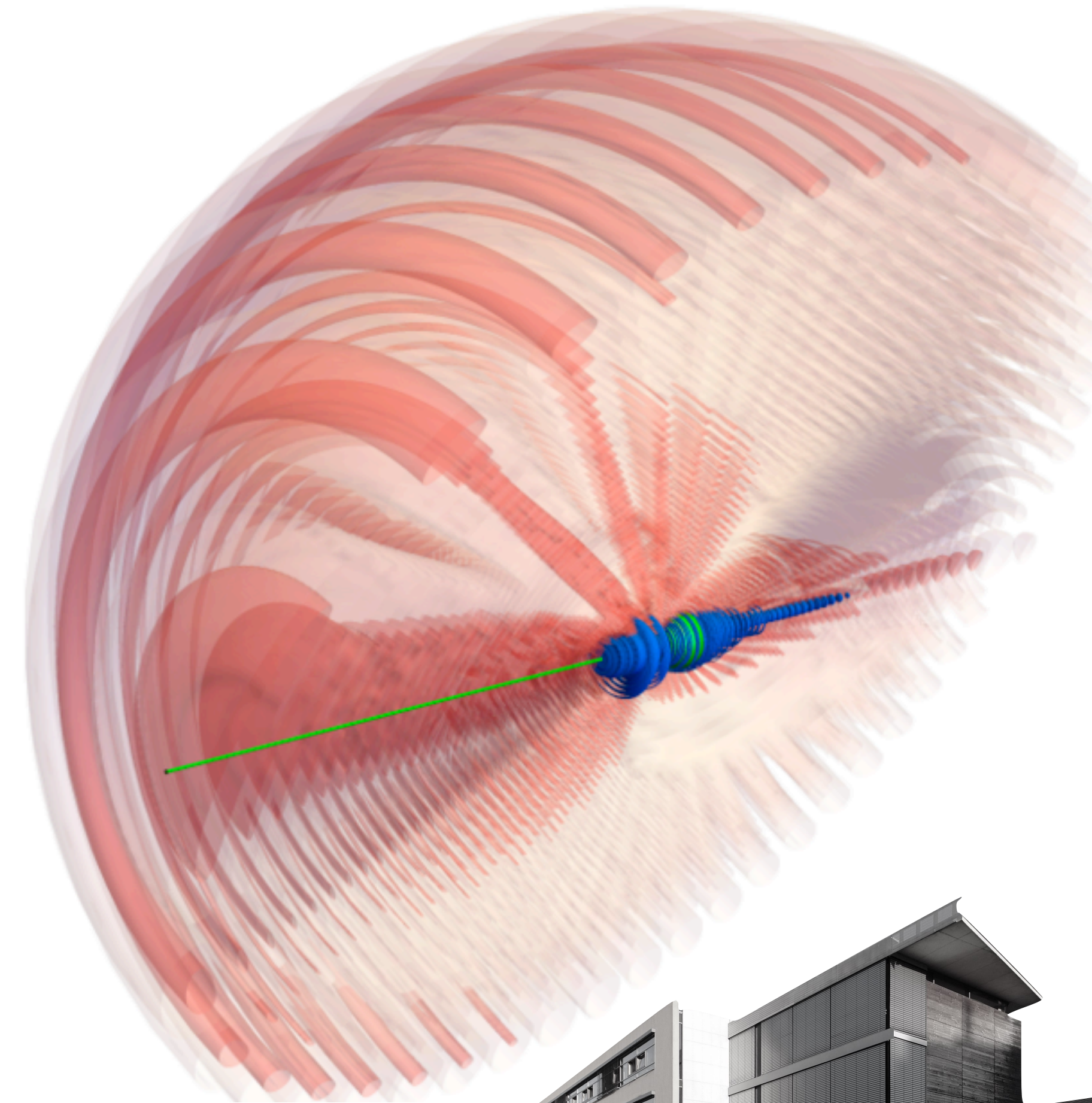


Quantum simulation from first principles

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

What this is:

- The first of two lectures on quantum simulation from **first principles** - in other words, from a few-body perspective.
- An introduction to / overview of **analog** quantum simulation with a very brief introduction to the experimental platforms highlighted this week.
- A discussion of several of the “first principles” concepts needed to understand them.
- A time to ask plenty of **questions** (perhaps to be answered tomorrow)
- ... and **discuss!**



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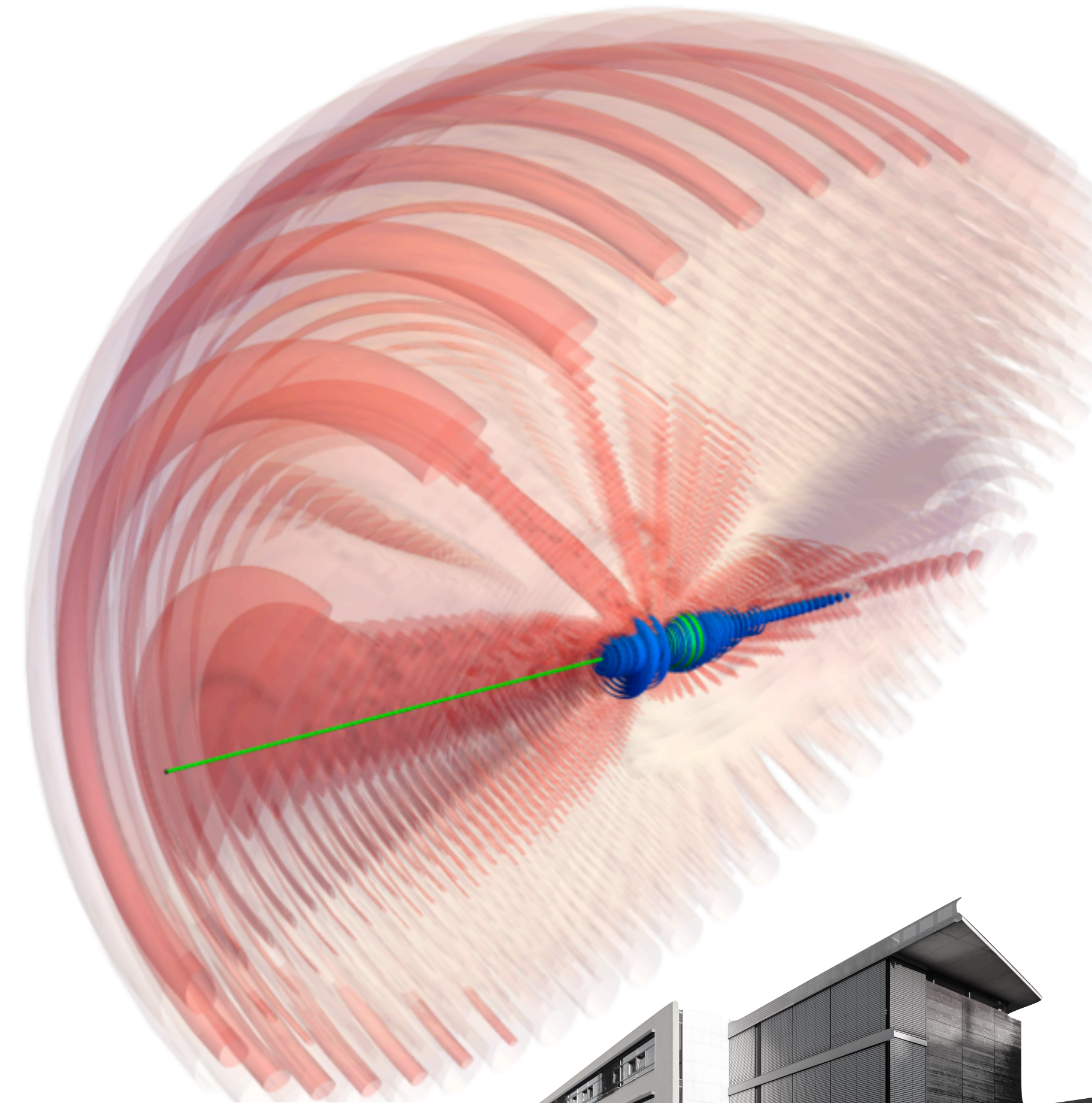
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Rough outline:

- What is analog quantum simulation, and how can we build the simulators?
- How to design a quantum **Rydberg atom simulator**.
 - What is the structure of an atom? Of a Rydberg atom?
 - How do atoms interact?
 - Long-range electrostatic interactions. (break!)
 - **Review!**
 - Scattering theory: phase shifts, zero energy scattering length, time delay, and the Fermi / Huang-Yang pseudopotential.
 - Put it all together + more.



What is quantum simulation?

- **Obligatory Feynman quote (1981):** “Nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy.”



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- **The obligatory basic idea (2014, quoting many earlier papers):** “As an example the standard “threshold” $N = 40$ [spin-1/2] frequently cited in the literature...This implies storing $2^{40} \sim 10^{12}$ numbers....Assuming single precision, about $\sim 3.2 \times 10^{13}$ bits, that is 4 TB (terabytes) are required to represent the spin state of 40 particles in a computer memory. In order to put this in perspective, the U.S. Library of Congress has almost 160 TB of data. Double the number of spins, and $\sim 3.8 \times 10^{25}$ bits (or 5×10^{12} TB) would be required. This is roughly 10^4 times more than the amount of information stored by humankind in 2007.



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Key idea: find an experimental system governed by the same Hamiltonian as a model we want to study, and then probe that experimental system instead of doing the (difficult or even "impossible") calculations.



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- **Some good resources:**
 - **Quantum Simulation** Georgescu, Ashhab, and Nori Rev. Mod. Phys. **86** (2014)
 - **What is a quantum simulator?** Johnson, Clark, and Jaksch EPJ Quantum Tech. **1** (2014)
 - **Can one trust quantum simulators?** Hauke, Cucchietti, Tagliacozzo, Deutsch, and Lewenstein Rep. Prog. Phys. **75** (2012).



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- (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.
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We should demand that the mimicked models are not purely of academic interest but that they rather describe some interesting physical systems and solve open problems. This also means that the simulated models should be computationally very hard for classical computers (see also requirement (d))



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It is in particular desirable to be able to set the parameters in a regime where the model becomes tractable by classical simulations, because this provides an elementary instance of validating the QS.



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'computationally very hard for classical computers' may have several meanings: (i) an efficient classical algorithm to simulate the model might not exist / be known; (ii) the efficient scalable algorithm is known, but the required size is too large to be simulated. ALSO: it is desirable to realize QSs to simulate and to observe novel phenomena that so far are only theoretically predicted. Simulating and actually observing in the lab is **more than just simulating abstractly** on a classical computer.



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The requirements of reliability and efficiency are interrelated. In fact, we could try to improve the precision of a QS by averaging more experiments, but in hypersensitive regimes (like those close to quantum-phase transitions) the necessary number of repetitions can grow rapidly, bringing the overall efficiency of the QS down to the level of classical computers.

We conclude that the answer to the question 'Can we trust quantum simulators?' is **...to some extent.**



We just learned what Qs are and what they should do...
...next we will see some examples!

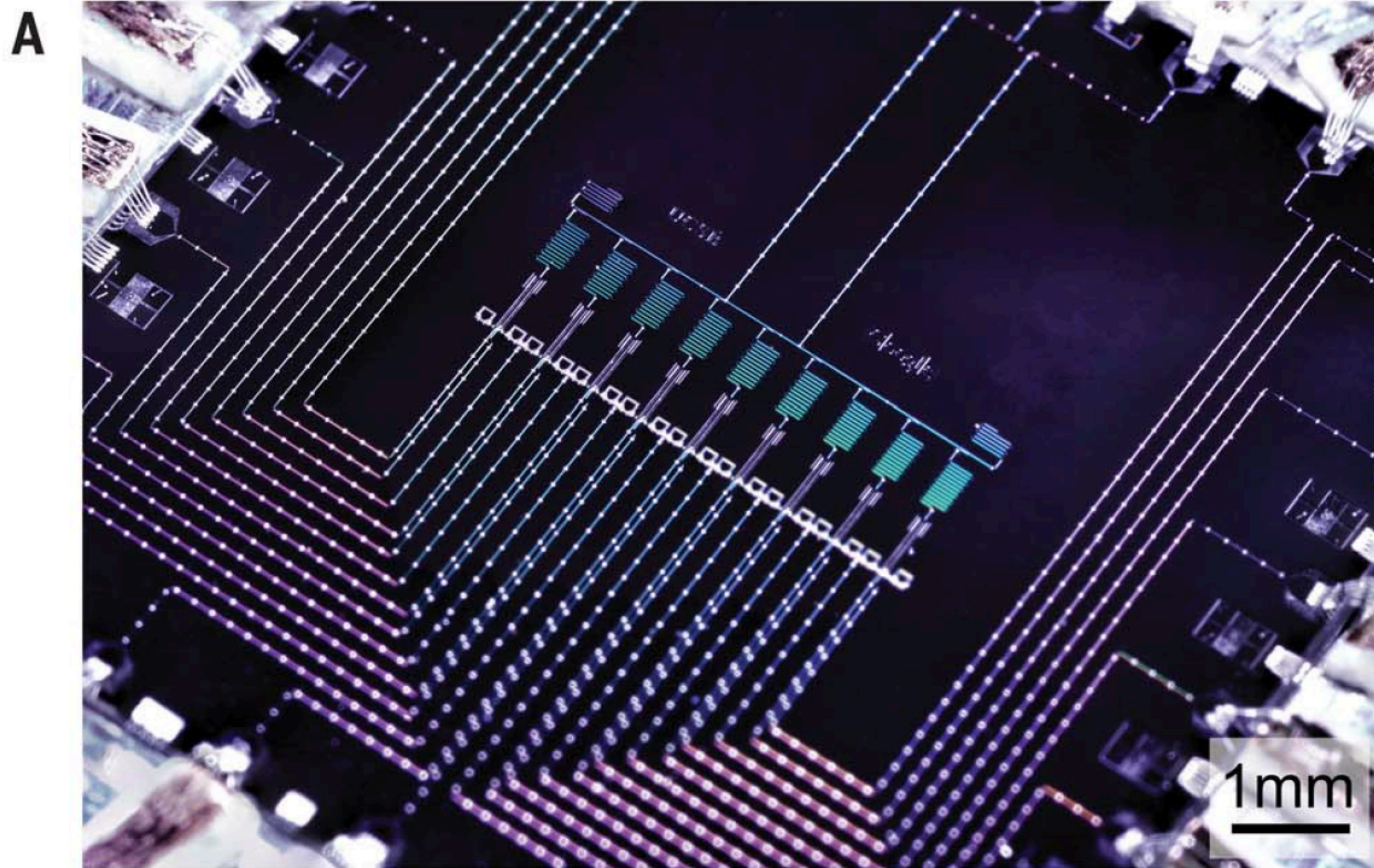


Quantum simulator exhibit A:

QUANTUM SIMULATION Roushan et al Science **358** (2017)

Spectroscopic signatures of localization with interacting photons in superconducting qubits

P. Roushan,^{1*} C. Neill,^{2†} J. Tangpanitanon,^{3†} V. M. Bastidas,^{3†} A. Megrant,¹ R. Barends,¹ Y. Chen,¹ Z. Chen,² B. Chiaro,² A. Dunsworth,² A. Fowler,¹ B. Foxen,² M. Giustina,¹ E. Jeffrey,¹ J. Kelly,¹ E. Lucero,¹ J. Mutus,¹ M. Neeley,¹ C. Quintana,² D. Sank,¹ A. Vainsencher,¹ J. Wenner,² T. White,¹ H. Neven,¹ D. G. Angelakis,^{3,4*} J. Martinis^{1,2}

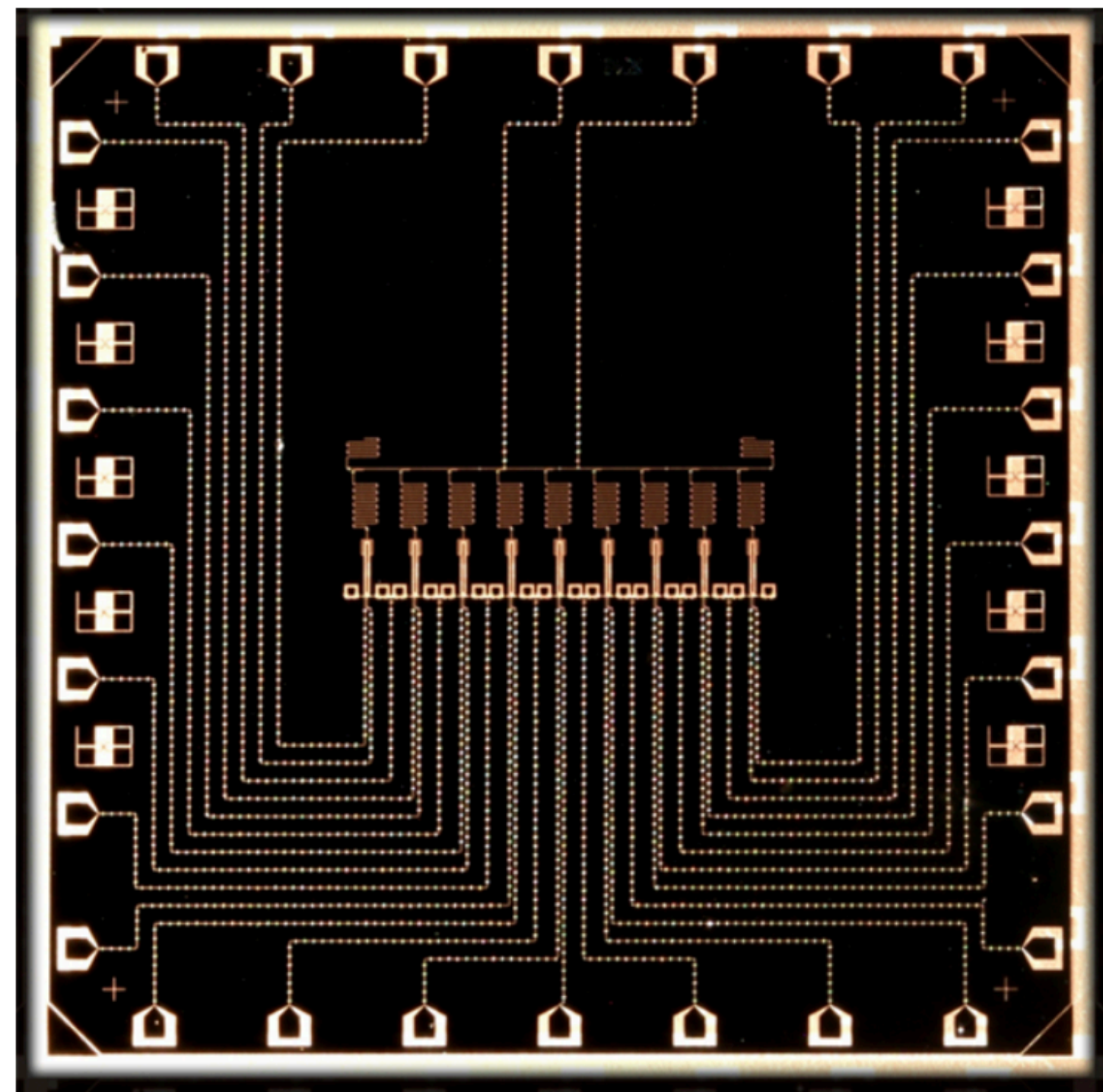


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1 cm

A quantum simulator of a 9-site **Bose-Hubbard model**:

$$H_{\text{BH}} = \sum_{n=1}^9 \mu_n a_n^\dagger a_n + \frac{U}{2} \sum_{n=1}^9 a_n^\dagger a_n (a_n^\dagger a_n - 1) + J \sum_{n=1}^8 a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1} \quad (2)$$

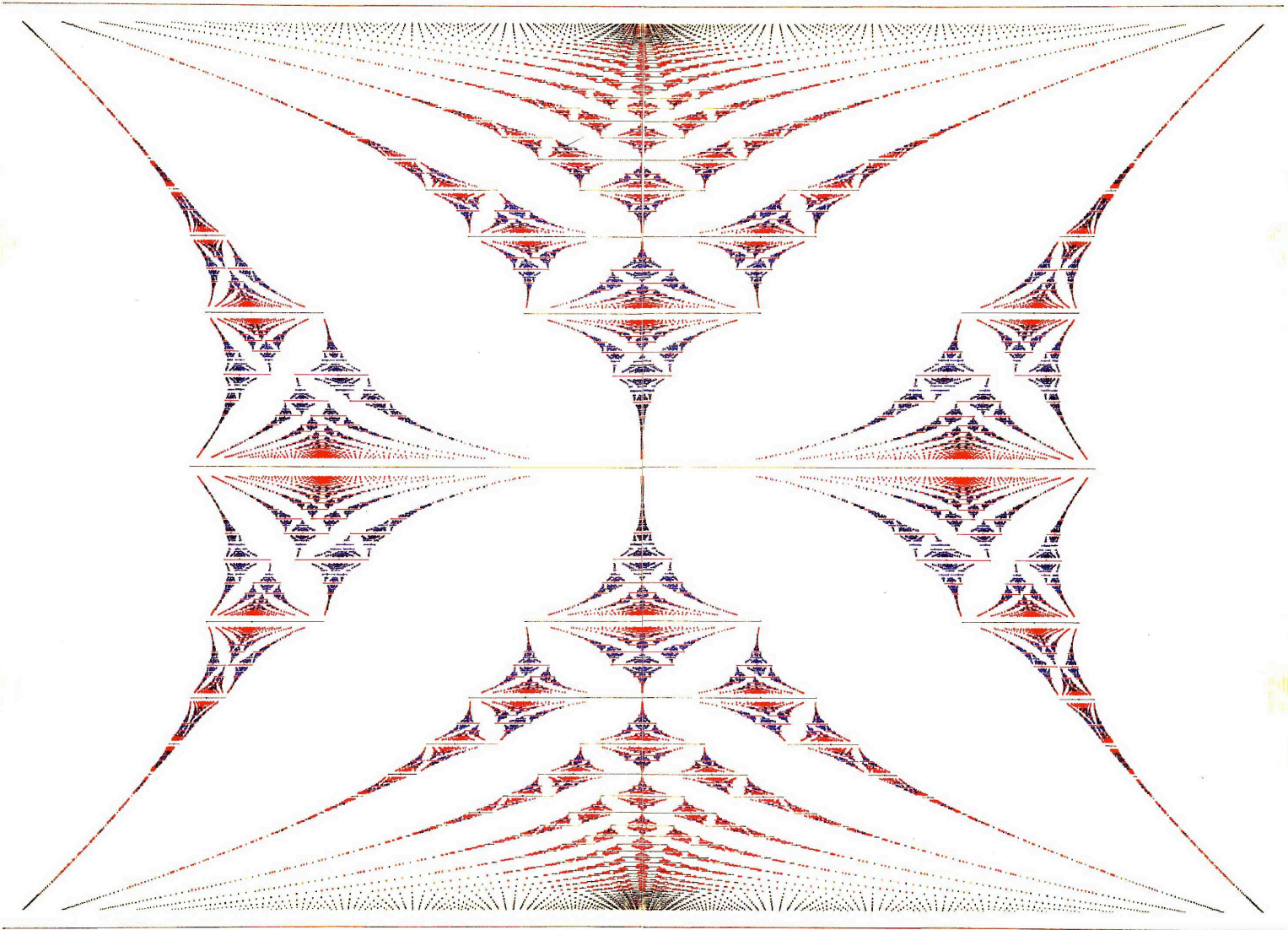
“Each of our qubits can be thought of as a nonlinear photonic resonator in the microwave regime...the qubit frequency, nearest-neighbor coupling, and nonlinearity set the on-site potential, the hopping rate, and the interaction, respectively”



Quantum simulator exhibit A:

First “simulation” tests **relevance, controllability, and reliability.**

A quantum simulator of a 9-site **Bose-Hubbard model:**



$$H_{\text{Harper}} = \Delta \sum_{n=1}^9 \cos(2\pi nb) a_n^\dagger a_n + J \sum_{n=1}^8 a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1}$$

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Relevance: “We simulate the problem of Bloch electrons on a 2D lattice subject to a perpendicularly applied magnetic field B. For typical crystals, the magnetic field required to “squeeze” one flux quantum through the unit cell is of the order of several tens of thousands of tesla, **too high to be experimentally feasible.**”

Reliability: “Recently, some features associated with the Hofstadter’s butterfly **were experimentally realized by using superlattices in graphene and cold-atom systems.**”

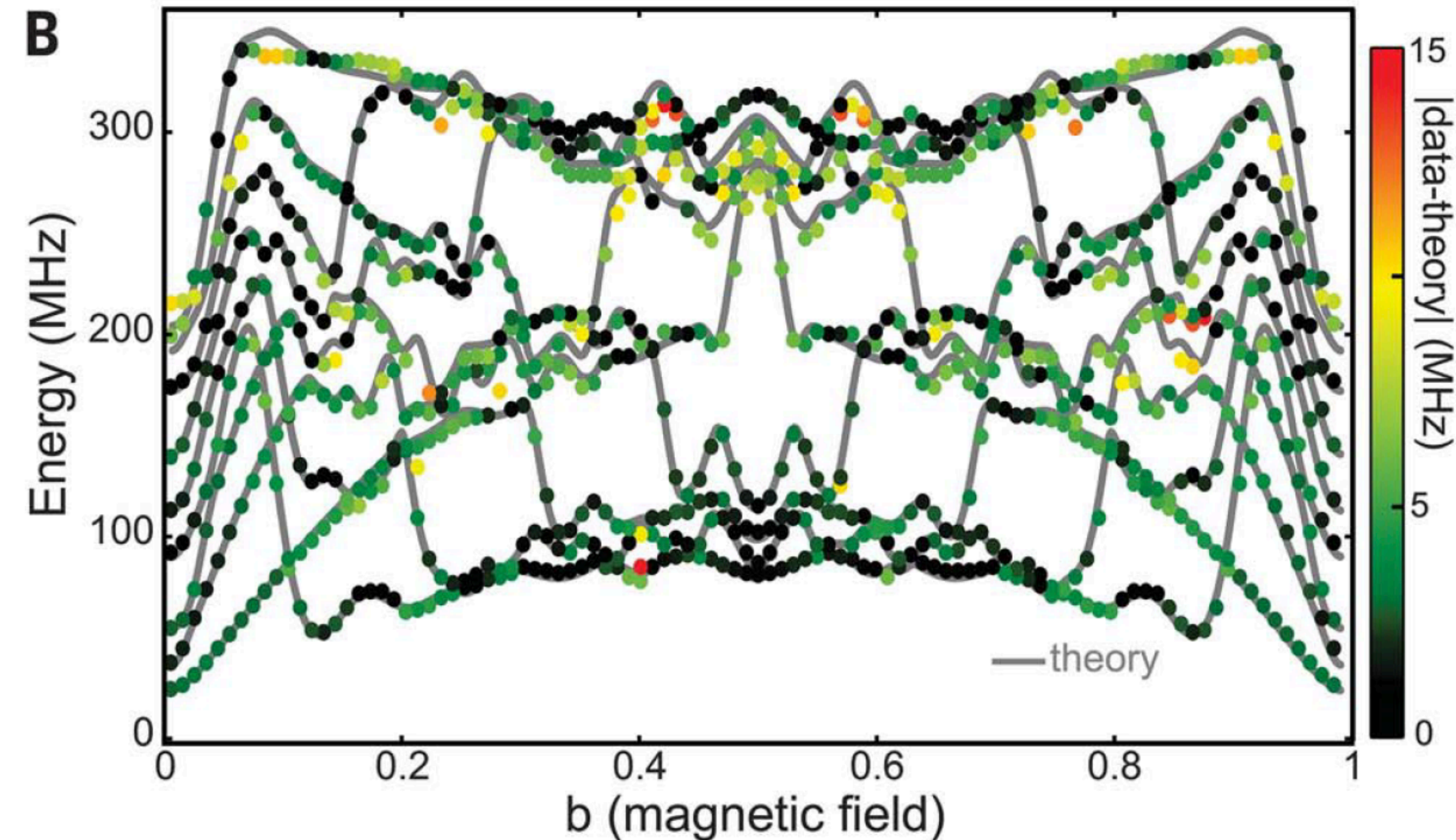
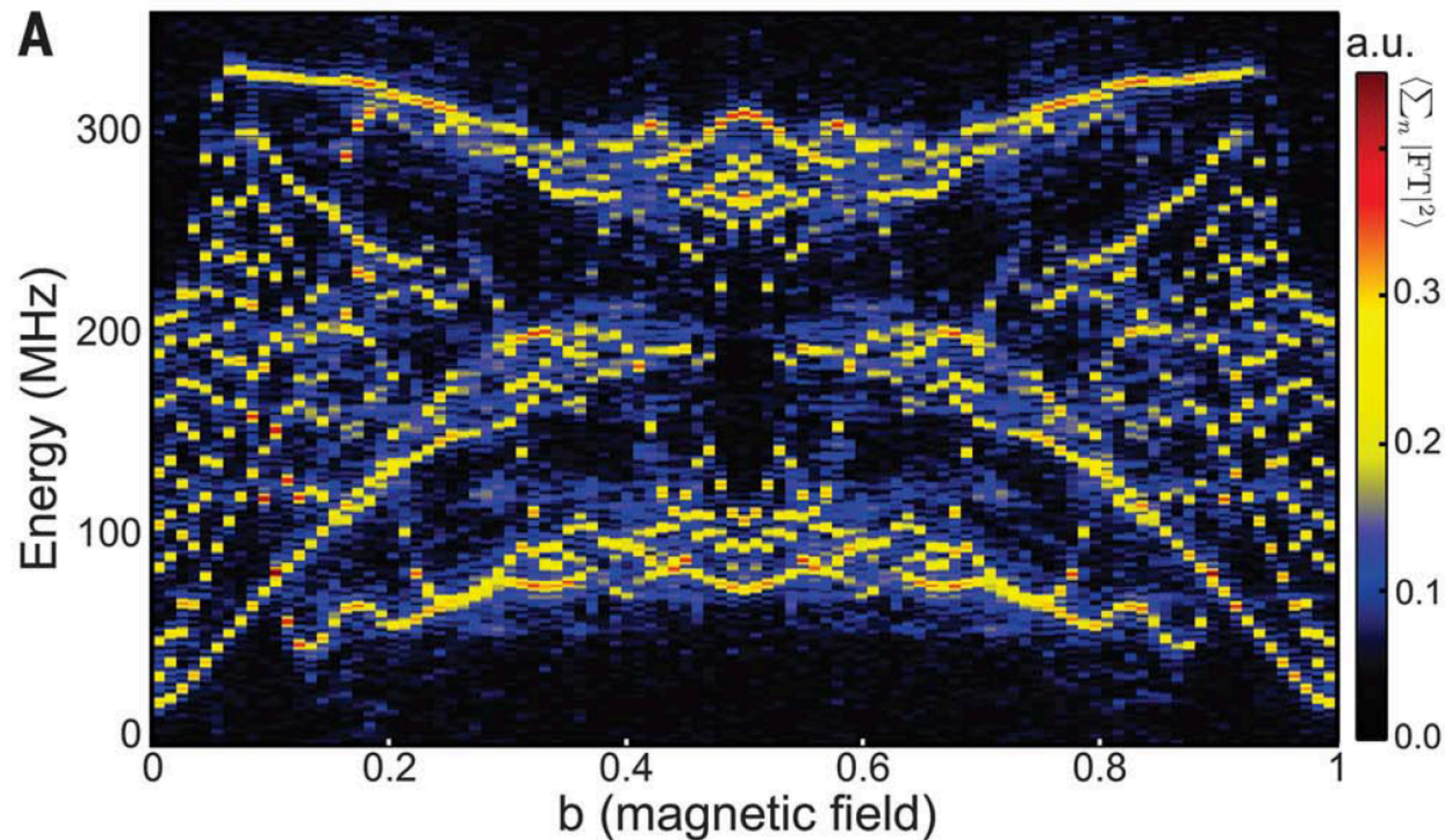
Controllability: Is claimed; will be proven if it works!



Quantum simulator exhibit A:

Experiment

Theory



“The average deviation is 3.5 MHz. This implies that we can set the matrix elements of the Hamiltonian, which in this case includes 17 terms, with <2% error. This capability of controlling a large quantum system is achieved through careful modeling of the qubits as nonlinear resonators.”



Quantum simulator exhibit A:

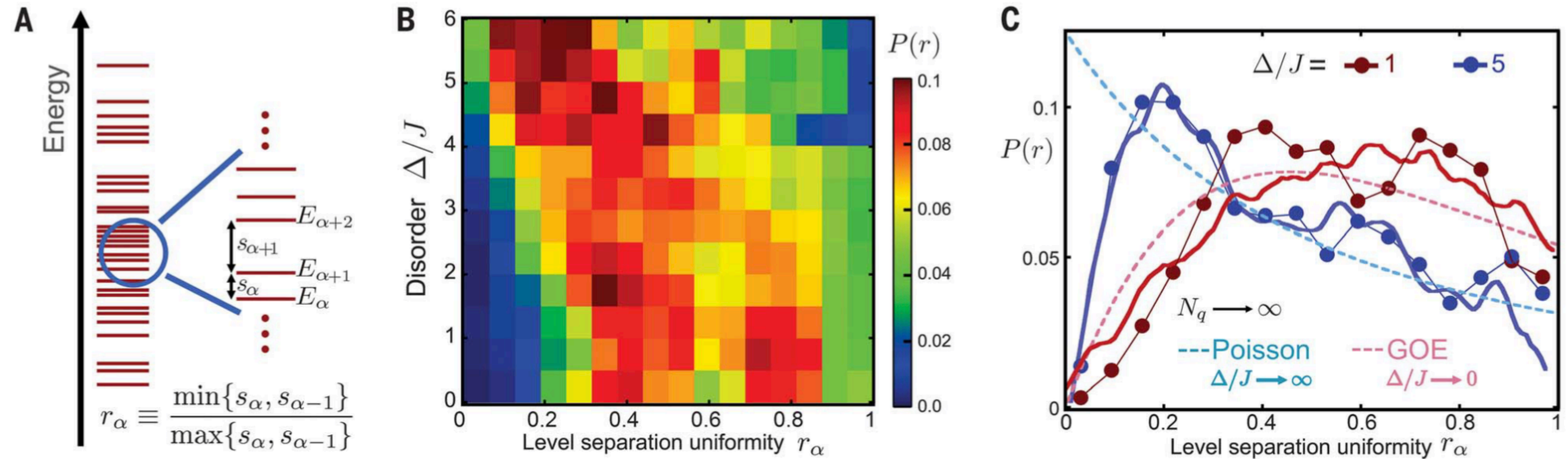


Fig. 3. Level statistics in a disordered potential. In Eq. 2, we set hopping to $J/2\pi = 50$ MHz, which fixes $U/J = 3.5$. To obtain a disordered potential, we set $\mu_n = \Delta \cos(2\pi n b)$ with four different irrational values of $b \in [0, 1]$ chosen and the results averaged over b . **(A)** The schematic of energy levels shows how r_α is defined. **(B)** The histogram of $P(r)$ measured

for various values of disorder Δ/J is presented as a color plot. **(C)** The measured histogram $P(r)$ of $\{r_\alpha\}$ for $\Delta/J = 1$ and 5. The dashed lines are plots of P_{Poisson} and P_{GOE} according to Eq. 4, and the solid lines are numerical simulations (21). The change from the GOE toward the Poisson distribution is indicative of vanishing of level repulsion with increase in Δ .

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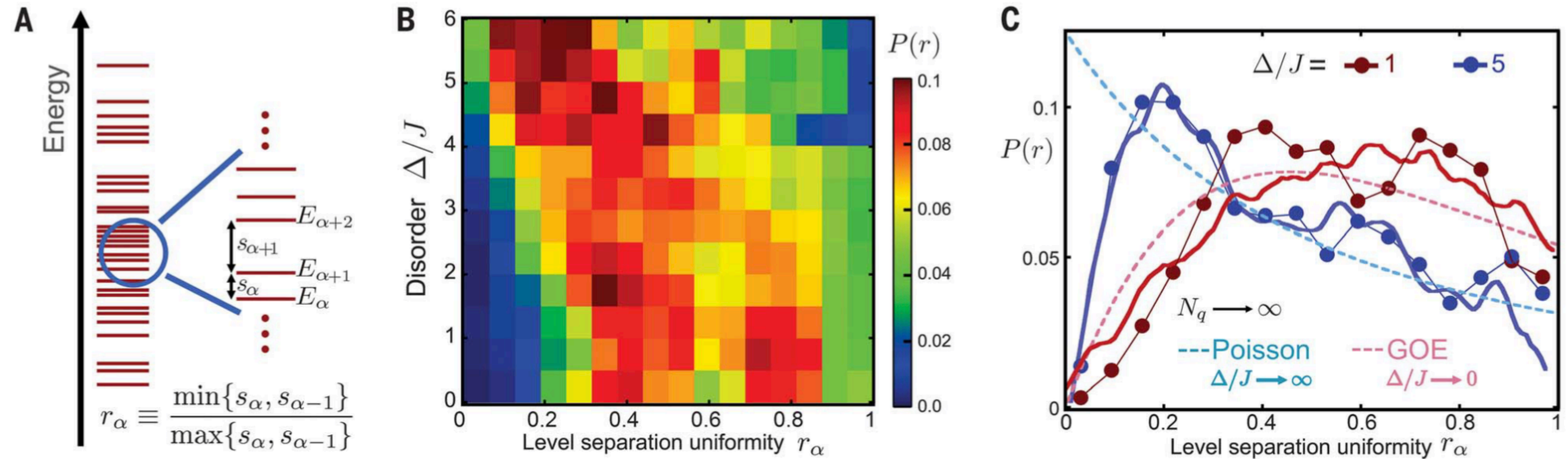


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Relevance: For larger numbers of qubits this will be relevant!

Reliability: ??

Efficiency: ~two days of measurements for this plot of a system with 45 states.



LETTERS

Quantum simulation of the Dirac equation

R. Gerritsma^{1,2}, G. Kirchmair^{1,2}, F. Zähringer^{1,2}, E. Solano^{3,4}, R. Blatt^{1,2} & C. F. Roos^{1,2}

The Dirac equation for a spin-1/2 particle with rest mass m is given by¹

$$i\hbar \frac{\partial \psi}{\partial t} = (c\boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + \beta mc^2)\psi$$

Here c is the speed of light, $\hat{\mathbf{p}}$ is the momentum operator, α_j ($j = 1, 2, 3$; $(\boldsymbol{\alpha})_j = \alpha_j$) and β are the Dirac matrices (which are usually given in terms of the Pauli matrices, σ_x , σ_y and σ_z), the wavefunctions ψ are four-component spinors and \hbar is Planck's constant divided by 2π . A general Dirac spinor can be decomposed into parts with positive and negative energies $E = \pm \sqrt{p^2 c^2 + m^2 c^4}$. Zitterbewegung is under-

“One of the most astonishing predictions of the single free-particle solutions of the Dirac equation is the fast quivering motion called Zitterbewegung. It is unexpected because it predicts an oscillatory motion of a freely propagating electron. The Zitterbewegung phenomenon has not been observed so far for a real relativistic electron, given that the predicted frequency, 10^{21} Hz, and amplitude, 10^{-11} cm, are difficult to access experimentally.”



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For the simulation, we trapped a single $^{40}\text{Ca}^+$ ion in a linear Paul trap²² with axial trapping frequency $\omega_{\text{ax}} = 2\pi \times 1.36$ MHz and radial trapping frequency $\omega_{\text{rad}} = 2\pi \times 3$ MHz. Doppler cooling, optical pumping and resolved sideband cooling on the $S_{1/2} \leftrightarrow D_{5/2}$ transition in a magnetic field of 4 G prepare the ion in the axial motional ground state and in the internal state $|S_{1/2}, m_j = 1/2\rangle$ (m_j , magnetic quantum number). A narrow-linewidth laser at 729 nm couples the states $\binom{0}{1} \equiv |S_{1/2}, m_j = 1/2\rangle$ and $\binom{1}{0} \equiv |D_{5/2}, m_j = 3/2\rangle$, which we identify as our spinor states. A bichromatic light field resonant with the upper and lower axial motional sidebands of the $\binom{1}{0} \leftrightarrow \binom{0}{1}$ transition with appropriately set phases and frequency realizes the Hamiltonian⁷

$$H_D = 2\eta\Delta\tilde{\Omega}\sigma_x\hat{p} + \hbar\Omega\sigma_z \quad (1)$$

Here $\Delta = \sqrt{\hbar/2\tilde{m}\omega_{\text{ax}}}$ is the size of the ground-state wavefunction, with \tilde{m} the ion's mass (not to be confused with the mass, m , of the

$$i\hbar\frac{\partial\psi}{\partial t} = H_D\psi = (c\hat{p}\sigma_x + mc^2\sigma_z)\psi$$

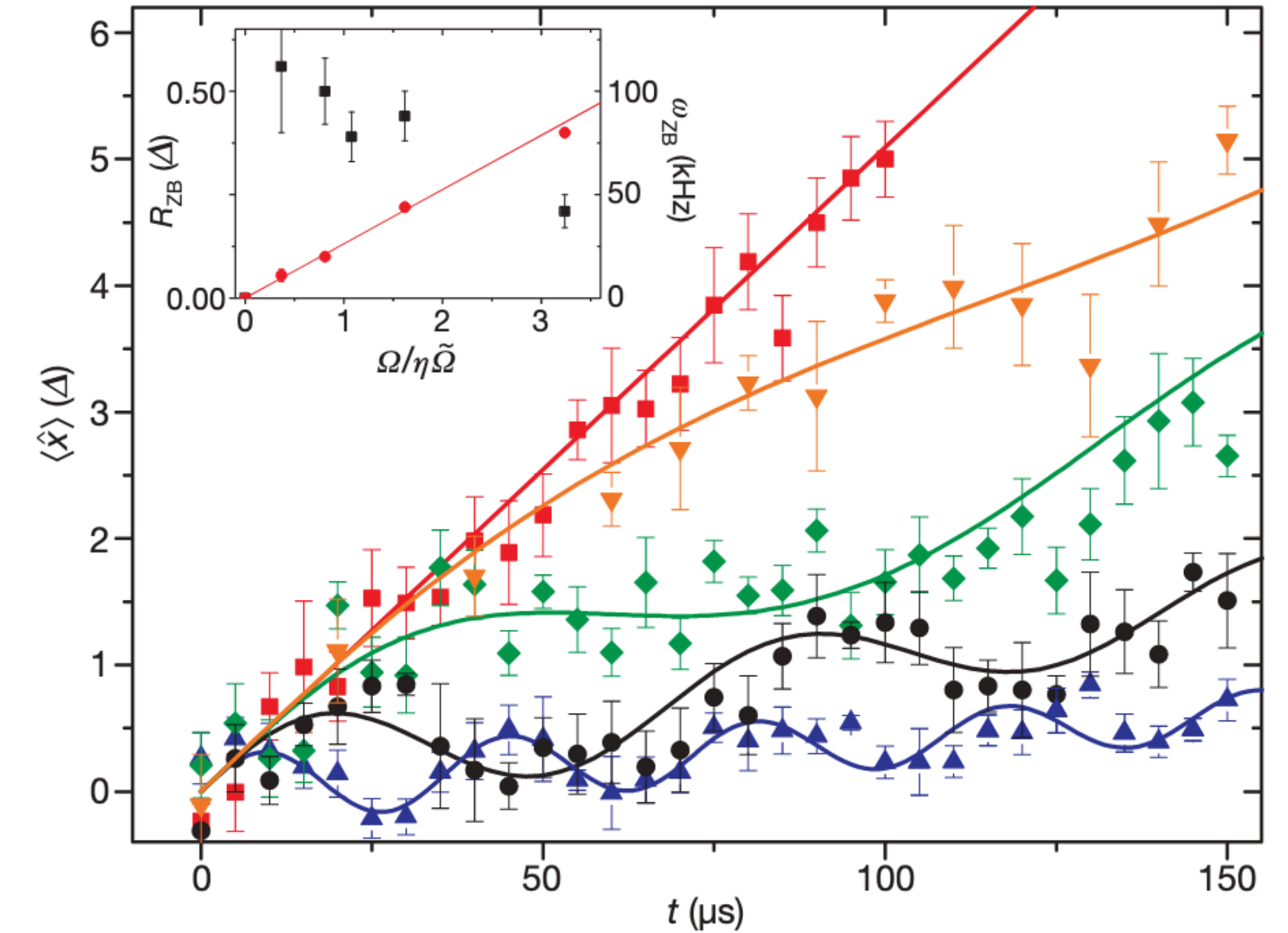


Figure 1 | Expectation values, $\langle\hat{x}(t)\rangle$, for particles with different masses. The linear curve (squares) represents a massless particle ($\Omega = 0$) moving at the speed of light, which is given by $c = 2\eta\tilde{\Omega}\Delta = 0.052\Delta \mu\text{s}^{-1}$ for all curves. From the top, the other curves represent particles of increasing masses. Their Compton wavelengths are given by $\lambda_C \equiv 2\eta\tilde{\Omega}\Delta/\Omega = 5.4\Delta$ (down triangles), 2.5Δ (diamonds), 1.2Δ (circles) and 0.6Δ (up triangles), respectively. The solid curves represent numerical simulations. The figure shows Zitterbewegung for the crossover from the relativistic limit, $2\eta\tilde{\Omega} \gg \Omega$, to the non-relativistic limit, $2\eta\tilde{\Omega} \ll \Omega$. Inset, fitted Zitterbewegung amplitude, R_{ZB} (squares), and frequency, ω_{ZB} (circles), versus the parameter $\Omega/\eta\tilde{\Omega}$ (which is proportional to the mass). Error bars, 1σ .

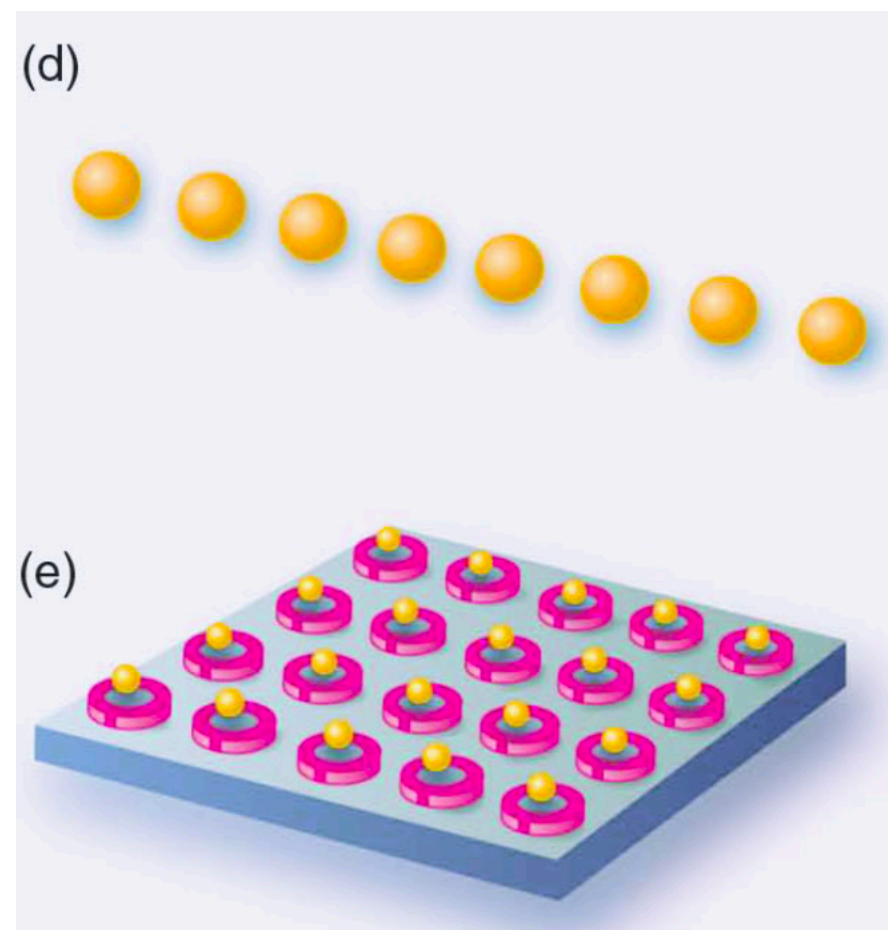


What are quantum simulators?

Lots of platforms have been proposed / exist to do analog (and sometimes digital as well) quantum simulation.
The four you will hear about this week are...

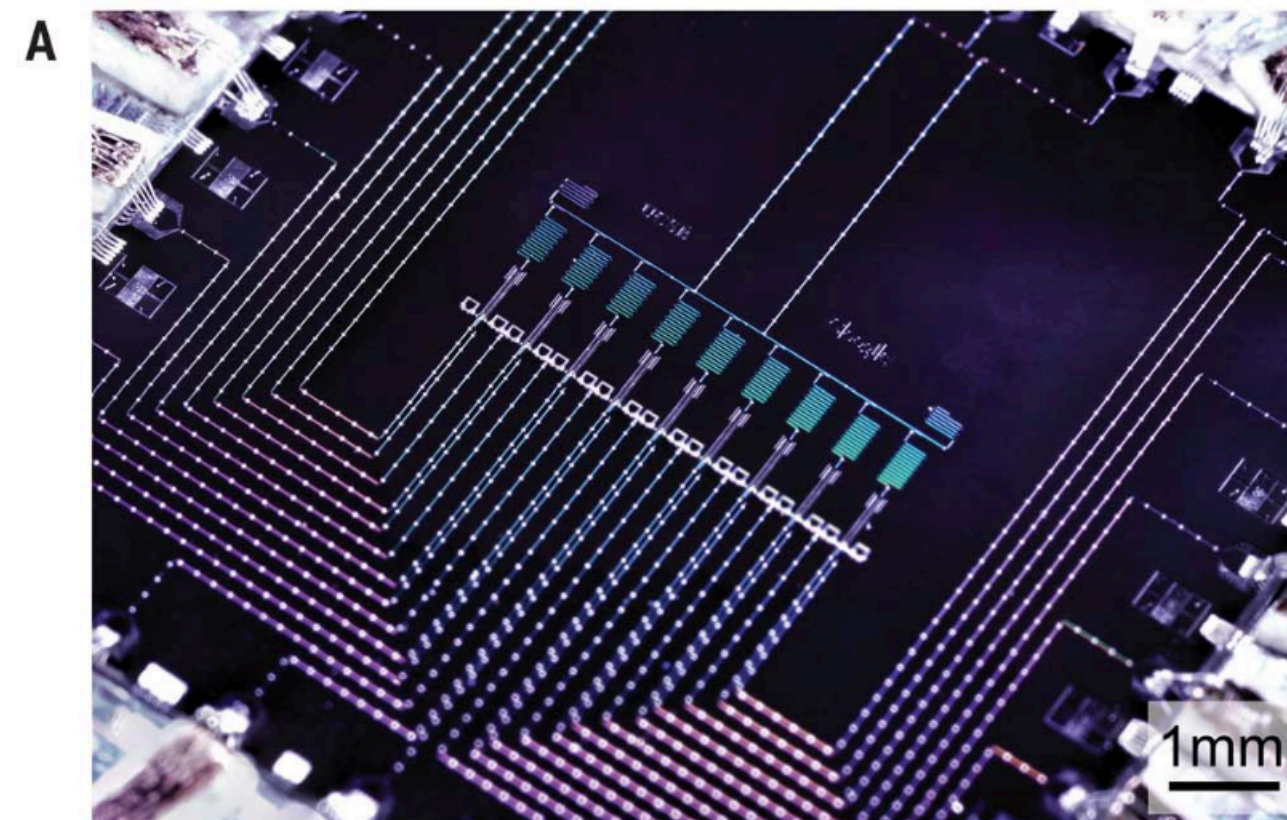
Trapped ions

Joshi Manoj, Wednesday



Superconducting qubits

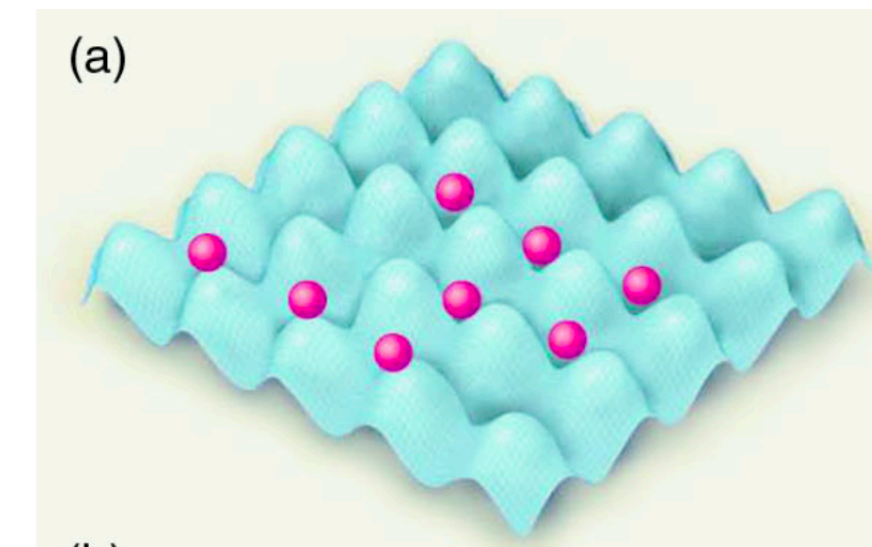
Andreas Wallraff, Tuesday



Neutral atoms

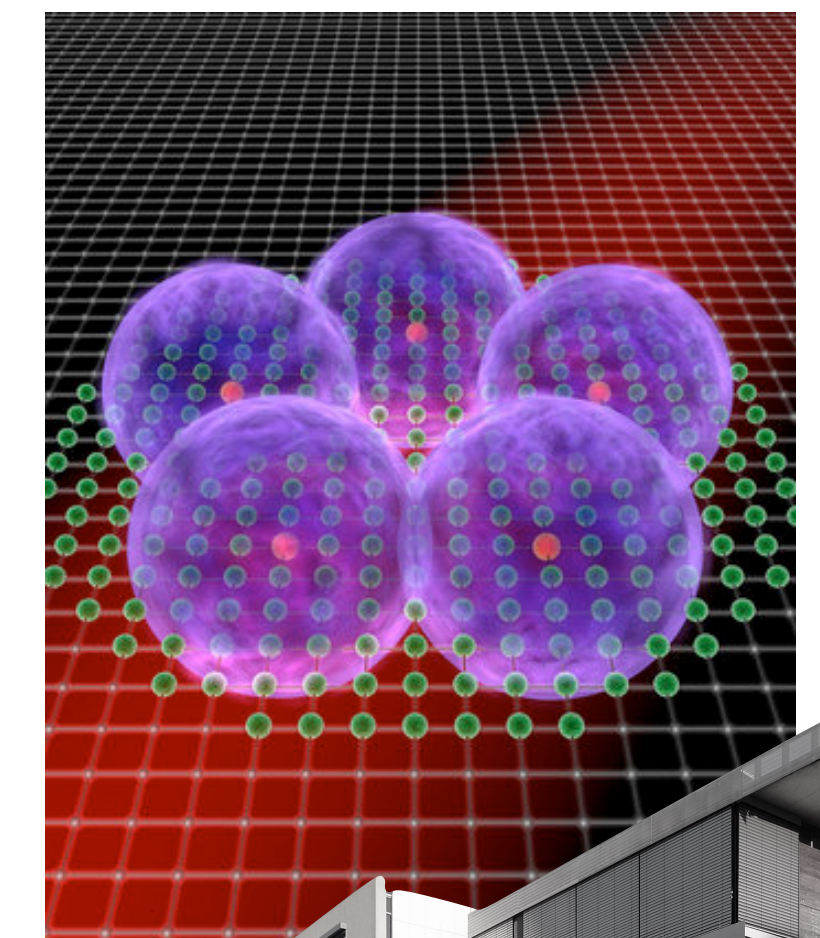
Optical lattices / quantum gases

Waseem Bakr, Tuesday



Rydberg atoms

Shannon Whitlock, Today



For what do we need quantum simulators?

- Georgescu, Ashhab, and Nori “Quantum Simulation”: RMP **86** (2014)

continued...

TABLE II. Potential applications of quantum simulators and the physical systems in which they could be implemented, along with relevant references. We note that this is not an exhaustive list.

Application	Proposed implementation
Condensed-matter physics:	
Hubbard models	Atoms (Jaksch <i>et al.</i> , 1998; Greiner <i>et al.</i> , 2002)* Ions (Deng, Porras, and Cirac, 2008) Polar molecules (Ortner <i>et al.</i> , 2009) Quantum dots (Byrnes <i>et al.</i> , 2008) Cavities (Greentree <i>et al.</i> , 2006; Hartmann, Brandao, and Plenio, 2006; Angelakis, Santos, and Bose, 2007)
Spin models	Atoms (Jané <i>et al.</i> , 2003; Garcia-Ripoll, Martin-Delgado, and Cirac, 2004, Simon <i>et al.</i> , 2011; Struck <i>et al.</i> , 2011)* Ions (Jané <i>et al.</i> , 2003; Porras and Cirac, 2004b; Deng, Porras, and Cirac, 2005; Bermudez, Porras, and Martin-Delgado, 2009; Edwards <i>et al.</i> , 2010; Lanyon <i>et al.</i> , 2011*; Kim <i>et al.</i> , 2011; Britton <i>et al.</i> , 2012)* Cavities (Cho, Angelakis, and Bose, 2008a; Chen <i>et al.</i> , 2010) Nuclear spins on diamond surface (Cai <i>et al.</i> , 2013) Superconducting circuits (Tsokomos, Ashhab, and Nori, 2010) Electrons on helium (Mostame and Schützhold, 2008)
Quantum phase transitions	Atoms (Greiner <i>et al.</i> , 2002)* Polar molecules (Capogrosso-Sansone <i>et al.</i> , 2010; Pollet <i>et al.</i> , 2010) Ions (Retzker <i>et al.</i> , 2008; Friedenauer <i>et al.</i> , 2008)*; Ivanov <i>et al.</i> , 2009; Giorgi, Paganelli, and Galve, 2010 NMR (Peng, Du, and Suter, 2005; Roumpos, Master, and Yamamoto, 2007; Zhang <i>et al.</i> , 2008) Superconducting circuits (van Oudenaarden and Mooij, 1996)*

Spin glasses	DQS (Lidar and Biham, 1997) Superconducting circuits (Tsokomos, Ashhab, and Nori, 2008)
Disordered systems	Atoms (Schulte <i>et al.</i> , 2005; Fallani <i>et al.</i> , 2007*; Billy <i>et al.</i> , 2008; Roati <i>et al.</i> , 2008)* Ions (Bermudez, Martin-Delgado, and Porras, 2010) Superconducting circuits (Garcia-Ripoll, Solano, and Martin-Delgado, 2008) NMR (Álvarez and Suter, 2010; Banerjee <i>et al.</i> , 2013)*
Frustrated systems	Ions (Porras and Cirac, 2006b; Kim <i>et al.</i> , 2010)* Photons (Ma <i>et al.</i> , 2011)*
High- T_c superconductivity	DQS (Yamaguchi and Yamamoto, 2002) Quantum dots (Manousakis, 2002) NMR (Yang <i>et al.</i> , 2006)*
BCS pairing	Atoms (Regal, Greiner, and Jin, 2004; Zwierlein <i>et al.</i> , 2005)*
BCS-BEC crossover	Superconducting circuits (Rakhmanov <i>et al.</i> , 2008)
Metamaterials	Superconducting circuits (Koch <i>et al.</i> , 2010)
Time-symmetry breaking	Atoms (Aguado <i>et al.</i> , 2008)
Topological order	Polar molecules (Micheli, Brennen, and Zoller, 2006) Linear optics (Lu <i>et al.</i> , 2009)* Superconducting circuits (You <i>et al.</i> , 2010)



For what do we need quantum simulators?

- Georgescu, Ashhab, and Nori "Quantum Simulation": RMP **86** (2014)

TABLE III. Continuation of Table II, but focused on applications other than condensed-matter physics. As in Table II, this is not an exhaustive list.

Application	Proposed implementation	Chemistry:
High-energy physics:		
Lattice gauge theories	DQS (Byrnes and Yamamoto, 2006) Atoms (Büchler <i>et al.</i> , 2005)	
Dirac particles	Ions (Lamata <i>et al.</i> , 2007; Casanova <i>et al.</i> , 2010, 2011; Gerritsma <i>et al.</i> , 2010*; Rusin and Zawadzki, 2010) Atoms (Goldman <i>et al.</i> , 2009; Hou, Yang, and Liu, 2009; Cirac, Maraner, and Pachos, 2010)	Quantum chaos:
Nucleons	Photons (Semiao and Paternostro, 2012)	
Cosmology:		Interferometry:
Unruh effect Hawking radiation	Ions (Alsing, Dowling, and Milburn, 2005) Atoms (Giovanazzi, 2005) Ions (Horstmann <i>et al.</i> , 2010) Superconducting circuits (Nation <i>et al.</i> , 2009)	
Universe expansion	BEC (Fischer and Schützhold, 2004) Ions (Schützhold and Mostame, 2005; Menicucci, Olson, and Milburn, 2010)	Other applications:
Atomic physics:		
Cavity QED Cooling	Superconducting circuits (You and Nori, 2003; Wallraff <i>et al.</i> , 2004)* Superconducting circuits (Grajcar <i>et al.</i> , 2008)*; You and Nori, 2011)	Schrödinger equation Quantum thermodynamics
Open systems:		
	NMR (Tseng <i>et al.</i> , 2000)* Ions (Piilo and Maniscalco, 2006; Barreiro <i>et al.</i> , 2011)* Superconducting circuits (Li <i>et al.</i> , 2013)*	

continued...

Thermal rate calculations
Molecular energies

Chemical reactions

DQS (Lidar and Wang, 1999)
DQS (Aspuru-Guzik *et al.*, 2005)
Linear optics (Lanyon *et al.*, 2010)*
NMR (Du *et al.*, 2010)*
DQS (Kassal *et al.*, 2008)
Quantum dots (Smirnov *et al.*, 2007)

NMR (Weinstein *et al.*, 2002)*
Linear optics (Howell and Yeaze, 1999)

Ions (Leibfried *et al.*, 2002*; Hu, Feng, and Lee, 2012; Lau and James, 2012)
Photons (Aaronson and Arkhipov, 2011; Broome *et al.*, 2013*; Crespi *et al.*, 2013; Spring *et al.*, 2013; Tillmann *et al.*, 2013)*
Superconducting circuits (Zhou, Dong *et al.*, 2008; Liao *et al.*, 2010)

DQS (Boghosian and Taylor, 1998a)
Superconducting circuits (Quan *et al.*, 2006, 2007)



For what do we need theorists?

A QS is an experimental system that mimics a **simple model, or a family of simple models.**

- (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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“Finding the mapping in an AQS might, at first glance, look simpler than obtaining the most efficient gate decomposition for a given Hamiltonian in DQS. Sometimes the mapping is indeed straightforward, but this is not always the case, and quite often clever mappings have to be devised, sometimes involving additional externally applied fields or ancillary systems to mediate various interactions.”

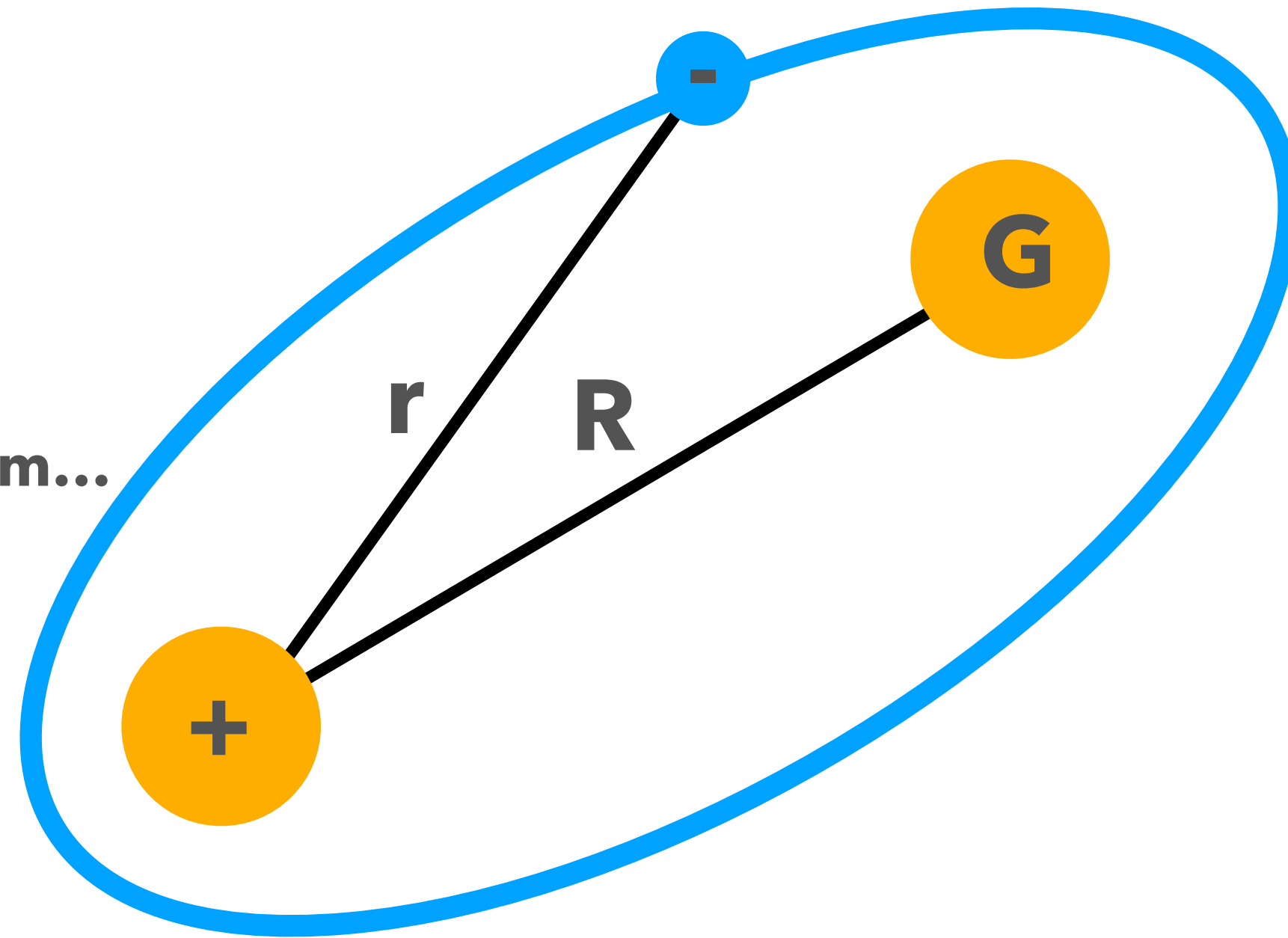


We just learned some more about what Qs are and what they do...
...now we will build one!



Building a quantum simulator of a Rydberg atom

Using a Rydberg atom...



...and a ground state atom...

...We want to simulate the Hamiltonian of an electron moving in a Coulomb potential!

$$H = -\frac{\nabla^2}{2M} - \frac{Z}{r}$$

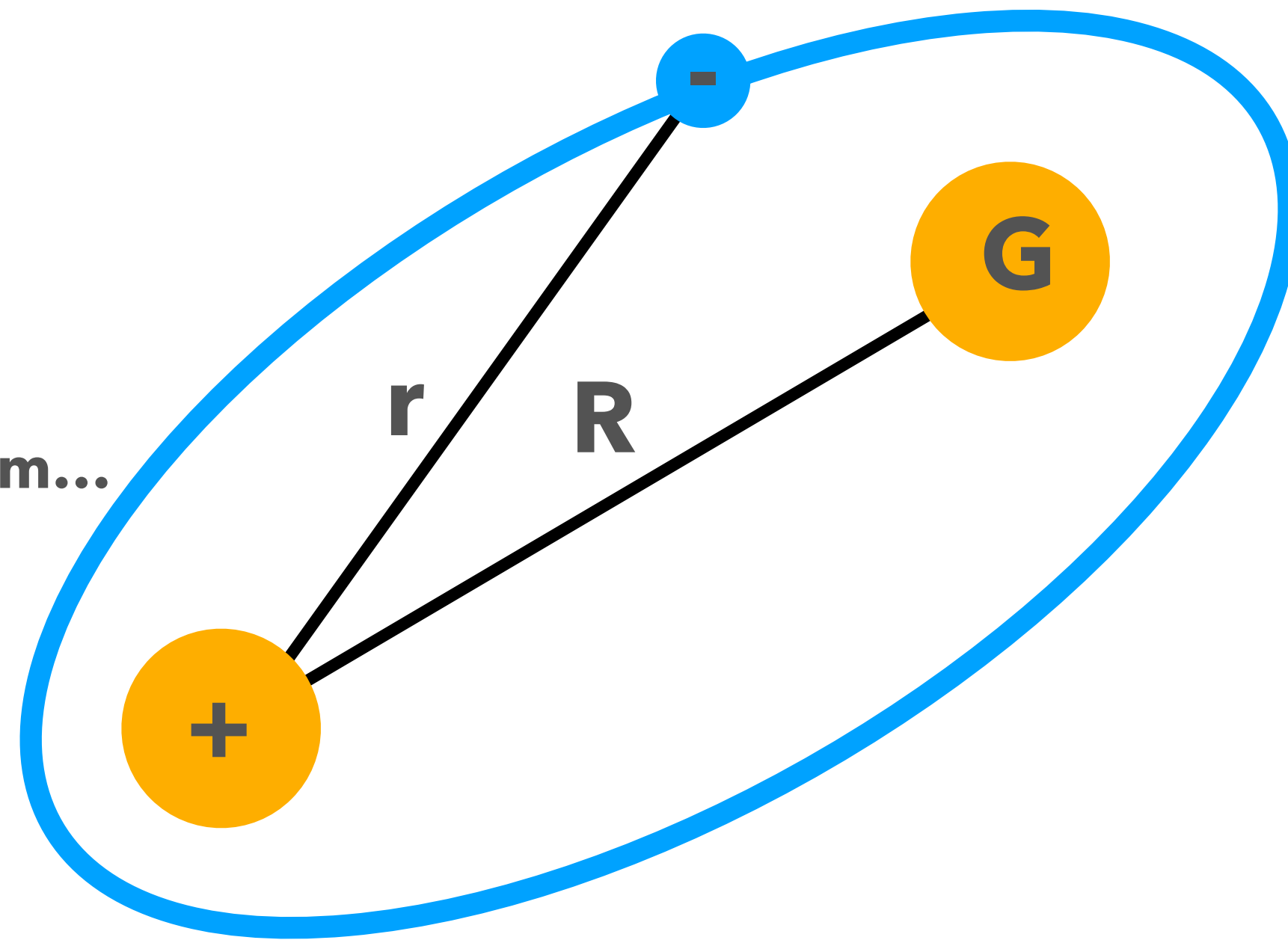
Why? (what is the relevance??)

- Large, even infinite, Hilbert space -> "tough to simulate classically".
- Test predictions in regimes inaccessible in typical Rydberg atoms (as long as we have controllability)



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Why? (what is the relevance??)

- Large, even infinite, Hilbert space -> "tough to simulate classically".
- Test predictions in regimes inaccessible in typical Rydberg atoms (as long as we have controllability)
- **Because doing so will introduce many of the atomic physics topics we want for a "first principles" lecture (and maybe in a less boring way!) and will help us think critically about quantum simulation!**



A quick survey of atomic structure

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. To understand their spectra and wave functions, we (of course) begin with the best atom with a single valence electron: hydrogen.

Schrödinger equation:

$$0 = \left(-\frac{\nabla^2}{2} - \frac{1}{r} - E \right) \psi(\vec{r}). \quad (R1) \quad \dots \text{in atomic units where } \hbar = e = m_e = 1$$



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Eq. R1 separates in spherical coordinates (among many other coordinate systems)

$$\psi(\vec{r}) = \frac{u_{\nu l}(r)}{r} Y_{lm}(\hat{r}) \quad (R2)$$



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$$\psi(\vec{r}) = \frac{u_{\nu l}(r)}{r} Y_{lm}(\hat{r}) \quad (R2)$$

Simplifying Eq. R1 with Eq. R2 yields the radial Schrödinger equation

$$0 = -\frac{1}{2} u''_{\nu l}(r) + \left(\frac{l(l+1)}{2r^2} - \frac{1}{r} - \left(-\frac{1}{2\nu^2} \right) \right) u_{\nu l}(r). \quad (R3)$$

centrifugal barrier at nonzero angular momentum

parametrize the energy (we are looking for negative energy bound states, so nu is positive)



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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.

$$u_{\nu l}(r) \sim f_{\nu l}(r) - \tan \delta_{\nu l} g_{\nu l}(r). \quad (R4)$$

(f and g are given by hypergeometric functions... lots of fun!)





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To apply boundary conditions, we need the asymptotic behavior of f and g :**

$$r \rightarrow 0 : \quad f_{\nu, l}(r) \propto r^{l+1}, \quad g_{\nu, l}(r) \propto r^{-l} \quad (R5)$$



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$$r \rightarrow \infty : \quad f_{\nu, l}(r) \rightarrow Ar^{-\nu} e^{r/\nu} \sin \pi(\nu - l) - Br^{\nu} e^{-r/\nu} \cos \pi(\nu - l) \quad (R6)$$

$$g_{\nu, l}(r) \rightarrow -Ar^{-\nu} e^{r/\nu} \cos \pi(\nu - l) - Br^{\nu} e^{-r/\nu} \sin \pi(\nu - l) \quad (R7)$$

(A and B are constants)



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$$u_{\nu l}(r) \sim f_{\nu l}(r) - \tan \delta_{\nu l} g_{\nu l}(r). \quad (R4)$$

Feynman said, "I don't want to have an explosion", and the wave function agrees!

$$\delta_{\nu l} = 0, \nu - l = n_r + 1, E_n = -\frac{1}{2n^2} \quad (R8)$$

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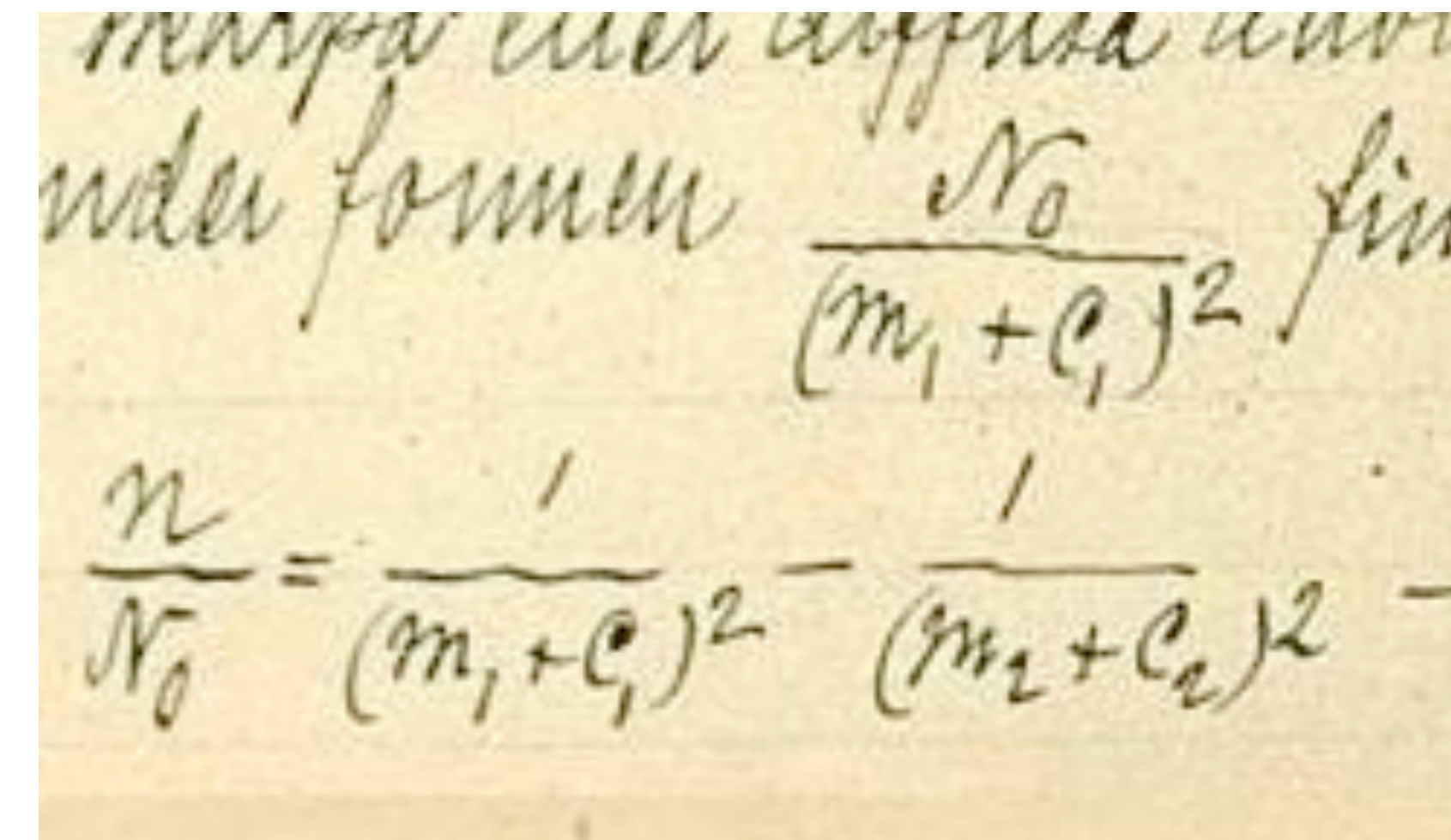
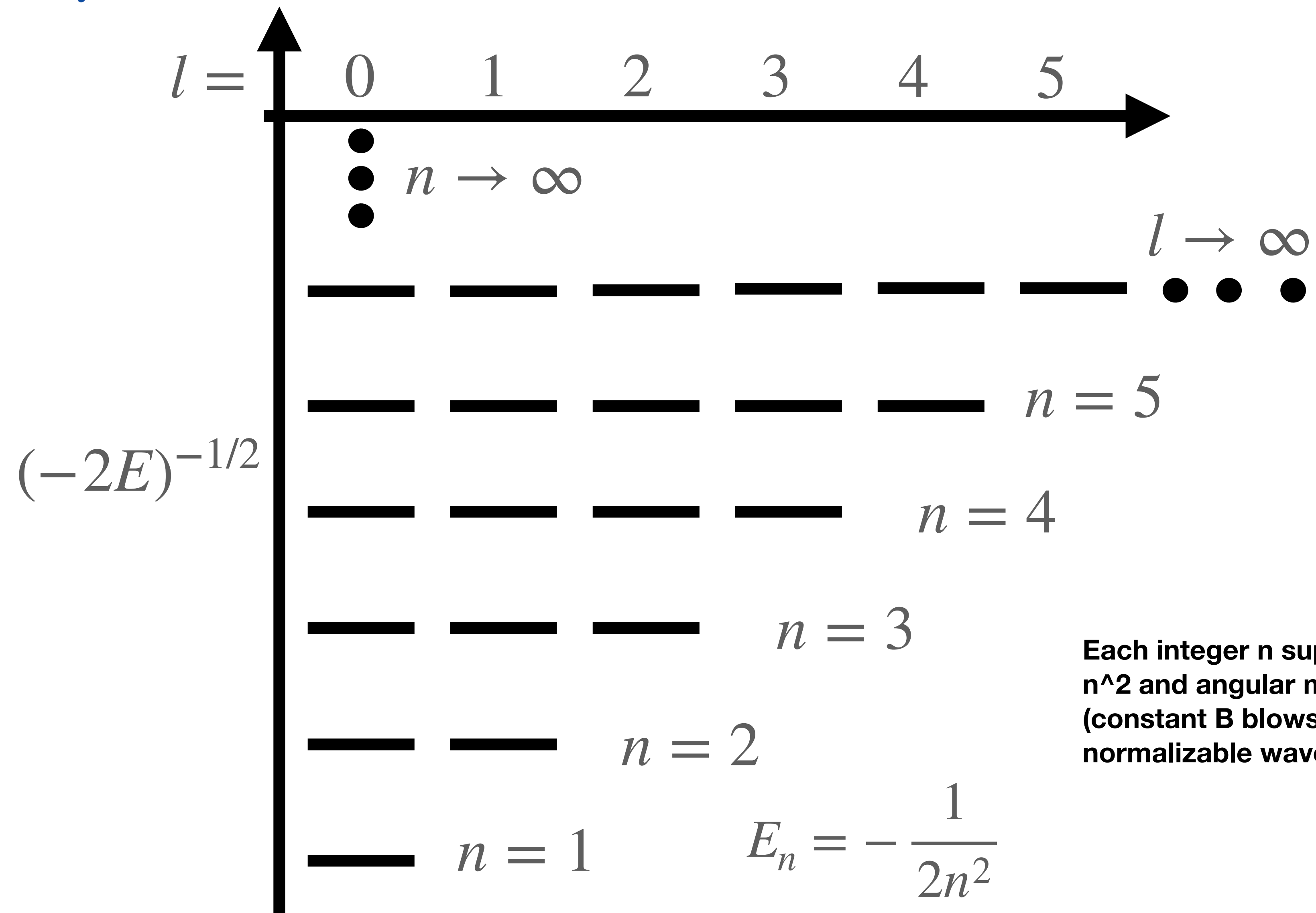
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A quick survey of atomic structure: hydrogen

For hydrogen: an infinite series of highly degenerate bound states



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

Each integer n supports n^2 degenerate levels with energy n^2 and angular momentum values $l = 0, \dots, n-1$ (constant B blows up when $n = l$, so we could not have a normalizable wave function...)

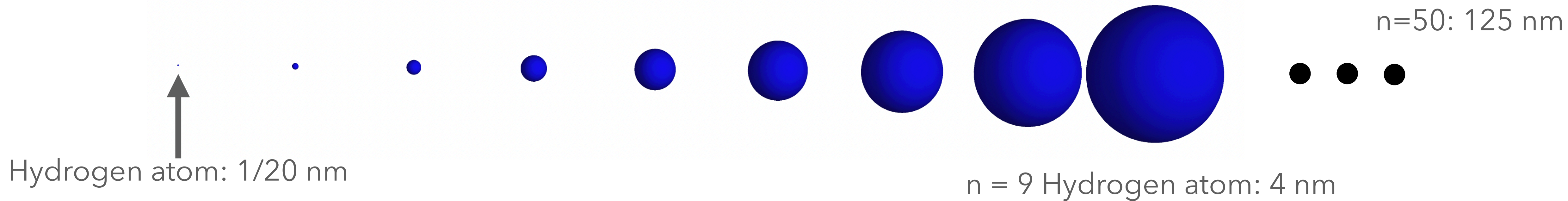


A quick survey of atomic structure: excited states of H

Because Rydberg's formula predicts an infinite series of excited bound states in hydrogen, we call atoms – of any species – which have been excited to high principal quantum numbers ($n > 10$ or so) **Rydberg atoms**.

Such atoms are fascinating because their properties are **extreme!**

$$E = T + V \implies -\frac{1}{2n^2} = \frac{k^2}{2} - \frac{1}{r} \implies r_0 = 2n^2$$

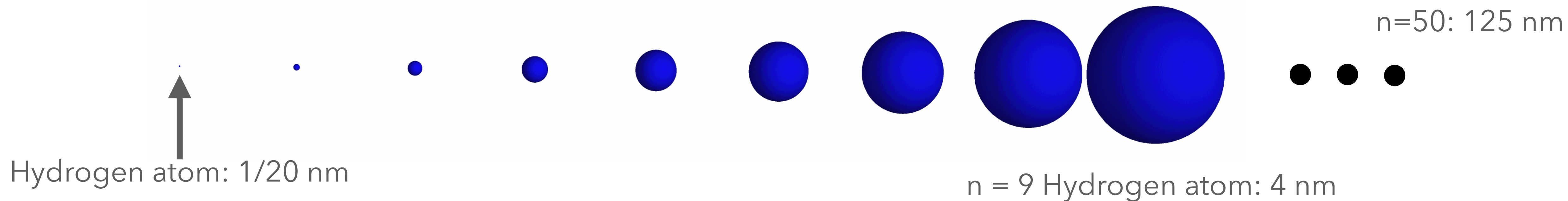


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Rydberg atoms are friendly: their properties obey robust scaling laws.

$$\langle n | r^\alpha | n \rangle \sim n^{2\alpha}, \alpha > 0. \quad (R9)$$



A quick survey of atomic structure: excited states of H

For further scaling laws, we need normalized wave functions.

Easiest to do with **WKB**:

$$u(r) \sim \frac{N \sin \int_{r_<}^r k(r) dr}{\sqrt{k(r)}}$$



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$$\Rightarrow \quad 2 = N^2 \int_0^{2n^2} \frac{1}{\sqrt{-\frac{1}{n^2} + \frac{2}{r}}} dr = \pi n^3 .$$



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So the normalization constant is $N = \sqrt{\frac{2}{\pi n^3}}$.

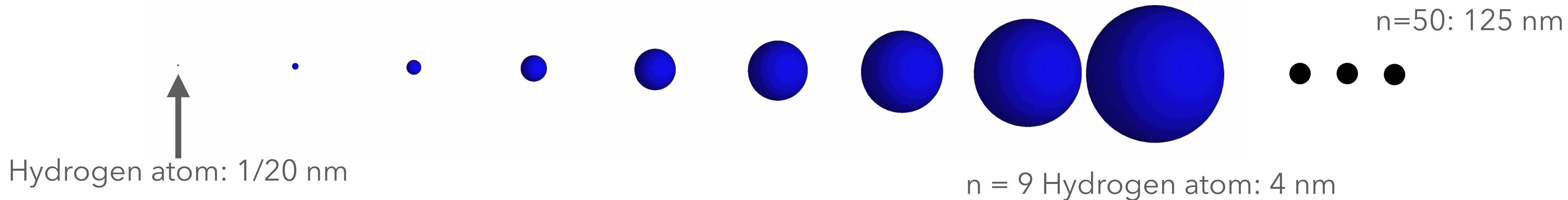


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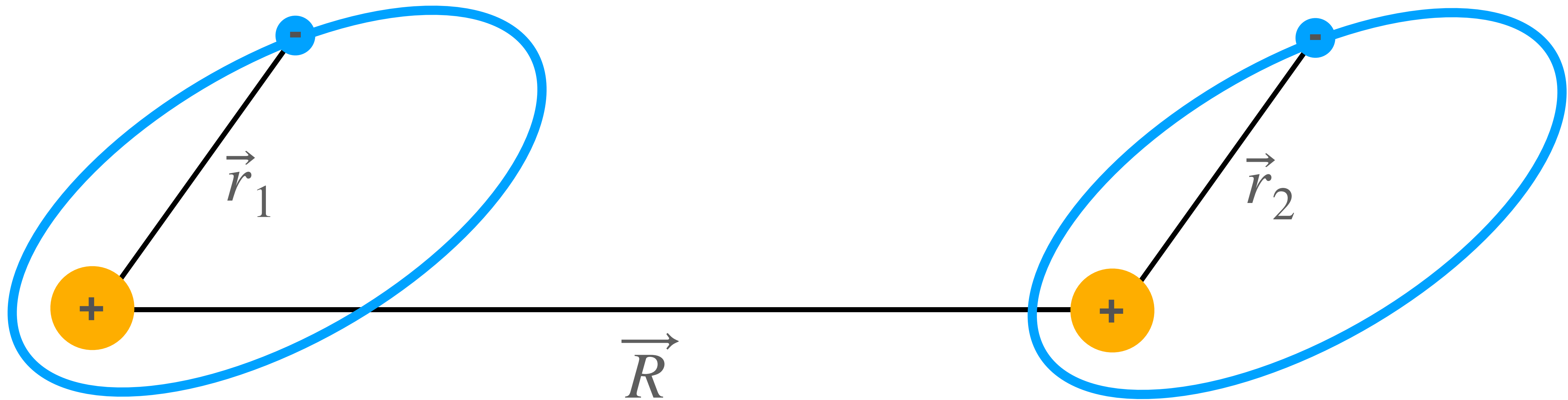
$$\langle n | r^\alpha | n \rangle \sim n^{2\alpha}, \alpha > 0. \quad (R9) \quad \langle n | r^\alpha | n \rangle \sim n^{-3}, \alpha > 0. \quad (R10)$$

Anything which depends on small r values will scale as n^{-3} due to the normalization constant...



Interlude: How do two atoms interact at a distance?

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



Since the atoms are far apart: R will be much larger than the typical distances of either electrons.
A great opportunity to do a Taylor expansion!



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$$\begin{aligned} \vec{r}_{12} &= \vec{r}_1 - \vec{r}_2 \\ |\vec{r}_{12}|^2 &= r_1^2 - 2\vec{r}_1 \cdot \vec{r}_2 + r_2^2 \end{aligned}$$

$$\frac{1}{|\vec{R} - \vec{r}_1 + \vec{r}_2|} = \frac{1}{R\sqrt{1 - \frac{2\vec{r}_{12} \cdot \hat{z}}{R} + \frac{r_{12}^2}{R^2}}} \approx \frac{1}{R} \left(1 + \frac{\vec{r}_{12} \cdot \hat{z}}{R} - \frac{1}{2} \frac{r_{12}^2}{R^2} + \frac{3(\vec{r}_{12} \cdot \hat{z})^2}{2R^2} \right)$$



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

$$\begin{aligned}\vec{r}_{12} &= \vec{r}_1 - \vec{r}_2 \\ |\vec{r}_{12}|^2 &= r_1^2 - 2\vec{r}_1 \cdot \vec{r}_2 + r_2^2\end{aligned}$$

$$\begin{aligned}\frac{1}{|\vec{R} - \vec{r}_1 + \vec{r}_2|} &= \frac{1}{R\sqrt{1 - \frac{2\vec{r}_{12} \cdot \hat{z}}{R} + \frac{r_{12}^2}{R^2}}} \approx \frac{1}{R} \left(1 + \frac{\vec{r}_{12} \cdot \hat{z}}{R} - \frac{1}{2} \frac{r_{12}^2}{R^2} + \frac{3(\vec{r}_{12} \cdot \hat{z})^2}{2R^2} \right) \\ &= \frac{1}{R} \left(1 + \frac{\vec{r}_1 \cdot \hat{z}}{R} - \frac{r_2 \cdot \hat{z}}{R} + \frac{-r_1^2 + 2\vec{r}_1 \cdot \vec{r}_2 - r_2^2}{2R^2} + \frac{3}{2R^2} \left((\vec{r}_1 \cdot \hat{z})^2 - 2(\vec{r}_1 \cdot \hat{z})(\vec{r}_2 \cdot \hat{z}) + (\vec{r}_2 \cdot \hat{z})^2 \right) \right) \\ \frac{1}{|\vec{R} - \vec{r}_1|} &= \frac{1}{R\sqrt{1 - \frac{2\vec{r}_1 \cdot \hat{z}}{R} + \frac{r_1^2}{R^2}}} \approx -\frac{1}{R} \left(1 + \frac{\vec{r}_1 \cdot \hat{z}}{R} - \frac{1}{2} \frac{r_1^2}{R^2} + \frac{3(\vec{r}_1 \cdot \hat{z})^2}{2R^2} \right) \\ \frac{1}{|\vec{R} + \vec{r}_2|} &= \frac{1}{R\sqrt{1 + \frac{2\vec{r}_2 \cdot \hat{z}}{R} + \frac{r_2^2}{R^2}}} \approx -\frac{1}{R} \left(1 - \frac{\vec{r}_2 \cdot \hat{z}}{R} - \frac{1}{2} \frac{r_2^2}{R^2} + \frac{3(\vec{r}_2 \cdot \hat{z})^2}{2R^2} \right)\end{aligned}$$



Interlude: How do two atoms interact at a distance?

After the dust settles...

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



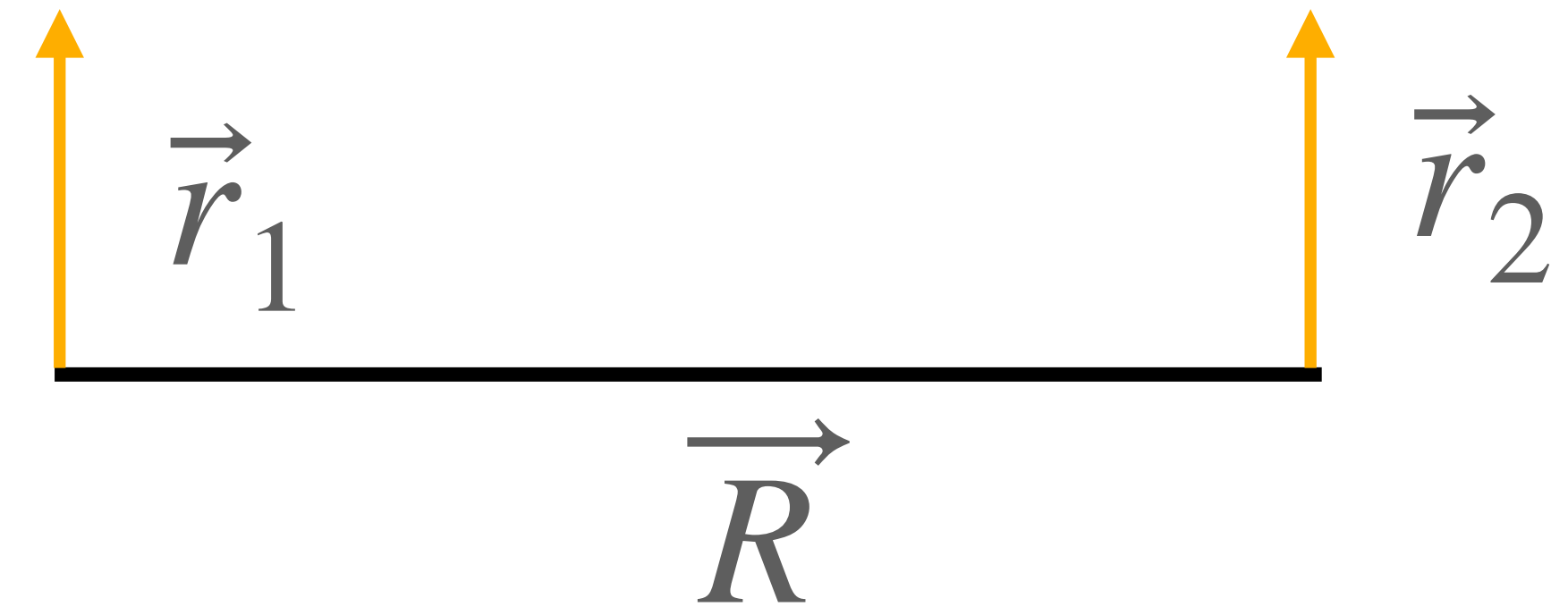
Interlude: How do two atoms interact at a distance?

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Now, for simplicity:

$$H \approx \frac{-\nabla_1^2}{2} - \frac{1}{r_1} + \frac{-\nabla_2^2}{2} - \frac{1}{r_2} + \frac{r_1 r_2}{R^3}$$



Let's go to the Born Oppenheimer picture (maybe: details tomorrow) to find the interaction between these atoms

$$H \approx \frac{-\nabla_1^2}{2} - \frac{1}{r_1} + \frac{-\nabla_2^2}{2} - \frac{1}{r_2} + \frac{r_1 r_2}{R^3}$$

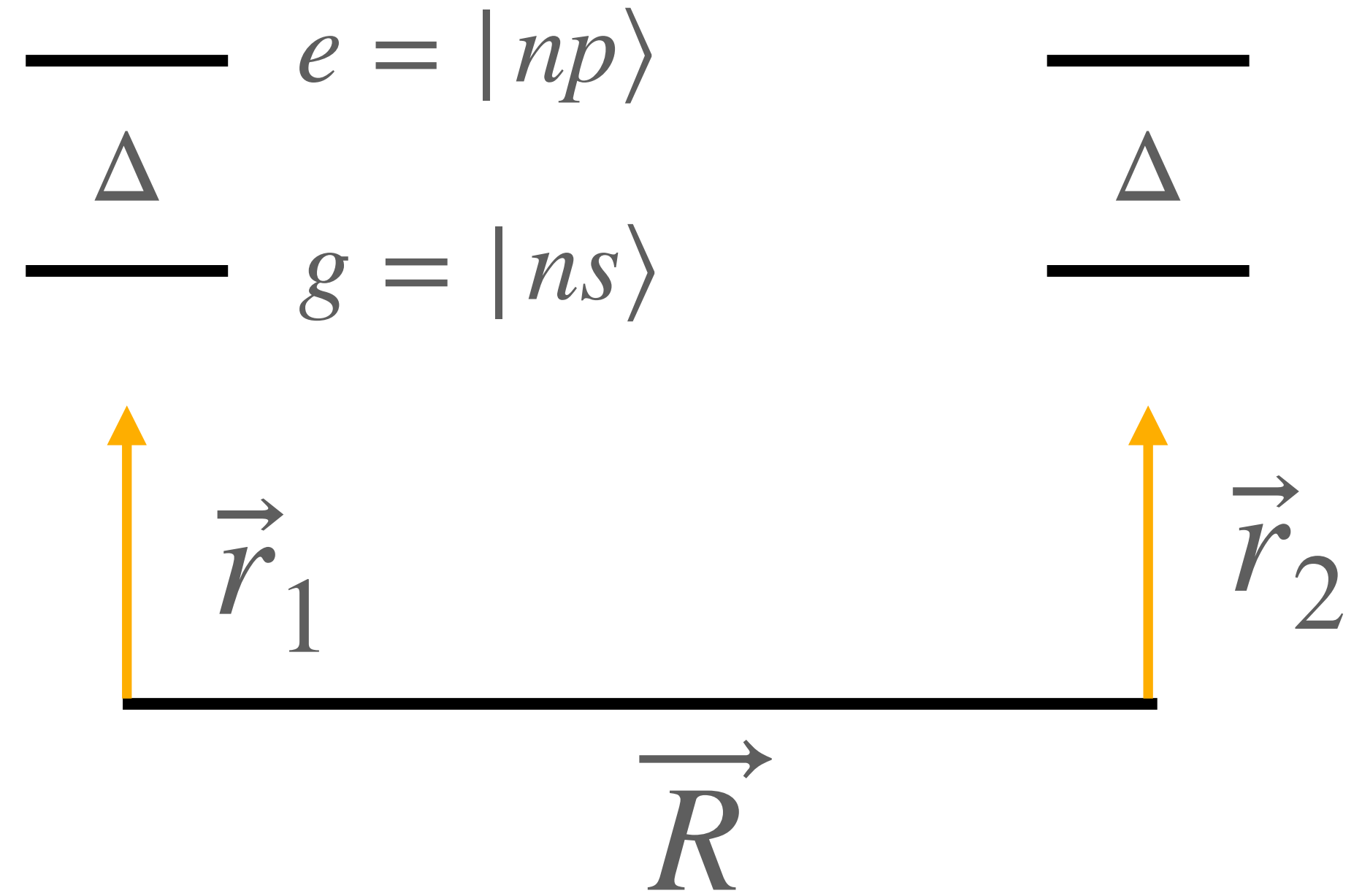
Integrate out electronic degrees of freedom. What basis?



Interlude: How do two atoms interact at a distance?

Choose just two electronic states for each atom.

-> four state basis $|ee\rangle, |gg\rangle, |eg\rangle, |ge\rangle$



Interlude: How do two atoms interact at a distance?

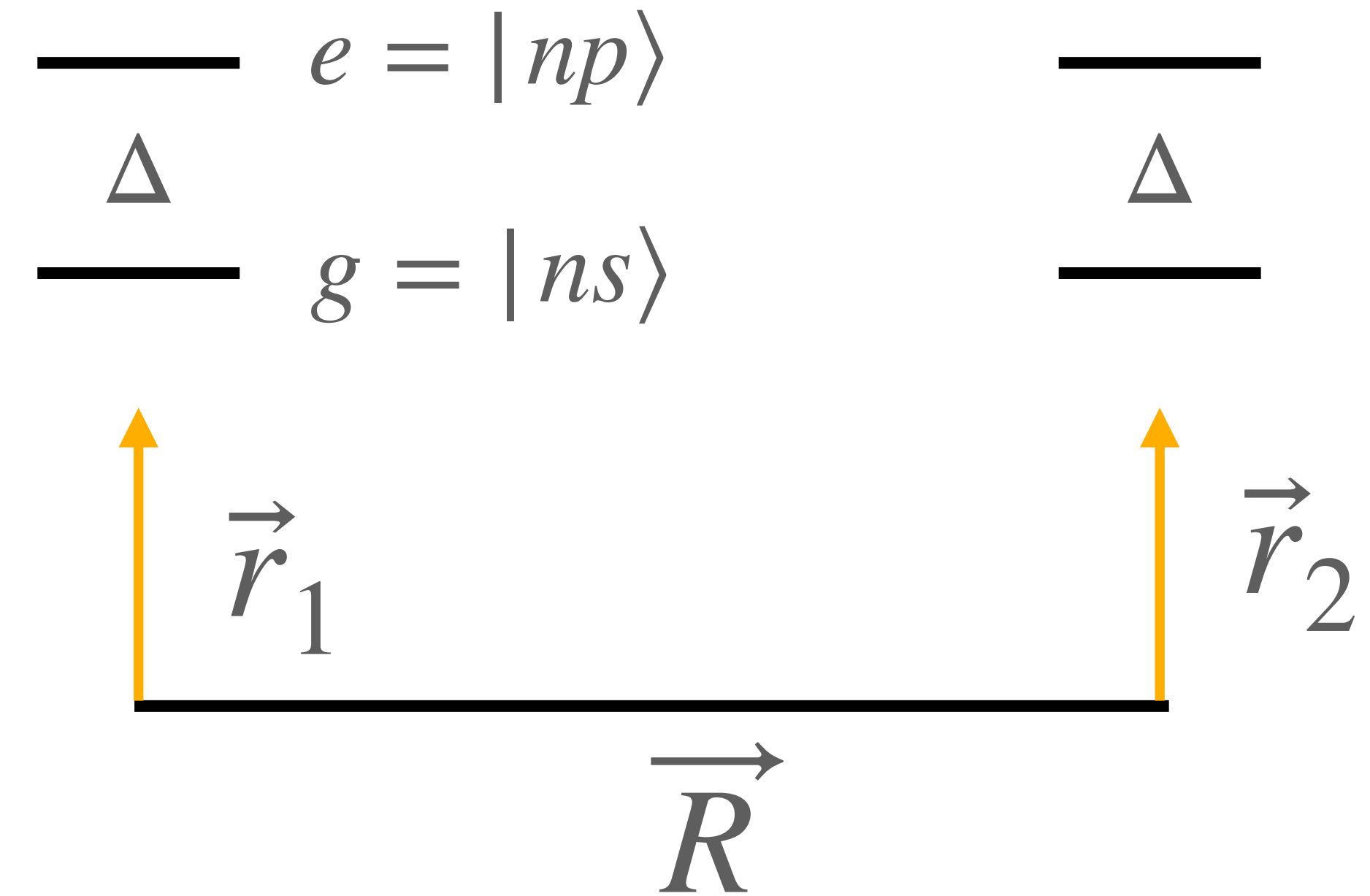
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(normally a pretty good approximation!)

$$H \approx \frac{-\nabla_1^2}{2} - \frac{1}{r_1} + \frac{-\nabla_2^2}{2} - \frac{1}{r_2} + \frac{r_1 r_2}{R^3}$$

$$\underline{V}(R) = \begin{pmatrix} 0 & \frac{d_1 d_2}{R^3} & 0 & 0 \\ \frac{d_1 d_2}{R^3} & 2\Delta & 0 & 0 \\ 0 & 0 & \Delta & \frac{d_1 d_2}{R^3} \\ 0 & 0 & \frac{d_1 d_2}{R^3} & \Delta \end{pmatrix}$$



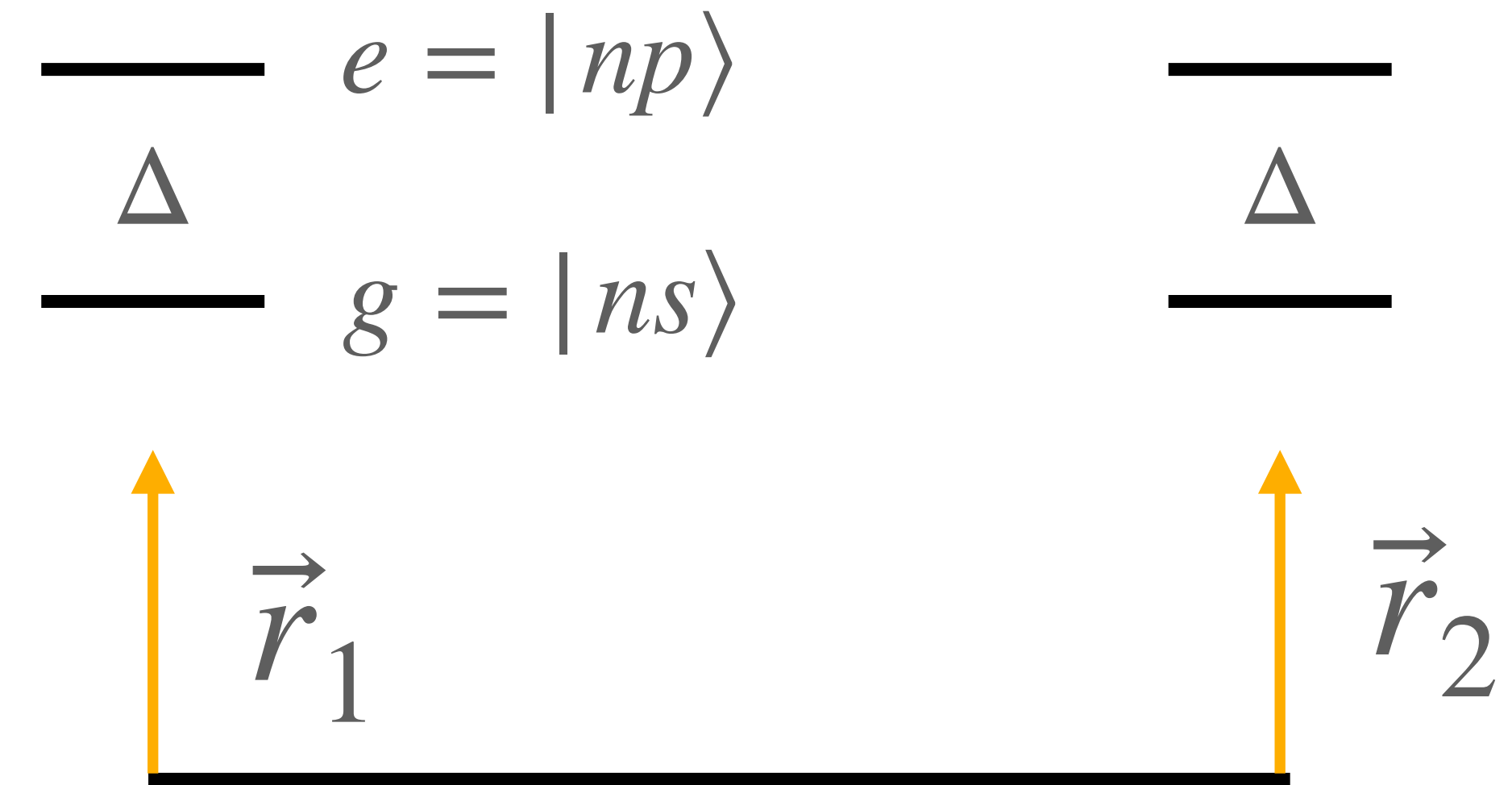
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$$\begin{pmatrix} a & b \\ b & c \end{pmatrix} \rightarrow 2u_{\pm} = (a + c) \pm \sqrt{4b^2 + (a - c)^2}$$

Two classes of interaction:

$$u_{\pm} = \Delta \pm \frac{d_1 d_2}{R^3}$$

$$u_+ \approx 2\Delta + \frac{(d_1 d_2)^2 / (2\Delta)}{R^6}$$

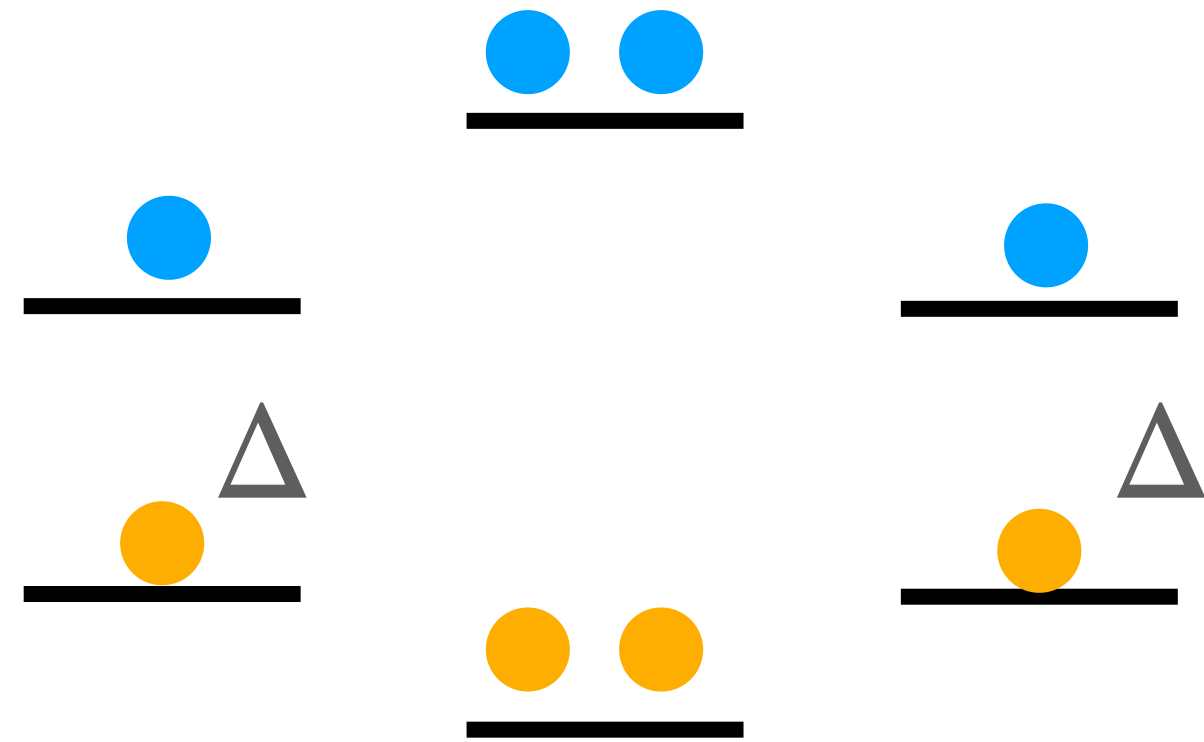
$$u_- \approx 0 - \frac{(d_1 d_2)^2 / (2\Delta)}{R^6}$$



Interlude: How do two atoms interact at a distance?

This simple two-state model shows atoms interact at long-range in two different regimes:

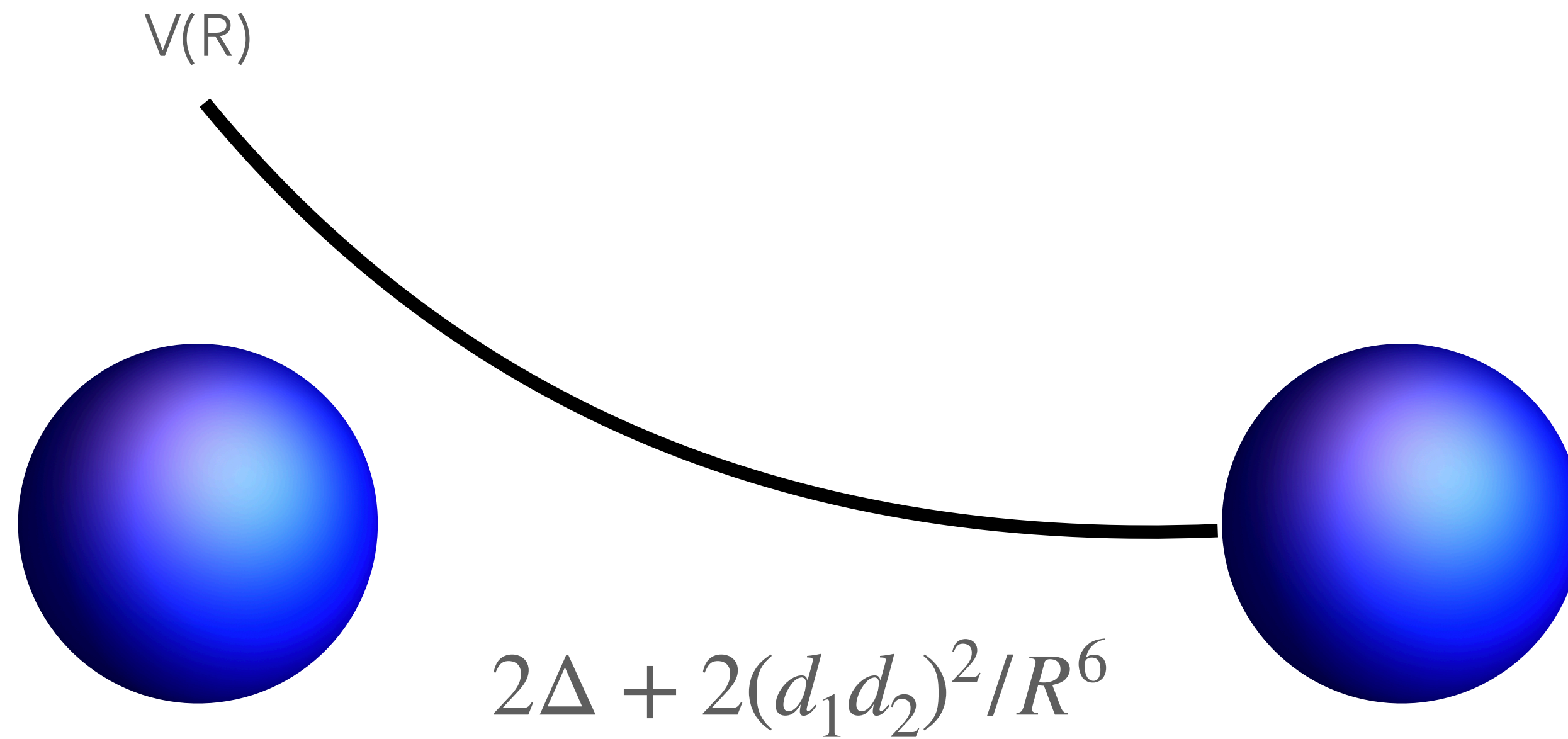
Both atoms in same state:



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

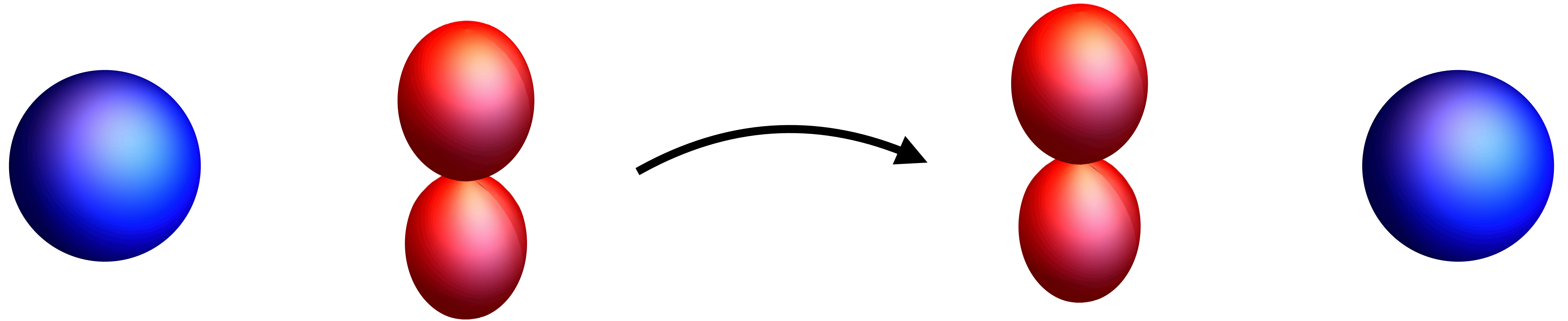
$$E_- \approx -\frac{(d_1 d_2)^2 / (2\Delta)}{R^6}$$

This *non-resonant* van der Waals interaction is at the core of ground-state – ground-state atom scattering as well as the source of Rydberg blockade: the ultra-strong interaction between Rydberg atoms prevents their mutual excitation!

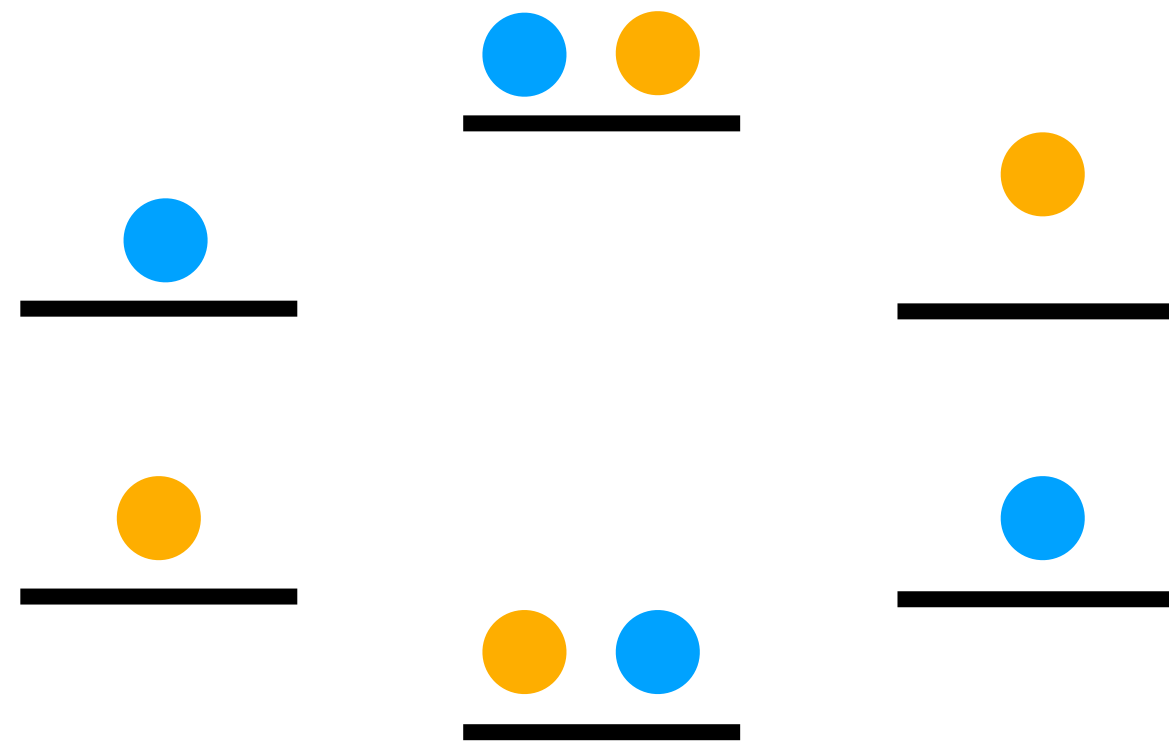


Interlude: How do two atoms interact at a distance?

This simple two-state model shows atoms interact at long-range in two different regimes:



Each atom in a different state:



$$u_{\pm} = \Delta \pm \frac{d_1 d_2}{R^3}.$$

This *resonant* dipolar interaction leads to a “flip-flop” or exchange interaction between atoms; in the full picture this interaction is *anisotropic*!



Interlude: How do two atoms interact at a distance?

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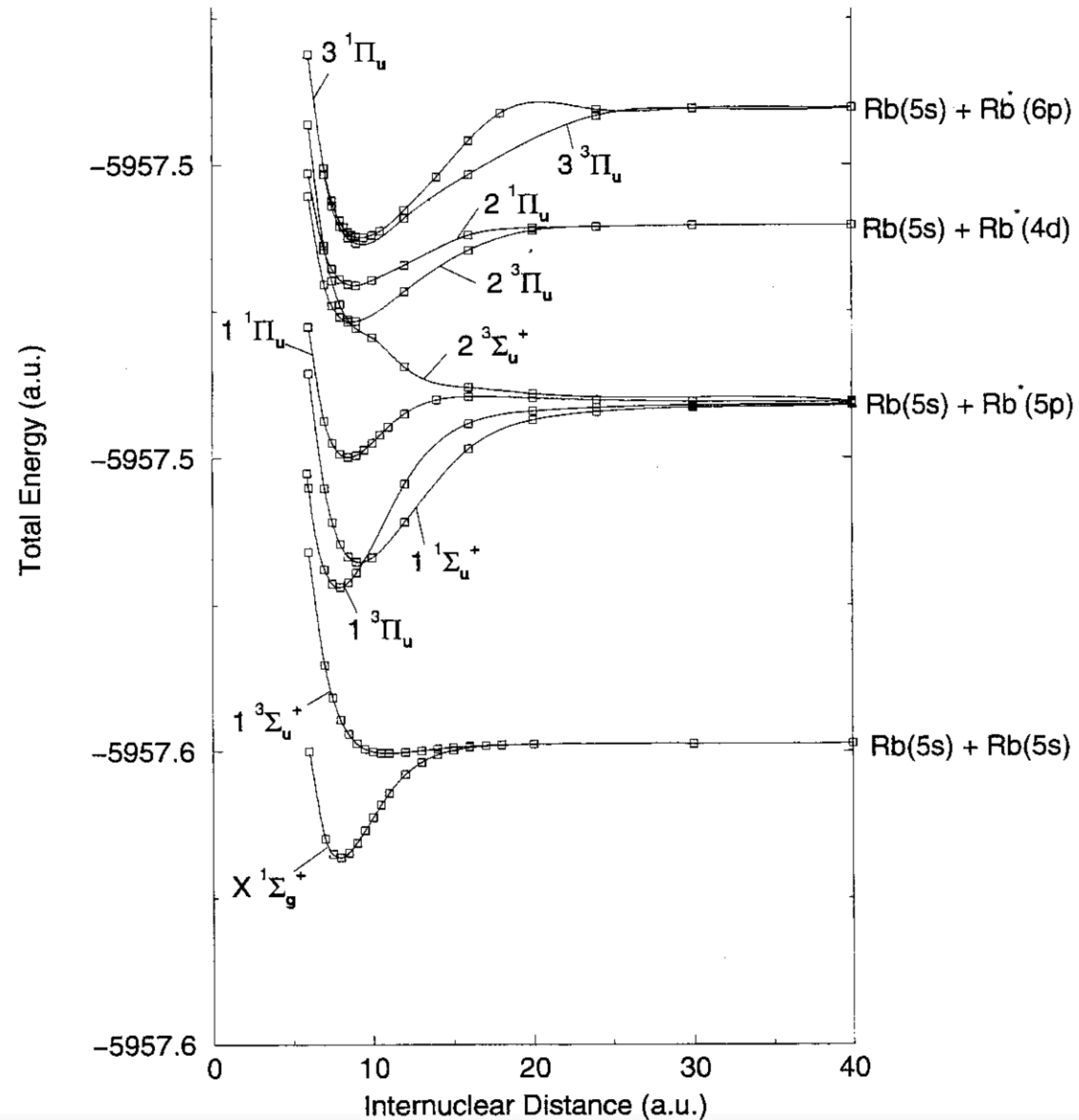


Figure 1. Calculated potential energy curves of electronic AS states in Rb_2 .

The interaction between atoms in the same state is characterized by a "C6 coefficient"

$$V_{vdW} = - \frac{(d_1 d_2)^2 / (2\Delta)}{R^6} = - \frac{C_6}{R^6}.$$

This simple two-state calculation we just did gives C_6 values for the ground state which are very close to the exact values for all of the bi-alkali molecules!

For example in Rb: C_6 in the ground state is 4691 (in atomic units); this calculation (using experimentally obtained dipole moments and energies) gives ~ 4100 .



Interlude: How do two atoms interact at a distance?

The amazing thing with Rydberg atoms is how these interactions scale...

<https://github.com/pairinteraction/pairinteraction>

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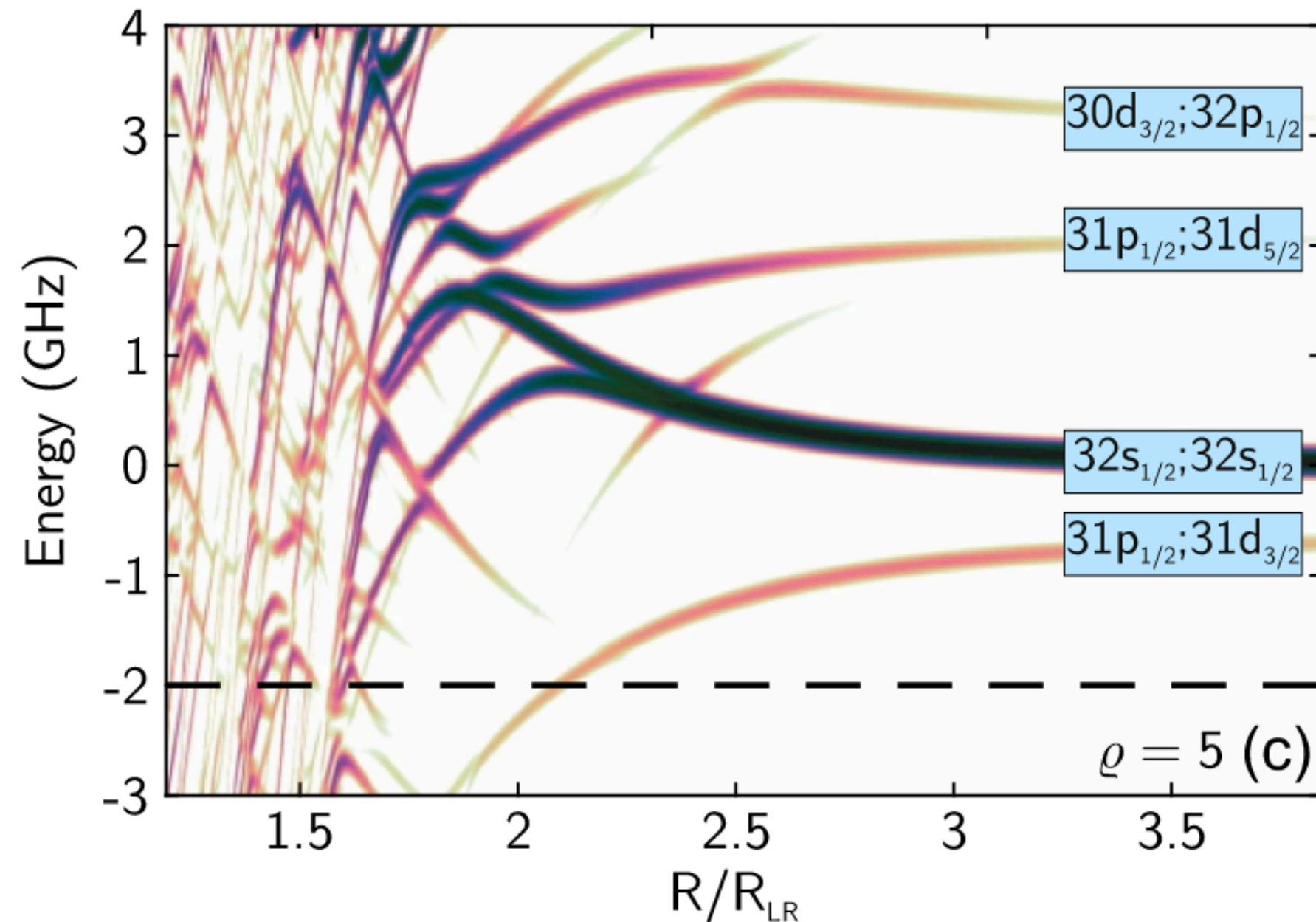
J. Phys. B: At. Mol. Opt. Phys. **50** (2017) 133001 (18pp)

<https://doi.org/10.1088/1361-6455/aa743a>

Tutorial

Calculation of Rydberg interaction potentials

Sebastian Weber^{1,7}, Christoph Tresp^{2,3}, Henri Menke⁴, Alban Urvoy^{2,5}, Ofer Firstenberg⁶, Hans Peter Büchler¹ and Sebastian Hofferberth^{2,3,7}



$$V_{vdW}(n) = \frac{1}{R^6} \sum_{n'_1, n'_2} \frac{|\langle n_1 s n_2 s | \vec{r}_1 \cdot \vec{r}_2 - 3 \vec{r}_1 \cdot \hat{z} \vec{r}_2 \cdot \hat{z} | n'_1 p n'_2 p \rangle|^2}{E_{n'_1 p} + E_{n'_2 p} - 2E_{ns}}$$

We could already see from the ground state calculation, but it's also clear here...



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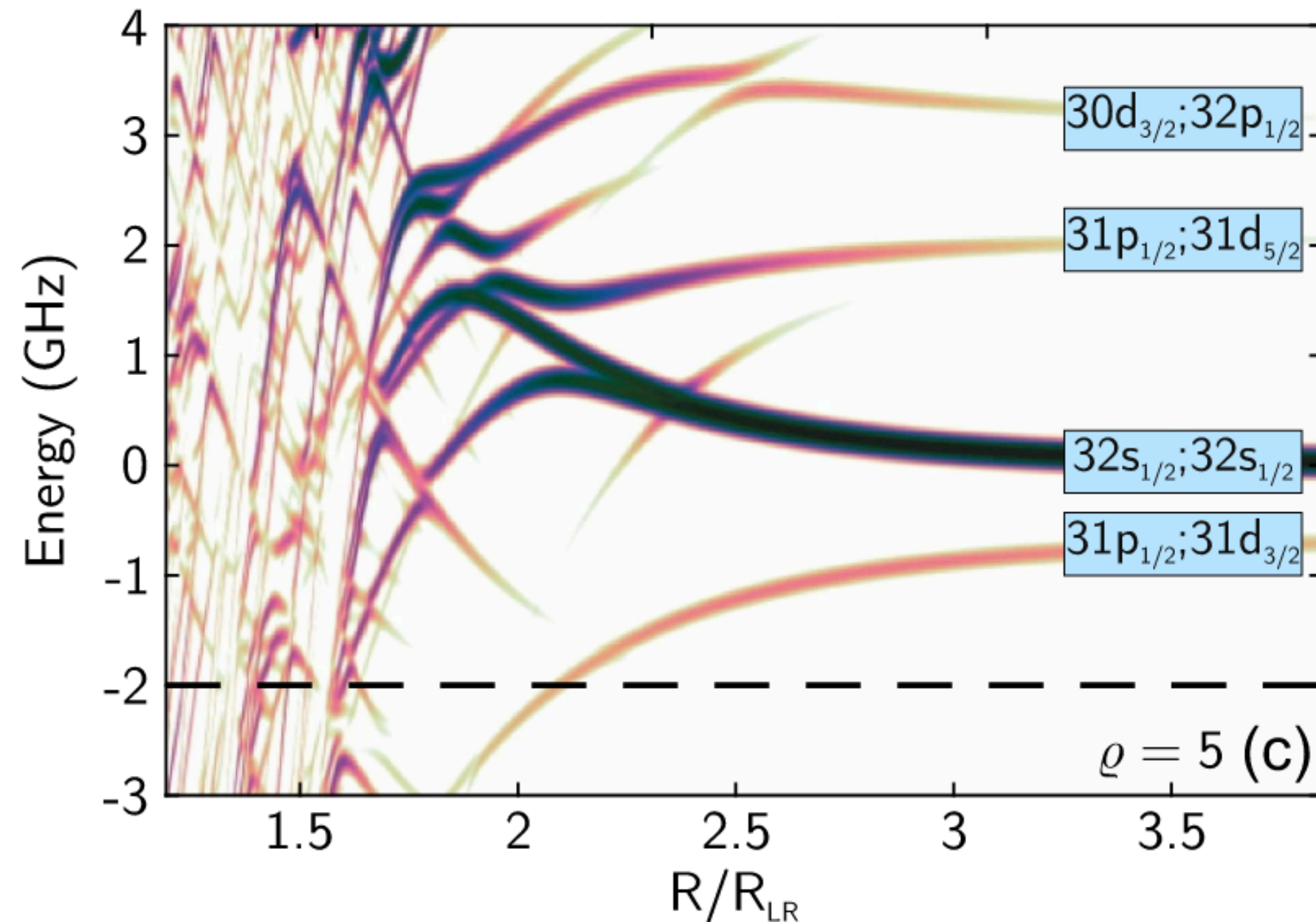
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We could already see from the ground state calculation, but it's also clear here...

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



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 $r > r_0$.

Our new radial equation is:

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



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.

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 !

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

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



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



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.

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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$$r \rightarrow \infty : \quad f_{\nu,l}(r) \rightarrow Ar^{-\nu} e^{r/\nu} \sin \pi(\nu - l) - Br^{\nu} e^{-r/\nu} \cos \pi(\nu - l) \quad (R6)$$

$$g_{\nu,l}(r) \rightarrow -Ar^{-\nu} e^{r/\nu} \cos \pi(\nu - l) - Br^{\nu} e^{-r/\nu} \sin \pi(\nu - l) \quad (R7)$$

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



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

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



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.

And finally:

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

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

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

Table 2. Measured frequencies for the $nP_{3/2}$ 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

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[doi:10.1088/0953-4075/42/16/165004](https://doi.org/10.1088/0953-4075/42/16/165004)

Precision measurements of quantum defects in the $nP_{3/2}$ 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

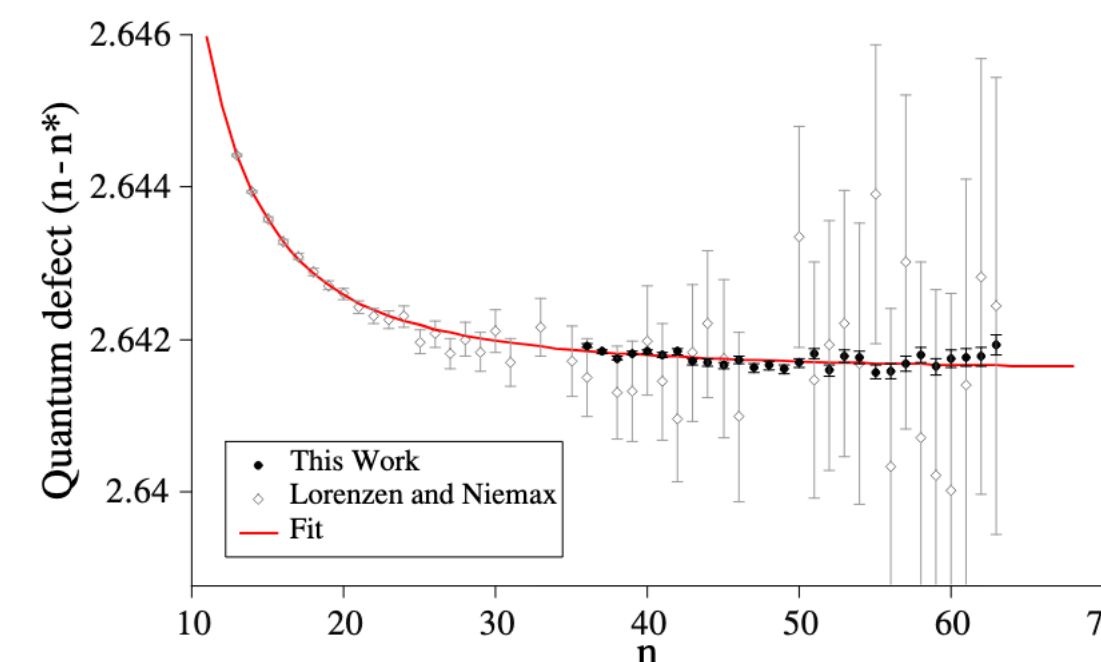
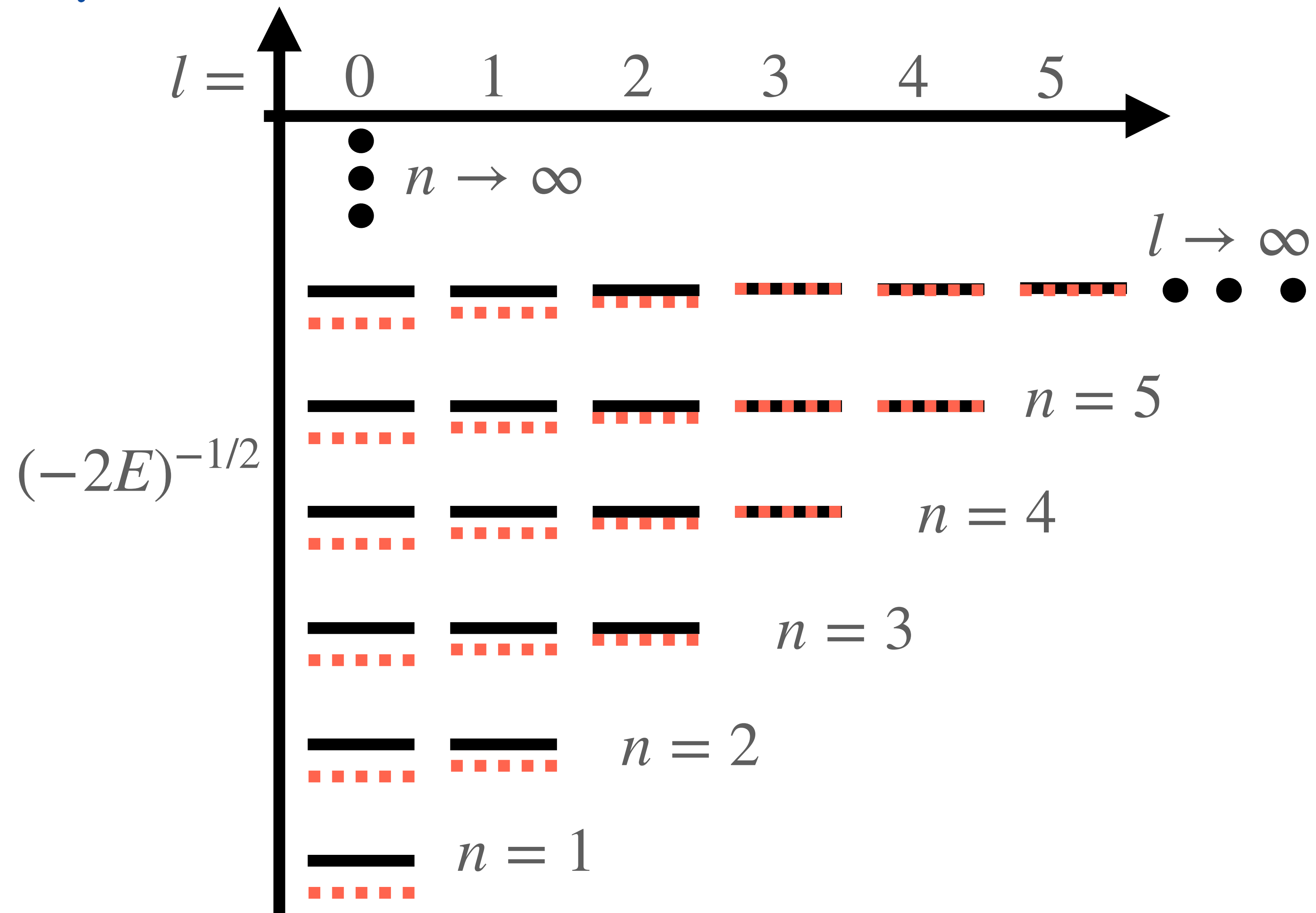


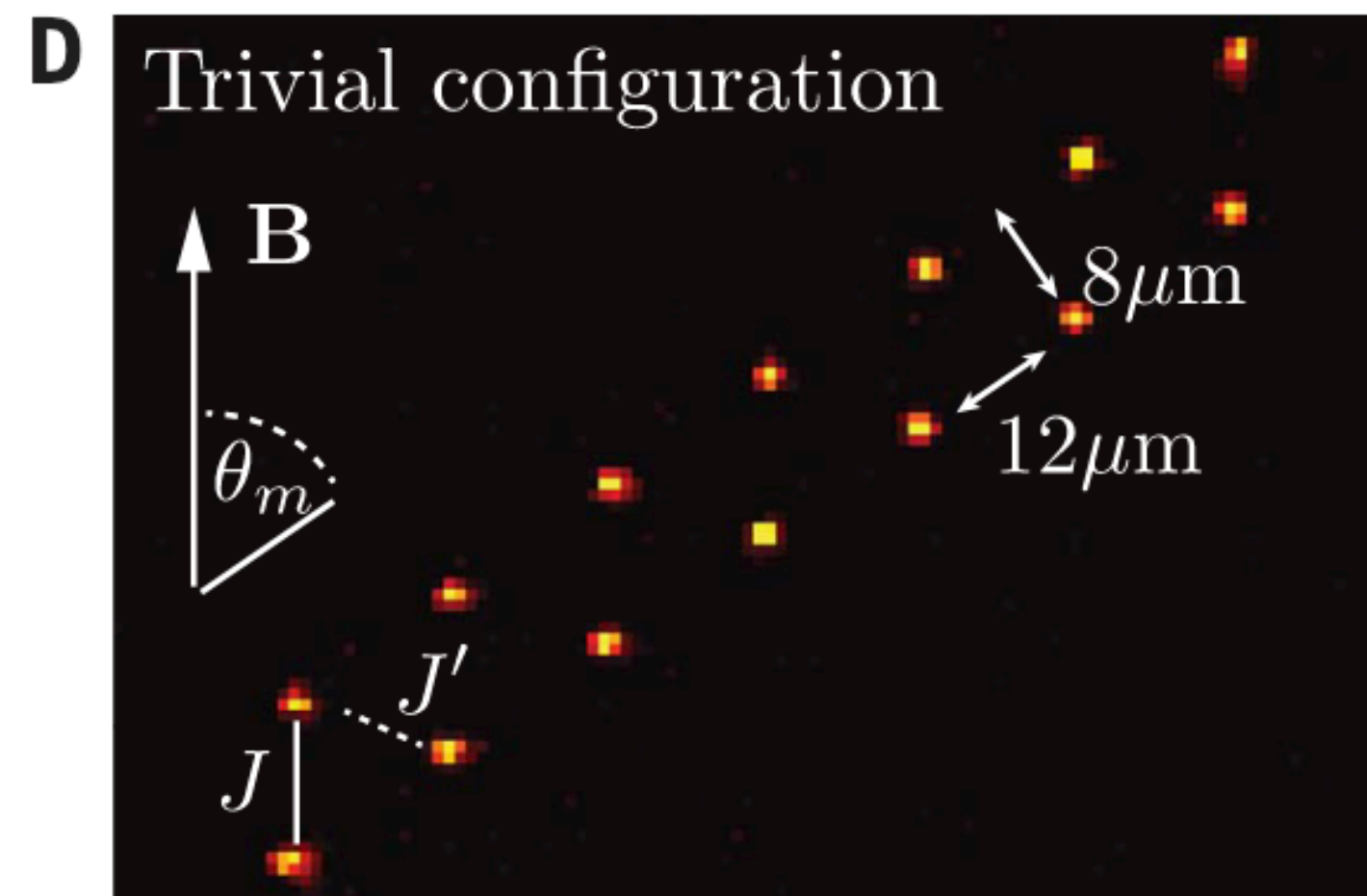
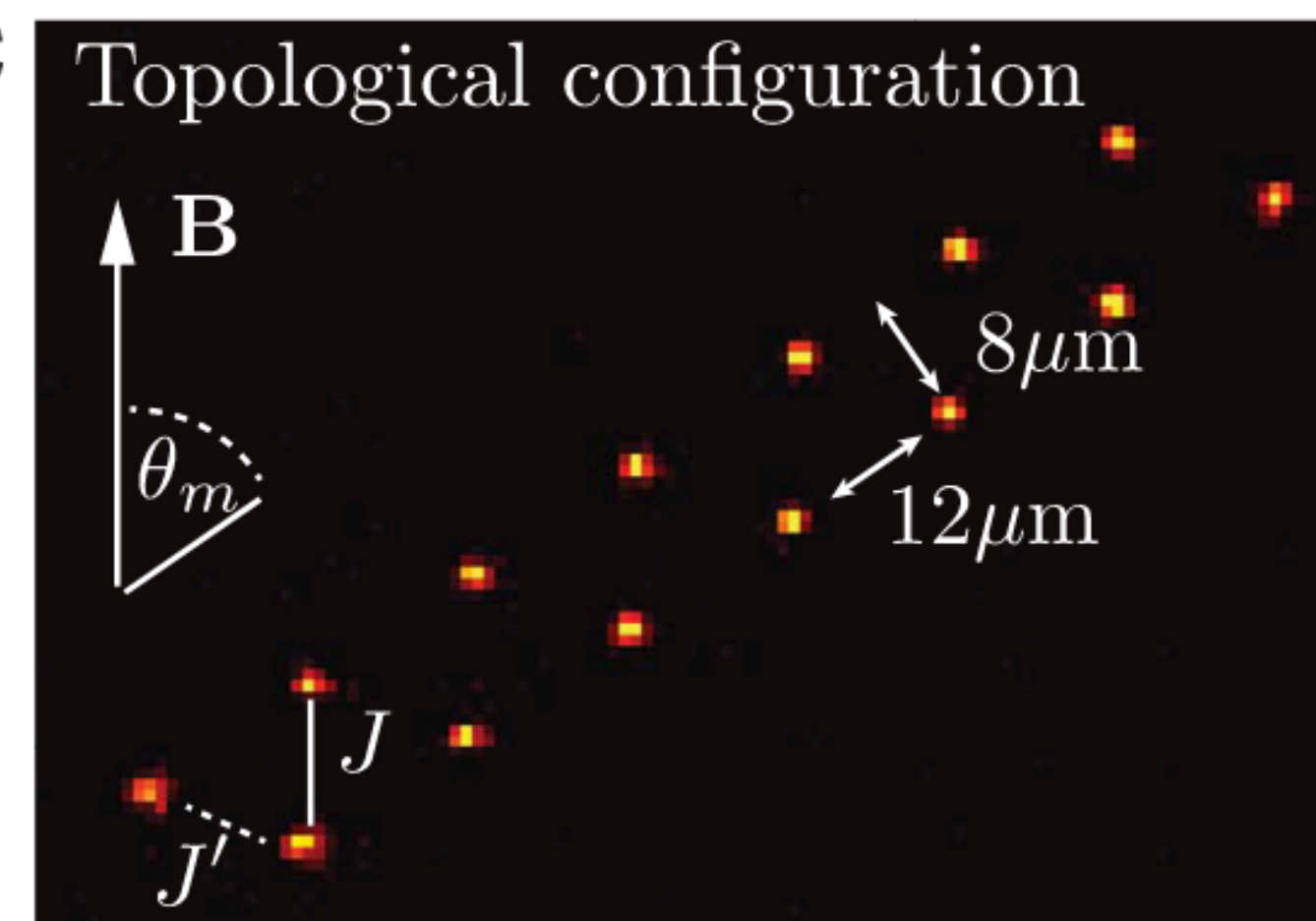
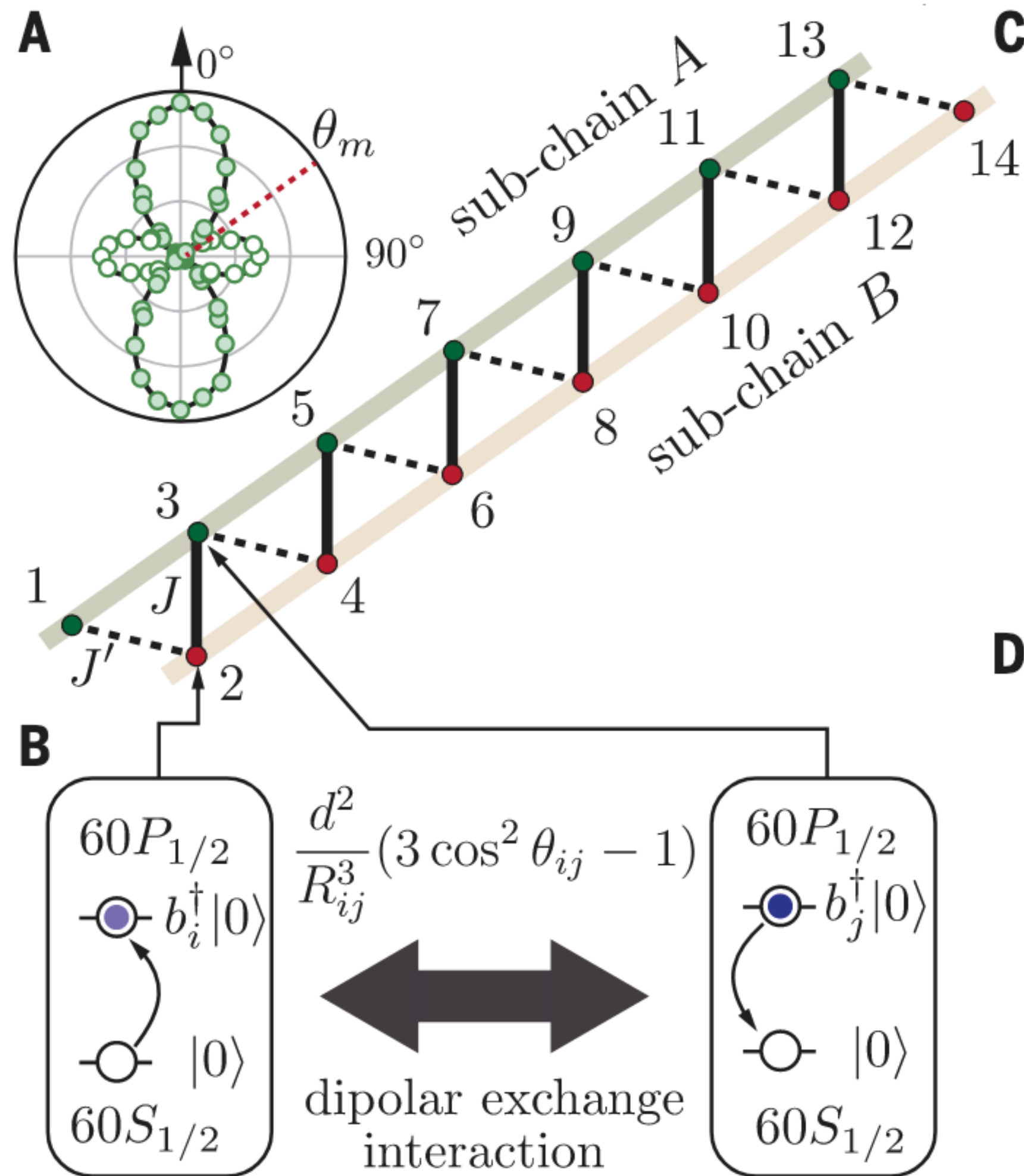
Figure 6. Quantum defects from the three different fitting methods. Data points for $n = 5$ and $n = 6$ were included in the calculations but are not shown, as their quantum defects are off the scale: 2.707 178 and 2.670 358, respectively.



A quick survey of atomic structure: hydrogen

Energy spectrum of hydrogen and an alkali atom.





RESEARCH ARTICLE

QUANTUM SIMULATION

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

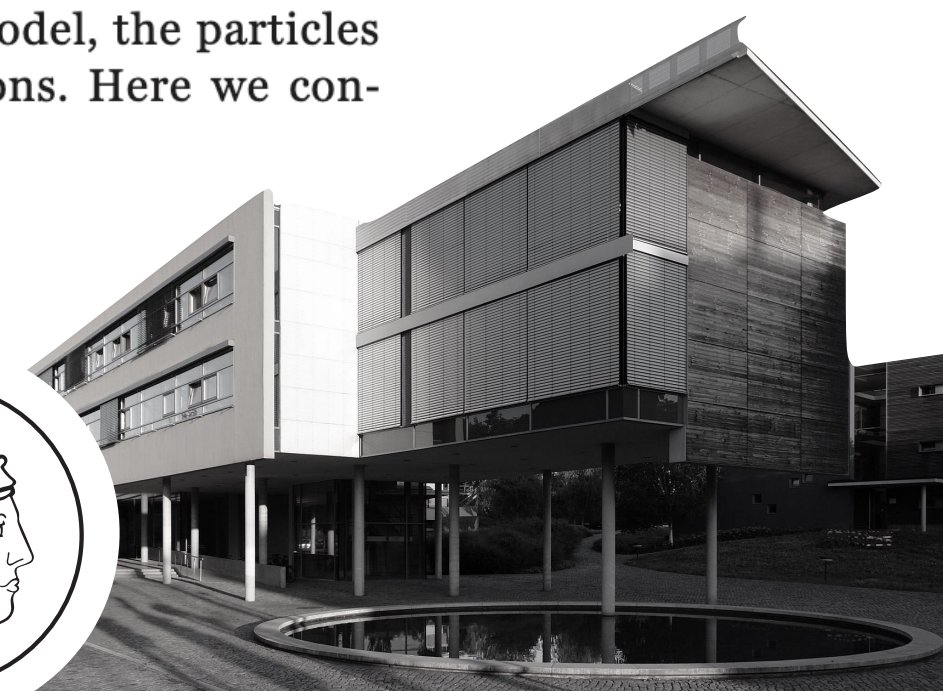
Sylvain de Léséleuc^{1*†}, Vincent Lienhard^{1*}, Pascal Scholl¹, Daniel Barredo¹, Sebastian Weber^{2*}, Nicolai Lang^{2*}, Hans Peter Büchler², Thierry Lahaye¹, Antoine Browaeys¹

SSH model for hard-core bosons

The SSH model is formulated on a one-dimensional lattice with an even number of sites N and staggered hopping of particles (Fig. 1A). It is convenient to divide the lattice into two sublattices: $A = \{1, 3, \dots, N - 1\}$, involving odd lattice sites, and $B = \{2, 4, \dots, N\}$, with even sites. Then, a particle on site i of one sublattice can hop to a site j of the other sublattice with a hopping amplitude J_{ij} (we do not restrict the system to nearest-neighbor hopping). The many-body Hamiltonian is

$$H = - \sum_{i \in A, j \in B} J_{ij} [b_i^\dagger b_j + b_j^\dagger b_i] \quad (1)$$

with b_i^\dagger (b_i) being the creation (annihilation) operator of a particle on site i . In the original formulation of the SSH model, the particles are noninteracting fermions. Here we con-



Quantum simulator exhibit C:

