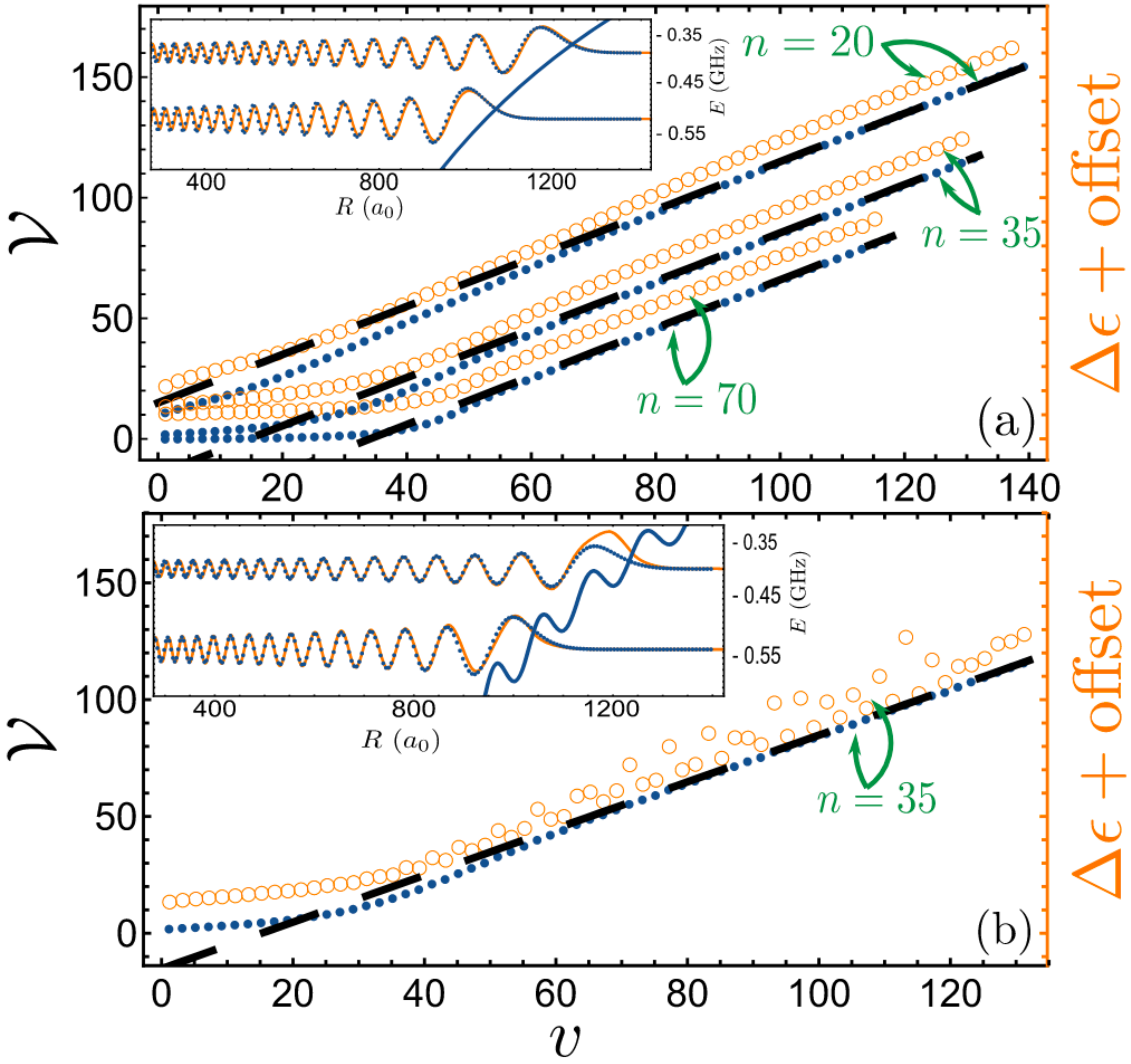
A Rydberg molecule simulator of a Rydberg atom



Giannakeas, **MTE**, Robicheaux, and Rost PRL **125** 123401 (2020); Giannakeas, **MTE**, Robicheaux, and Rost PRA **102** 033315

A Rydberg molecule simulator of a Rydberg atom

Does this quantum simulator obey our criteria?

Why or why not?

If we can calculate it, do we need to "simulate" it?