Cold Rydberg atoms for quantum simulation of exotic condensed matter interactions

J.P. Hague · S. Downes · C. MacCormick · P.E. Kornilovitch

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Abstract Quantum simulators could provide an alternative to numerical simulations for understanding minimal models of condensed matter systems in a controlled way. Typically, cold atom systems are used to simulate e.g. Hubbard models. In this paper, we discuss a range of exotic interactions that can be formed when cold Rydberg atoms are loaded into optical lattices with unconventional geometries; such as long-range electron-phonon interactions and extended Coulomb like interactions. We show how these can lead to proposals for quantum simulators for complex condensed matter systems such as superconductors. Continuous time quantum Monte Carlo is used to compare the proposed schemes with the physics found in traditional condensed matter Hamiltonians for systems such as high temperature superconductors.

Keywords Superconductivity · Stripes · Quantum simulators

1 Introduction

The recent implementation of quantum simulators for Hubbard models has been a triumph of experimental technique [1,2]. The simulation of Hubbard models has been a success, however the most basic form of the Hubbard model misses some crucial physics found in many condensed matter systems, including: (1) The electron-phonon interaction and (2) Longer range instantaneous interactions. In this paper we will discuss the potential for systems of dressed Rydberg atoms to become toolkits for examining the physics of more complicated, yet more realistic interactions such as these. Rydberg interactions are particularly timely, because interactions between small numbers of cold Rydberg atoms have recently been measured experimentally [3].

Rydberg atoms have been used to propose simulators for various different types of interactions in condensed matter systems. For example, chains of Rydberg ions have high energy phonons that can be used as part of a mapping to spin systems [4,5]. Other uses of Rydberg states in cold ion crystals are the investigation of structural distortions [6]. Simulators for Su-Schrieffer-Heeger polarons relevant to strongly deformable materials such as polymers may be achievable using excitons in Rydberg chains [7]. Cold polar molecules offer a similar platform to Rydberg states and have been proposed for simulators of Holstein and Su-Schrieffer-Heeger polarons [8,9]. In this paper, the use of Rydberg atoms to simulate long range electron-phonon couplings for arbitrary filling and extended Hubbard interactions is discussed. The bilayer scheme discussed here (see also [10]) has major advantages over previous proposals for electron-phonon interactions since arbitrary filling factors could be achieved in principle, whereas previous proposals concerned only the low density polaron limit. We have not previously discussed extended Hubbard interactions between Rydberg atoms.

2 Control over Rydberg interactions

Rydberg atoms have a high principal quantum number. As such, the electron is far from the nucleus and the atom has a large polarisability. When atoms are in
the \( |ns_{1/2}/2 \rangle \) state, separated by a displacement \( \mathbf{R} \), the dipole-dipole interaction can be calculated by analysing the appropriate interaction:

\[
V_{\text{dip}} = \frac{1}{4\pi\varepsilon_0} \left( \frac{\mu_1 \cdot \mu_2}{R^3} - \frac{3(\mu_1 \cdot \mathbf{R})(\mu_2 \cdot \mathbf{R})}{R^5} \right) \tag{1}
\]

which couples pairs of \( |ns_{1/2}/2; ns_{1/2}/2 \rangle \) states to pairs of other states (e.g. \( |n'p_f; n''p_f' \rangle \) which differs in energy by \( \Delta_{sp} \)). Here the dipole moments, \( \mu_i = e\mathbf{r}_i \), with \( e \) the electron charge and \( \mathbf{r}_i \) the position operator for atom \( i \). The Hamiltonian matrix is then:

\[
V_{\text{int}} = \begin{pmatrix}
0 & V(R) \\
V(R) & \Delta_{sp}
\end{pmatrix}
\tag{2}
\]

where \( V(R) = \langle ns_{1/2}/2; ns_{1/2}/2 | V_{\text{dip}} | n'p_f; n''p_f' \rangle \). The average over states ensures that \( V(R) \) has no preferential direction. Diagonalizing the matrix leads to the interaction strength,

\[
V_{\text{int} \pm} = \Delta_{sp}/2 \pm \sqrt{V(R)^2 + \Delta_{sp}^2}/4 \tag{3}
\]

If \( V(R) \ll \Delta_{sp} \), the standard van der Waals interaction is recovered. Of more use for condensed matter quantum simulators is the limit \( V(R) \gg \Delta_{sp} \) where the interaction has the form \( V_{\text{int}} = \alpha/R^3 \) (\( \alpha \) may also be written as \( C_3 \)). This regime is appropriate for this paper as \( \alpha \) is large and distances in an optical lattice (compared to the size of Rydberg states) are small. Control over Rydberg states (and the lifetime of the states) can be improved by illuminating the atoms with laser light offset by a value \( \Delta \) from the transition between the ground and Rydberg states to form virtual Rydberg atoms.

We propose to load cold Rydberg atoms into a bilayer optical lattice, similar to that shown in Fig. 1. Each layer represents different parts of the condensed matter system: Atoms in the upper layer take the place of itinerant electrons (itinerant layer), and those in the lower layer vibrating nuclei (phonon layer). Since each atom in a condensed matter system has a nucleus, the atoms in the lower (phonon) layer should be in a Mott insulating state so that there is a single atom (which can vibrate to make phonons) per site - as such the optical lattice for the phonon layer needs to be deep. The depth of the phonon layer also means that the phonon layer fills before the itinerant layer so that it is always completely filled, whereas the itinerant layer can be partially filled to simulate the effects of doping. In order to get small phonon frequencies in that layer, two optical pancakes can be separated by a small distance, \( D \), or two spots a distance \( D \) apart can be made using the painted potential technique [11].

The bilayer scheme offers significant control over the interactions and energy scales in the system. The depth of the itinerant layer can be varied to change energy scales such as the hopping, \( t \), the local Hubbard \( U \), the extended Hubbard interaction between atoms within the itinerant plane, \( V_{ij} \). Spots in the phonon layer can be changed to affect the Rydberg-phonon (electron-phonon) interaction between planes, \( g_{ij} \) and the phonon frequency, \( \omega_0 \). The strength of \( V_{ij} \) and \( g_{ij} \) can also be varied by changing the offset \( \Delta \) from the transition when dressing the Rydberg state, and also by selecting a different principal quantum number of the Rydberg state. A major advantage of the bilayer scheme over previous proposals for electron-phonon interactions is that arbitrary filling factors can be achieved - previously, only proposals for low density polaron states were available.

Hopping, \( t^{(it)} \), Hubbard \( U^{(it)} \) and phonon frequencies \( \omega_0^{(it)} \) in the itinerant layer have the standard values [12]:

\[
t^{(it)} \approx \frac{4}{\sqrt{\pi}} E_{\text{rec}} \left( \frac{V_0}{E_{\text{rec}}} \right)^{3/4} \exp \left[ -2 \left( \frac{V_0}{E_{\text{rec}}} \right)^{1/2} \right] \tag{4}
\]

\[
U^{(it)} \approx \sqrt{\frac{2\pi}{\pi}} k_0 E_{\text{rec}} \left( \frac{V_0}{E_{\text{rec}}} \right)^{3/4} \tag{5}
\]

\[
\hbar \omega_0^{(it)} = 2E_{\text{rec}} \left( \frac{V_0}{E_{\text{rec}}} \right)^{1/2} \tag{6}
\]

where \( V_0 \) is the depth of the lattice, \( E_{\text{rec}} \) has the value, \( \hbar^2 k^2/2M \), \( M \) is the atomic mass of the Rydberg atoms, \( k = \pi/a, \bar{a} \) is the s-wave scattering length and \( a \) is the lattice constant. Both \( t^{(it)} \) and \( U^{(it)} \) may be adjusted to represent hopping and Hubbard \( U \) in the resulting electron-phonon problem. Note that the phonon...
frequency $\omega_0^{(it)}$ is not the phonon frequency in the simulated problem, rather in this case it is only important that $\omega_0^{(it)}$ is very large as it essentially represents the separation between bands in the problem (energy levels of the simulated electron).

The phonon frequency for the electron-phonon Hamiltonian is provided by the phonon layer. The potential provided by the spot potentials is:

$$-\frac{V_0^{(ph)}}{2} \left[ \exp \left( -\frac{(x-D)^2}{2u_0^{(ph)^2}} \right) + \exp \left( -\frac{(x+D)^2}{2u_0^{(ph)^2}} \right) \right]$$

(7)

(Where the depth of the potential in the phonon layer is $V_0^{(ph)}$ and $u_0^{(ph)}$ is the waist size of the beam forming the painted potential, or in the case of 2 slightly separated optical pancakes is the width of each pancake). The Taylor expansion leads to the phonon frequency,

$$\left(\omega_0^{(ph)}\right)^2 = V_0^{(ph)} \exp \left( -\frac{D^2}{2u_0^{(ph)^2}} \right) \frac{(w_0^{(ph)^2} - D^2)}{Mw_0^{(ph)^2}}.$$  
(8)

Taylor expansion of the dipole-dipole interactions between Rydberg atoms in itinerant and phonon layers and assuming only c-axis phonons (which can be achieved by making the phonon layer from 2 optical pancakes separated by a small distance, $D$, as with the phonon frequency) leads to an electron-phonon (Rydberg-phonon) interaction $g_{ij}$:

$$g_{ij} = \frac{\Omega^2}{4\Delta^2} \frac{3\mu^2b}{2 \left( b^2 + r_{ij}^2 \right)^{3/2}} \sqrt{\frac{\hbar}{2M\omega_0}}$$

(9)

where $\Omega$ is the Rabi frequency and $b$ is the interplane distance.

Taking these values together, a dimensionless electron-phonon coupling can be defined,

$$\lambda = \frac{1}{2\omega_0^{(it)/2}MW} \left[ \frac{3\Omega^2\mu^2}{4\Delta^2} \sum_i b_i^2 \left( b_i^2 + r_{ij}^2 \right)^3 \right]$$

(10)

where $W = 4\ell^{(it)}$.

Finally, it should be noted that there are dipole-dipole interactions between Rydberg atoms in the itinerant plane that contribute an extended Hubbard V to the Hamiltonian,

$$V_{ij} = \frac{(2M\omega_0^{(it)/2}W)^{1/2}}{3r_{ij}^2} \left[ \sum_k \frac{b_k^2}{\left( b_k^2 + r_{ij}^2 \right)^{3/2}} \right]^{-1/2}.$$  
(11)

In the limit of low phonon frequency, this does not contribute to the physics as demonstrated elsewhere [12]. Alternatively, it is possible to manipulate the Rydberg system so that this extended Hubbard physics dominates, and in this case we use the shorthand $V_{ij} = \alpha/r_{ij}^3$.

Thus, the full Hamiltonian that is simulated by the proposed bilayer Rydberg quantum simulator is:

$$H = -t^{(it)} \sum_{\langle ij \rangle} c^\dagger_i c_j + U^{(it)} \sum_i n_i \hat{n}_i + \sum_{ij} V_{ij} n_i n_j + \sum_{ij} g_{ij} n_i (d_j^\dagger + d_j^\dagger) + \hbar \omega_0^{(ph)} \sum_i d_i^\dagger d_i$$  
(12)

3 Tests of the proposed simulator

The Rydberg-phonon interaction in Eqn. [9] differs slightly from the standard Fröhlich form of the electron-phonon interaction, $g_{ij}^{(Fr)} \propto \exp(\frac{-R_{\text{sc}}r_{ij}}{a^2 + r_{ij}^2})^{-3/2}$. In the limit that $b \rightarrow 0$, the standard Holstein interaction $g_{ij}^{(Hol)} \propto \delta_{ij}$ is recovered. It is necessary to check that the difference in the tails of the interaction does not lead to any major qualitative changes in the physics of the Hamiltonian. Here, continuous time quantum Monte Carlo (CTQMC) [13] is used to examine the polaron and bipolaron physics, as shown in Fig. 2. The figure shows results from QMC for both Fröhlich interactions, and the Rydberg-phonon interaction considered here. Effective nearest-neighbour interactions have been matched by modifying the distance $b$ between the two planes, so only the tails of the interactions differ as would be the case when making an experimental implementation of the scheme. The agreement between the two schemes is excellent.

As yet unexplored is the potential to use Rydberg atoms for extended Hubbard interactions. A 1D simplification of the complex bilayer geometry allows the simulation of many particle ensembles using CTQMC without sign problems. Fig. 3 shows the correlation function of particle positions $(n_i n_j)$ (including auto-correlation). 12 particles were simulated on a ring of 48 sites (density $1/4$). For large $\alpha$, short range correlations can be observed as a modulation of the correlation function. As $\alpha$ decreases, the range of the correlations decreases until the tails of the correlation function show the uncorrelated value of 0.25. Correlations and extended Hubbard interactions from Rydberg atoms will be described in more detail in an extended paper.

4 Summary and outlook

We have proposed that systems of Rydberg atoms could be used to simulate exotic long-range interactions in condensed matter systems. States of dressed Rydberg atoms can be chosen such that the dipole-dipole interactions between them have the form $1/R_{ij}^3$. Appropriate layering of Rydberg atoms into bilayers where an itinerant layer represents the physics of itinerant
Fig. 2 Polaron and bipolaron energies for different interaction ranges within the bilayer Rydberg scheme proposed here, and for a screened Fröhlich interaction. The near-neighbor interaction strengths have been matched. $U_{ij}^{(it)} = 4t_{ij}^{(it)}$, $h_{ij}^{(ph)} = t_{ij}^{(it)}$, $\lambda = \Phi(0)/8t_{ij}^{(it)} M_{ij}^{(it)}$. Unless shown, error bars are smaller than the points. The lower plots show the residual between the Rydberg and Fröhlich schemes, which is less than 0.1 per particle. Both the interaction type in the proposed quantum simulator and the screened Fröhlich interaction have quantitatively similar physics. The effects of a harmonic potential are also shown, and do not lead to significant deviations from the free lattice case.

Fig. 3 Density-density correlation function vs relative particle positions, for a range of interaction strengths, $\alpha$. For large $\alpha$, the system forms a state with local order. As $\alpha$ is decreased, the long range behaviour becomes unordered (see the long tail of $C_{ij} = 0.25$ when $\alpha = 1$). Error bars are typically too small to be distinguishable.

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