Quasi-Static Lineshape Theory for Rydberg Excitations in Various Bose-Einstein Condensates

Giorgi Kharchilava[1] and Jesus Perez-Rios[2,3]
1: Department of Physics, University of Notre Dame, Notre Dame, IN, 46556
2: Department of Physics, Stony Brook University, Stony Brook, NY, 11794
3: Institute of Advanced Computational Science, Stony Brook University, Stony Brook, NY, 11794

Introduction

- Rydberg atom: an atom with a very excited electron (n>25). In such atoms, the core resembles a hydrogen nucleus.
- Lineshape: a distribution of relative frequencies of detunings for electron excitations.
- Detuning: the difference in energetic shift between an undisturbed excitation and an excitation in the presence of perturbers, which are atoms within the electron's orbit.

Theoretical Approach

The detuning of an excitation is the effect of perturbers on initial and final energies during photon absorption:

$$\omega = (E_f - E_i) + (\Delta\, E_f \; - \Delta\, E_f) = \omega_0 + \Delta\omega \quad (1)$$

The interaction between the Rydberg electron and perturber has a 1st and 2nd order component associated with s/p wave scattering respectively. The pseudopotential in (2) shows a dirac function (a semiclassical analog) instead of the wave function squared, which reflects a quantum perspective [3]:

$$V_{e-p} = 2\pi a_s(k)\delta^{(3)}(\boldsymbol{r}-\boldsymbol{R}) + 6\pi(a_p(k))^3\delta^{(3)}(\boldsymbol{r}-\boldsymbol{R})\nabla^2 \quad (2)$$

The neutral perturbers will also polarize and interact with the ionic Rydberg core as follows [3]:

$$V_{c-p} = \frac{-\alpha}{2r^4} \quad (3)$$

The perturber distributions are calculated using statistical mechanics. The Rydberg atom is positioned at the center of an harmonic trap in a gaseous Bose-Einstein condensate. The density distribution can be represented as the sum of BEC and Thermal atom densities [3, 4]:

$$N_{BEC}(\rho) = \begin{cases} \frac{m^2\omega^2}{8\pi a_{bb}}(R_{TF}^2 - \rho^2) & 0 \le \rho \le R_{TF} \\ 0 & \rho > 0 \end{cases} \quad (4)$$

$$N_{th}(\rho) = \frac{1}{\lambda_T^3} Li_{3/2}\left(e^{\frac{-1}{k_B T}\left(\frac{1}{2}m\omega^2|\rho^2 - R_{TF}^2| + \frac{8\pi a_{bb}}{m} N_{th}(p)\right)}\right) \quad (5)$$

Bose-Einstein Condensate

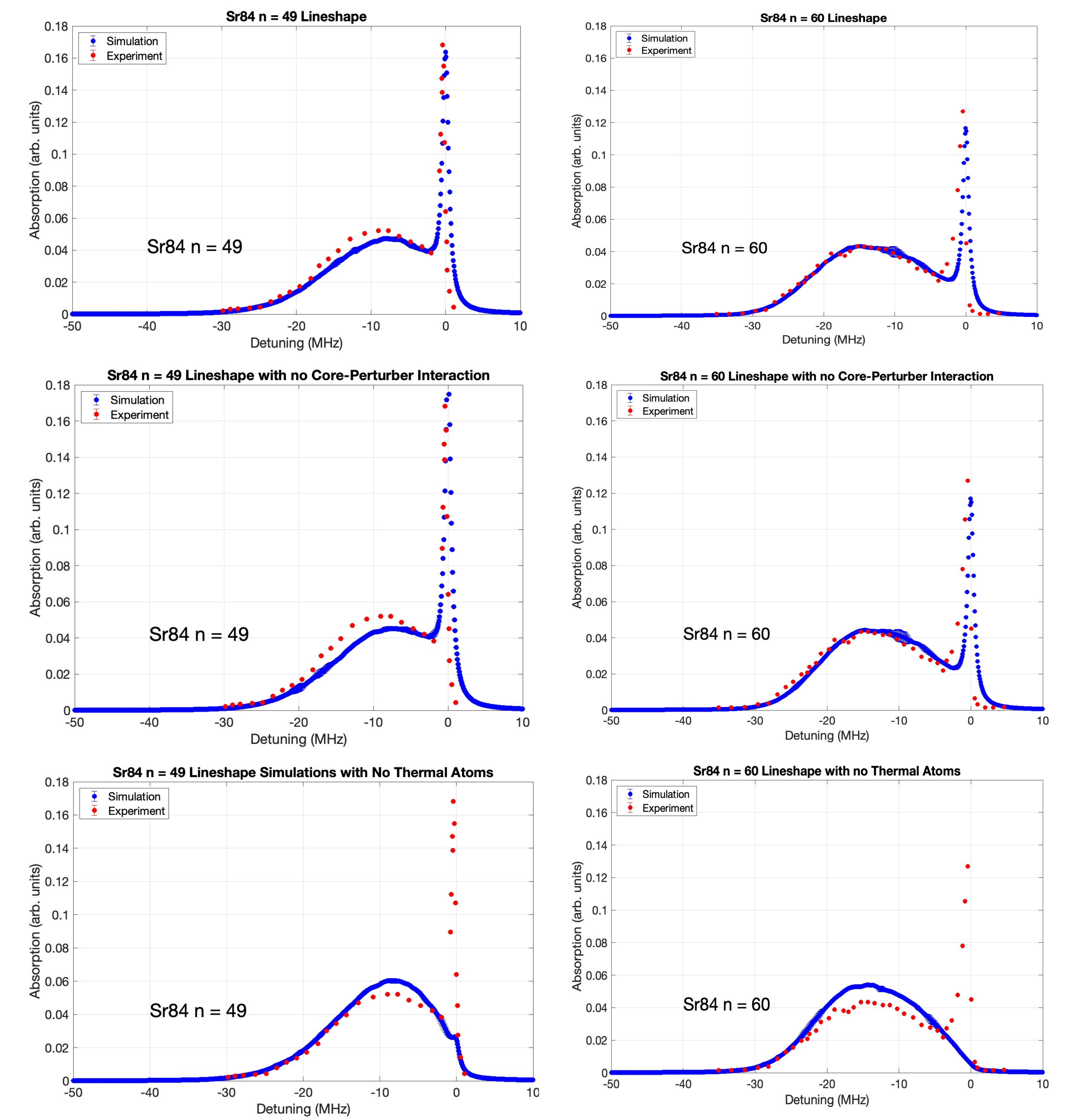
Indian physicist Satyendra Bose postulated that at low temperatures, the wave-particle duality of matter would result in wave packets with a macroscopic thermal de Broglie wavelength [1]:

$$\lambda = \frac{h}{p} = \sqrt{\frac{h^2}{mk_BT}} \quad (6)$$

At sufficiently low temperature, every particle's associated wavelength would become long enough to overlap with the others, leading every particle to occupy the same ground state and act as a unified quantum system. The BEC arises as a novel state of matter that allows physicists to observe and study quantum mechanics at a macroscopic scale.

Purpose

Develop a general computational method for simulating lineshapes of Rydberg atoms in a Bose-Einstein Condensate (BEC) and analyze the model's dependence on BEC density using Sr84 and Rb87 as test cases. Theoretical lineshape simulation is useful because lineshapes can illuminate certain hard-to-measure Rydberg properties, such as electron-neutral interactions or the density of the media.



Future Works

- Threshold densities: the current BEC densities ensure a single electron-perturber interaction and a relatively low dipole-dipole interaction potential
- Simulate higher densities to find transition to multiple perturbers and significant dipole-dipole interaction

References

1. L. de Broglie, "On the Theory of Quanta," 1925.
2. E. Fermi, "Sopra lo spostamento per pressione delle righe elevate delle serie spettrali," Il Nuovo Cimento (1924-1942), vol. 11, no. 3, p. 157, 2008.
3. J. Perez-Rios, "Introduction to Cold and Ultracold Chemistry", Springer, 2020.
4. T. Scheuing, J. Perez-Rios, "Quasi-Static Lineshape Theory for Rydberg Excitations." arXiv:2305.09010.

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Ultracold Regime

- At temperatures below 100 nK, The particles' de Broglie wavelengths are macroscopic and they each occupy the same quantum state (BEC) [3].
- The Rydberg atom is placed within an harmonic trap that contains a distribution of mostly BEC gas with a smaller number of thermal atoms.
- Rydberg electrons can bind to perturbers to form a diatom known as a Rydberg polaron , which has a very large dipole moment despite being homonuclear [3].

Considerations

- Quasi-static theory – Calculations assume negligible particle motion during excitation
- Perturbation Order – 1st/2nd (s/p)
- Thermal atoms
  - Internally excited beyond ground-state
- Multiple perturbers: 1<M<5
- Induced dipole-dipole interactions between perturbers

Methodology

- Mathematica – original coding language for simulations
- Matlab – simulation notebooks converted from Mathematica

The lineshape simulation process is as follows:

1. The harmonic trap probability distributions are scaled by radial distance from the center squared: $P(\rho) \sim N(\rho)\rho^2$ (7)
2. Choose number of nearby perturber atoms by designating the threshold radius as $2.5(n^*)^2$, and run different different numbers of perturbers according to a Poisson distribution.
3. Choose the distance of each perturber from the Rydberg core. The vicinal density is constant since the max perturber distance is much less than the trap radius. Thus, $P(r) \sim r^2$.
4. Total effect of perturbers is summed up using interaction potentials to get detunings:

$$V_{c-p} + \sum_{1}^{M} V_{e-p} + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} V_{p_i - p_j} \quad (8)$$

5. This set of detunings is converted to a histogram to generate an approximate lineshape, which is then converted to a proper lineshape by accounting for the light bandwidth [4]:

$$I(\nu) = \sum_i \frac{1}{(\nu - \nu_i^2) + (\Gamma/2)^2} \quad (9)$$