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Quantum simulation of electron–phonon interactions in strongly deformable materials

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Abstract. We propose an approach for quantum simulation of electron–phonon interactions using Rydberg states of cold atoms and ions. We show how systems of cold atoms and ions can be mapped onto electron–phonon systems of the Su–Schrieffer–Heeger type. We discuss how properties of the simulated Hamiltonian can be tuned and how to read physically relevant properties from the simulator. In particular, use of painted spot potentials offers a high level of tunability, enabling all physically relevant regimes of the electron–phonon Hamiltonian to be accessed.

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1. Introduction

Electron–phonon interactions lead to some dramatic effects in condensed matter systems, with lattice vibrations leading to phenomena such as superconductivity [1] and colossal magnetoresistance [2]. Even in the presence of overwhelming Coulomb repulsion, quasi-particle properties such as the effective mass can be strongly modified when electron–phonon interactions are strong. The importance of electron–phonon interactions has led to an industry in numerical simulation, but even very simplified models [3, 4] are significantly more difficult to treat than other standard models in condensed matter such as Hubbard’s model [5]. This difficulty lies in the very large Hilbert space that is needed to handle a potentially infinite number of phonons associated even with motion of a single electron.

Recently, there has been a move to use systems of cold atoms as quantum simulators to investigate standard models of condensed matter physics [6]. The model that has been most successfully simulated is the Hubbard model of instantaneous local repulsion between electrons [5]. An optical lattice loaded from a Bose–Einstein condensate (BEC) can be directly related to a Hubbard model, since there is a large energy penalty for two atoms to sit on the same lattice site [6]. The use of cold atoms to simulate Hubbard models has led to direct observation of important phenomena such as the superfluid to Mott insulator transition [7, 8]. However, there is no simple way of extending the approach to include phonons.

There are several classes of electron–phonon interaction that are of direct relevance to condensed matter systems. For polymers, which are very easy to deform, the hopping of electrons along the chain can be strongly modified by the presence of lattice vibrations. This leads to the Su–Schrieffer–Heeger (SSH) model, which describes a chain of CH groups in polyacetylene [4], which for a chain of $N$ groups of mass $M$ has the Hamiltonian,

$$
H_{SSH} = -\sum_{i} t_{i+1,i}(c_{i+1,\sigma}^\dagger c_{i,\sigma} + \text{H.c.}) + \frac{K}{2} \sum_{i} (u_{i+1} - u_{i})^2 + \frac{M}{2} \sum_{i} \dot{u}_{i}^2,
$$

where the intersite hopping, $t_{i+1,i} = t_0 - g(u_{i+1} - u_{i})$, $c_{i,\sigma}^\dagger$ creates an electron at site $i$, $g$ is the electron–phonon coupling strength, $t_0$ is the hopping in the absence of vibrations, $\sigma$ is the electron spin, $u_i$ is the group displacement and $K$ is the spring constant for the phonons.

The first term in this Hamiltonian is the electron kinetic energy from hopping, the second term is the potential energy from bond stretching and the third term the kinetic energy of the nuclei. In such strongly deformable materials, the vibrational amplitude of the atoms is large enough to affect the hopping integrals, since electrons typically hop more easily between atoms that are closer together. Thus the hopping, $t_0$, is augmented proportional to the relative displacement of neighbouring atoms. The energy spectrum for the second and third terms in the Hamiltonian, that relate to the phonon modes, may be solved in the absence of interaction by Fourier transforming, diagonalizing and introducing creation and annihilation operators [9]. In this way, they are rewritten as $\sum_{k,v} \hbar \omega_k \nu (d_k^\nu d_k^\dagger + 1/2)$, where each phonon mode has energy $\hbar \omega_k$. The combination $d_k^\nu d_k^\dagger$ is the number operator for phonons of mode $\nu$ with momentum $k$, where $d_k^\nu$ and $d_k^\dagger$ respectively represent phonon creation and annihilation operators.

General three-dimensional (3D) phonon fields are quantized in the usual way by substituting

$$
\mathbf{u}_i = \sum_{k,\nu} \sqrt{\frac{\hbar}{2NM\omega_{k\nu}}} \xi_{k\nu} \left( d_{k\nu} e^{-i\mathbf{k} \cdot \mathbf{R}_i} + d_{k\nu}^\dagger e^{i\mathbf{k} \cdot \mathbf{R}_i} \right),
$$

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with $\xi_{kv}$ the polarization vector [9]. In the case of the standard SSH model, there is a single phonon mode, so the model is simplified and $u_i = \sum_k \sqrt{\hbar/2MN} \omega_k (d_k e^{-ikR_i} + d_k^\dagger e^{ikR_i})$. Creation and annihilation operators may be Fourier transformed using the relation, $d_i^\dagger = \sum_k d_k^\dagger e^{ikR_i}/\sqrt{N}$, where $d_i^\dagger$ creates a phonon at site $i$. If the phonons are taken to be dispersionless Einstein modes of frequency $\omega_0$ (which are a mean field approximation to the phonons, and are often a good approximation to optical phonon modes) then the momentum sum can be performed to obtain the expression, $u_i = \sqrt{\hbar/2M}\omega_0(d_i + d_i^\dagger)$. In the case of polymers, out of chain phonon modes may also be permissible, and if Einstein phonons are used as an approximation, the polarization vectors $\xi_{kv}$ point in orthogonal directions.

There are a number of other models of electron–phonon interactions in condensed matter. One of the most prominent is Holstein’s molecular crystal model, which describes the type of interactions that can be found in many materials, where the local electron density couples to local optical phon modes which are usually associated with vibrations of other ions in the unit cell [3]. The Fröhlich model describes the continuum limit of interactions between electrons and strongly polarizable materials, which originate when itinerant electrons generate a dipole moment in a medium [10] and can be generalized to lattice models [11] (the latter are sometimes known as extended Holstein interactions). Holstein and extended Holstein interactions have the form,

$$H_{\text{Holstein}} = -t_0 \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ij\sigma} \tilde{g}_{ij} n_{i\sigma} (d_{j\sigma}^\dagger + d_{j\sigma}) + \hbar \omega_0 \sum_j (d_{j\sigma}^\dagger d_{j\sigma} + 1/2),$$

(3)

where $\tilde{g}_{ij}$ is related to the force between the electron and the ion, and for a standard Holstein model $\tilde{g}_{ij} = \delta_{ij}$, where $\delta_{ij}$ is the Kronecker delta. The local number operator for electrons of spin $\sigma$ at site $i$ is $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, and $d_{j\sigma}$ is the number operator for phonons at site $j$. The third term in the Hamiltonian represents a local Harmonic oscillator or Einstein mode. Since $d_{j\sigma}^\dagger + d_{j\sigma} \propto u_j$ where $u_j$ is the atomic displacement, a simple physical picture arises: when an electron hops onto a site, an atomic displacement is formed, and as the electron leaves a site, the displacement relaxes. The continual displacement and relaxation of atoms generates a phonon cloud that moves with the electrons, increasing their effective mass.

Even the simplest case of the electron–phonon model (the polaron) where a single electron moves on a chain has caused controversy since the polaron concept was introduced [12]. In particular, the existence of self-trapping, where distortions of the lattice generated by the electron prevent the electron from hopping, has remained an open question. It is now known that self-trapping is not possible in the Holstein model, where the effective mass increases exponentially at strong coupling, but never becomes infinite [13]. On the other hand, there is tantalizing evidence for self-trapping in the SSH model which may have consequences for polymer physics [14].

A number of schemes for quantum simulation of different interaction types between electrons and phonons have been suggested. A scheme for simulation of the Frenkel–Kontorova model to probe friction and energy transport has been proposed by Pruttivarasin et al [15]. Bruderer et al [16, 17] have proposed a system where an optical lattice is bathed in a BEC in which polaron effects have been observed [18]. The use of cold polar molecules to obtain Holstein polaron effects has been discussed by Herrera et al [19]. It is also appropriate to note the use of Rydberg ions to simulate spin systems, where high-energy phonon states are used as part of the mapping onto a spin system. Porras and Cirac [20] have made the mapping between a system of ions and an Ising model by making a Lang–Firsov transformation. Their
proposed system has the form of phonons coupled to a single Rydberg state via an interaction of the Holstein type, and the interaction is generated using a laser. Müller et al [21] have proposed the use of trapped Rydberg ions to simulate spin chains. Li and Lesanovsky [22] have discussed the structural distortions associated with exciting a high-energy Rydberg state in a cold ion crystal. We also note the proposed use of weakly dressed Rydberg states to simulate supersolids [23], strongly correlated gases [24] and collective many-body interactions [25].

In this paper, we present an approach to simulating the SSH polaron problem using Rydberg states of cold atoms and ions. We will show how a system of Rydberg atoms can be directly mapped to a SSH electron–phonon Hamiltonian, which is of direct interest in the modelling of polymers and other condensed matter phenomena relating to highly deformable materials, and to our knowledge has not been investigated before in the context of cold atoms. The simulator is introduced and the mapping to corresponding models is carried out. We then discuss how to read properties of electron–phonon interactions from the simulator, and describe a simple experiment to investigate the self-trapping problem.

2. Mapping between cold Rydberg atoms and a Su–Schrieffer–Heeger model

We now consider the various terms in the Hamiltonian that describes the motion of excited Rydberg states, the interaction of the Rydberg state with ions and atoms and the interaction of atoms and ions with each other. We begin by discussing how electron–phonon interactions can be simulated in a system of cold Rydberg atoms such as rubidium in a deep optical lattice where there is a single atom per lattice site. The deep optical lattice is essential in this case so that hoppings of atoms between sites are suppressed and there is no double occupancy of atoms. Systems of cold ions will be discussed later.

Following the prescription in [26], it is possible to set up a stable (long lifetime) Rydberg system where the excitations are superpositions of low-energy hyperfine and high-energy Rydberg states. Such a system is initialized with two hyperfine states \(|g\rangle\) and \(|h\rangle\), so that (for example) on a chain the system is in a state \(|\pi_i\rangle = |\cdots ggghggg \ldots\rangle\). Then two lasers detuned from the \(|g\rangle \leftrightarrow |nS\rangle\) and \(|h\rangle \leftrightarrow |nP\rangle\) transitions of the cold atoms from the ground to Rydberg states \(|nP\rangle\) and \(|nS\rangle\) are switched on so that all but one atom is in the dressed state \(|0\rangle = c_S|nS\rangle + c_h|g\rangle\). Excitons in state \(|1\rangle = c_p|nP\rangle + c_h|h\rangle\) hop in the system, as illustrated in figure 1. Here \(c_S, c_p, c_P\) and \(c_h\) are constants. As described in [26] the van Vleck perturbation theory (which acts to project an interacting Hamiltonian onto an effective hopping Hamiltonian) can be used to obtain an effective Hamiltonian for the motion of excitons,

\[
H_{\text{eff}} = \sum_i \left( E_2 + E_4 + W \right) |\tilde{\pi}_i\rangle\langle \tilde{\pi}_i| + \sum_{i \neq j} \tilde{V}_{ij} |\tilde{\pi}_i\rangle\langle \tilde{\pi}_j|,
\]

where the wavefunction \(|\tilde{\pi}_i\rangle\) represents a single exciton at site \(i\). There are onsite energy offsets as a direct result of the dressing of the Rydberg states, which are calculated to second order as,

\[
E_2 = (N - 1)\alpha_S^2 \Delta_S + \alpha_P^2 \Delta_P,
\]

and to fourth order in the van Vleck scheme as,

\[
E_4 = - (N - 1)\alpha_S^4 \Delta_S + \alpha_P^4 \Delta_P - (N - 1)\alpha_S^2 \alpha_P^2 (\Delta_S + \Delta_P),
\]
Figure 1. Schematic of the dressed Rydberg excitations. A set of cold atoms or ions is prepared. They are illuminated by two frequencies \( \Delta E_{gS} - \Delta_S \) and \( \Delta E_{hP} - \Delta_p \), where \( \Delta E_{gS} \) corresponds to the transition between the \(|g\rangle\) and \(|nS\rangle\) states, and \( \Delta E_{hP} \) to the transition between \(|h\rangle\) and \(|nP\rangle\) states. \(|g\rangle\) and \(|h\rangle\) are hyperfine levels and \(|nS\rangle\) and \(|nP\rangle\) Rydberg states with \( l = 0 \) and \( l = 1 \) respectively, both with \( m_l = 0 \). The lasers are de-tuned from the transition so that the particles spend only a short period of time in the Rydberg states. This increases the lifetime of the particles by reducing the incidence of ionization, and also stabilizes the particles against decay, although this reduces the effective dipole–dipole interactions between the atoms. Superpositions of the \(|h\rangle\) and \(|nP\rangle\) states move around the lattice as excitons.

and there is an additional energy shift due to dipole–dipole interactions of,

\[
W = \alpha_S^2 \alpha_P^2 \left( \sum_{k \neq j} \frac{1}{1 - \tilde{V}_{kj}^2} \right) (\Delta_S + \Delta_P).
\]  

(7)

A hopping term between exciton states on sites \( i \) and \( j \) also emerges from the perturbation theory,

\[
\tilde{V}_{ij} = \alpha_S^2 \alpha_P^2 \frac{V_{ij}}{1 - \tilde{V}_{ij}^2},
\]  

(8)

where \( \tilde{V}_{ij} = V_{ij} / (\Delta_S + \Delta_P) \). \( N \) is the number of ions in the chain. \( \alpha_S = \Omega_S / 2 \Delta_S \) and \( \alpha_P = \Omega_P / 2 \Delta_P \) are dressing parameters. \( \Delta_S \) and \( \Delta_P \) are the detunings of the illuminating radiation away from the frequencies corresponding to the \( g-nS \) gap, \( \Delta E_{gS} \), and the \( h-nP \) gap, \( \Delta E_{hP} \), respectively. The Rabi frequencies are denoted \( \Omega_S \) and \( \Omega_P \). The undressed interaction between Rydberg states on different ions is given by the dipole–dipole interaction,

\[
V_{kl} = \frac{\mu^2}{|R_k - R_l|^3},
\]  

(9)

where \( \mu \) is the effective dipole moment on the Rydberg atom and \( R_k \) is the vector to the \( k \)th atom in the optical lattice.
All states are set up with $m_l = 0$, and the atoms are illuminated with light which is polarized out of the plane. With this choice of laser polarization, transitions to the $|nP⟩$, $m_l = 1, -1$ states are suppressed \cite{27}. It is worth noting that the effective Hamiltonian can also be written using the second quantized notation as,

$$H_{\text{eff}} = \sum_i (E_2 + E_4 + W) a_i^\dagger a_i + \sum_{i \neq j} \tilde{V}_{ij} a_i^\dagger a_j,$$

where $a_i^\dagger$ creates an exciton and $a_i$ annihilates an exciton at site $i$. In the following, the excitons will take the place of the electrons in the SSH and Holstein models. Note that the excitons are hardcore as there cannot be more than one exciton per site (there is either an exciton associated with a site, or there is not).

Terms in the Hamiltonian (4) have the following origin. The first term $(E_2 + E_4)$ is simply an onsite, constant offset of the energy which would be absorbed into a chemical potential. It arises because of the interaction between the lasers and the atoms, and would be present even in the absence of dipole–dipole interactions between the atoms. The energy offset term $W$ arises because the local dipole moment induces moments in other atoms, which then cause an energy shift by re-interacting with the original dipole. The most important term here is the long-range hopping term $\tilde{V}_{ij}$ which is the origin of a SSH interaction as discussed below. The corrections to this interaction also have their origin in induced dipoles.

The following discussion is for arbitrary dimension and works equally well for optical lattices in planes and on chains, and for phonons that can vibrate on a line, plane or within a full 3D space. Phonons can be introduced to the system by displacing the atoms from their equilibrium positions. Atomic displacements within the optical lattice are independent as no interaction is carried through the optical lattice. Therefore, the vibrations of the atoms in the lattice are a faithful representation of Einstein phonons. One interesting possibility for 2D or 3D vibrations is to distort the harmonic potential of the optical lattice to lift the degeneracy of the phonon modes. The Hamiltonian for these modes will be,

$$H_{\text{ph}} = \sum_{\nu k} \hbar \omega_\nu (d_{\nu k}^\dagger d_{\nu k} + 1/2) = \sum_{\nu i} \hbar \omega_\nu (d_{\nu i}^\dagger d_{\nu i} + 1/2).$$

The introduction of small in-plane phonon displacements, $u_i$, at site $i$ causes the interaction between Rydberg states to become,

$$V_{ij} = \frac{\mu^2}{|R_i + u_k - R_j - u_j|^3},$$

which can be Taylor expanded if the displacement is small, noting that it is only necessary to expand to 1st order in $u$ as this is the lowest order for nontrivial interaction with phonons. This leads to:

$$V(R + u) \approx \frac{\mu^2}{|R|^3} - \frac{3 \mu^2 u \cdot \dot{R}}{|R|^4}.$$

This expansion can be applied to the off-site terms in equation (8) to obtain,

$$\tilde{V}_{ij}(u) \approx \frac{\alpha^2 \alpha_p \mu^2}{1 - \mu^4/R_{ij}^4} \left[ \frac{1}{R_{ij}^3} - \frac{3 u_{ij} \cdot \dot{R}_{ij}}{R_{ij}^4} - \frac{6 u_{ij} \cdot \dot{R}_{ij}}{R_{ij}^5} \frac{\tilde{\mu}^4}{1 - \mu^2/R_{ij}^6} + O(u^2) \right],$$

where $\tilde{\mu}^2 = \mu^2/(\Delta_S + \Delta_F)$ and $u_{ij} = u_i - u_j$. 

Quantization of the atomic displacements using equation (2) leads to an extended SSH model which is general for both cold ion or cold atom systems,

\[ H_{\text{ext--SSH}} = \sum_{ij} a_i^\dagger a_j \frac{\alpha_j^2 \alpha_i^2 \mu^2}{1 - \mu^4 / R_{kj}^6} \frac{1}{R_{ij}} \left[ 1 - \frac{3}{R_{ij}} \sum_k \sqrt{\frac{\hbar}{2NM\omega_{kv}}} \hat{R}_{ij} \cdot \xi_{kv} \right. \]

\[ \times \left( d_{kv} [e^{-ik \cdot R_i} - e^{-ik \cdot R_j}] + d_{kv}^\dagger [e^{ik \cdot R_i} - e^{ik \cdot R_j}] \right) . \]  

Here, \( a_i^\dagger / a_i \) create/annihilate excitons on site \( i \) and \( M \) is the mass of the atoms (or ions).

A further simplification can be made for atoms in the optical lattice because the oscillators are independent and local, thus there is no momentum dependence in the phonon modes and \( \omega_{kv} = \omega_{0v} \) and \( \xi_{kv} = \xi_{0v} \) so that the momentum sum only applies to the phonon creation and annihilation operators. Moreover, the set of \( \xi_{0v} \) is now orthogonal. Fourier transforming these operators, the local nature of the model with Einstein modes becomes clear,

\[ H_{\text{ext--SSH}} = \sum_{ij} a_i^\dagger a_j \frac{\alpha_j^2 \alpha_i^2 \mu^2}{1 - \mu^4 / R_{kj}^6} \frac{1}{R_{ij}} \left[ 1 - \frac{3}{R_{ij}} \sum_v \sqrt{\frac{\hbar}{2M\omega_{0v}}} \xi_{0v} (d_{jv} + d_{jv}^\dagger - d_{iv} + d_{iv}^\dagger) \right] . \]  

This Hamiltonian is an extended version of the SSH model. Note that there can still be several phonon modes since even if the atoms are arranged in a chain or sheet, the harmonic traps can be three dimensional. Making the comparison with the SSH Hamiltonian (equation (1)), it is possible to assign values to \( t_0 \) and \( g \). The form of the coefficients mean that the relative strength of the parameters can be tuned by changing the inter-ion spacing in the lattice since the Hopping term, \( t \), has \( 1/R^3 \) functionality, whereas the electron–phonon coupling term \( g \sim 1/R^4 \). The phonon frequencies can be changed by altering the depth of the optical lattice, giving full control over all parameters in the model. We will discuss this tuning in more detail in section 4.

Making a similar Taylor expansion, phonon interactions via the on-site term in equation (7) can also be considered,

\[ \sum_{k \neq j} \frac{1}{1 - \frac{\mu^4}{R_{kj}^6}} \approx \sum_{k \neq j} \frac{1}{1 - \frac{\mu^4}{R_{kj}^6} + 6u_{kj} \cdot \hat{R}_{kj} \mu^4 / R_{kj}^6} \]  

\[ = \sum_{k \neq j} \frac{1}{1 - \frac{\mu^4}{R_{kj}^6}} \left[ 1 - \frac{6u_{kj} \cdot \hat{R}_{kj} \mu^4}{R_{kj}^6 (1 - \frac{\mu^4}{R_{kj}^6})} \right] , \]  

so that the local Hamiltonian becomes,

\[ H_{\text{ext--Hol}}(\mathbf{u}) = \sum_i a_i^\dagger a_i (\Delta_S + \Delta_P) \alpha_i^2 \alpha_i^2 \sum_{k \neq i} \frac{1}{1 - \frac{\mu^4}{R_{ki}^6}} \left[ 1 - \frac{6u_{ki} \cdot \hat{R}_{ki} \mu^4}{R_{ki}^6 (1 - \frac{\mu^4}{R_{ki}^6})} \right] . \]  

the first term in this expression leads to a constant energy term. Once quantized, the second term leads to an extended Holstein type electron–phonon interaction. However, the prefactor \( 1/R^7 \) indicates that this term will be very small in comparison to the SSH style term.

Combining all Hamiltonian terms from the preceding discussion, the following Hamiltonian is found (up to a constant term):

\[ H = H_{\text{ext--SSH}} + H_{\text{ext--Hol}} + H_{\text{ph}} . \]  

A schematic of the simulator with the effective interactions is shown in figure 2.
In order to gain insight into any differences that long-range hopping make to the extended SSH Hamiltonian, we make perturbation theory calculations for three cases. The standard SSH model, an extended SSH model with $1/R^3$ hopping and the extended SSH model with both $1/R^3$ hopping and $1/R^4$ interaction strength. In all cases, the model is on the chain. A single Einstein phonon mode in one-dimension is considered. The lowest order perturbative contribution to the self-energy of the polaron at absolute zero is:

$$\Sigma(\omega, k) = \frac{\lambda^2}{\pi} \int_{-\pi}^{\pi} dq \frac{g_{k,k+q}^2}{\omega - \omega_0 - \epsilon_{k+q} + i\delta},$$  \hspace{1cm} (21)$$

where an integration over the energy has been performed for the phonon propagator. The Fourier transform of the interaction vertex is,

$$g_{k,k+q} = 2ig \sum_{n=1}^{\infty} \frac{1}{(R_n/R_1)^4} \left[ \sin(n(k+q)) - \sin(nk) \right],$$  \hspace{1cm} (22)$$

and the non-interacting dispersion,

$$\epsilon_k = -2t \sum_{n=1}^{\infty} \frac{\cos(nk)}{(R_n/R_1)^3}.$$  \hspace{1cm} (23)$$

The dimensionless electron–phonon coupling $\lambda = g^2/\omega_0t_0$ and $\delta$ is a small real number. From this, the polaron energy can be calculated through the expression,

$$\omega - \epsilon_k - \text{Re}\Sigma(\omega, k) = 0,$$  \hspace{1cm} (24)$$

and the effective mass from the second derivative of the polaron energy with respect to momentum, $k$.

Results from the perturbation theory are shown in figures 3 and 4. The polaron shift shown in figure 3 is the difference in energy between the interacting and non-interacting cases. For all three cases, the form of the polaron shift is qualitatively similar. Introduction of long-range hopping decreases the polaron shift as the polaron is essentially less tightly bound to a site and hopping becomes easier, whereas introducing the long-range interaction moderately increases...
Figure 3. Effect of long-range hopping and vertex on the polaron shift of the SSH polaron formed from interaction with one Einstein mode. Here $\lambda = g^2/\omega_0 t_0$ is the dimensionless electron–phonon coupling and $\omega_0 = 0.1t$. There is no qualitative change in the polaron shift as long-range effects are switched on.

Figure 4. Effect of long-range hopping and vertex on the effective mass of the SSH polaron formed from one Einstein mode. The shift because the effective interaction is slightly stronger. A stronger change can be seen in the effective mass as the hopping range is increased (figure 4) but the core physics remains the same. The divergence in the effective mass signifies the breakdown in the perturbation theory.

We note that the Rydberg excitation is bosonic. For polaron problems, which have a single electron, this is no problem because the electron has no other particle with which to exchange. It is also possible to simulate the ground state of a bipolaron (two interacting polarons) since the ground state of two interacting fermions is always a singlet with symmetric spatial component of the wavefunction, with the antisymmetry of the wavefunction imposed by the spin degrees of freedom \cite{28}. Thus, most observables in the absence of a magnetic field (e.g. total energy, effective mass) are identical in the two fermion or two boson ground states. Since there can only be one exciton per site, the bosons are hard core.
3. Cold Rydberg ions: interactions with acoustic phonons

An alternative possibility for tuning the Hamiltonian is to use cold ions instead of cold atoms. For a system of cold ions confined to 1D, the ions form a chain, held in place by the direct Coulomb repulsion between the ions. Cold ions confined to 2D will form a Wigner crystal with a triangular lattice. The phonon modes have been calculated in the harmonic approximation for the triangular lattice \([29, 30]\) and have an acoustic nature. Note that these modes are not independent and the full Hamiltonian \((15)\) applies here. The ions considered here are sufficiently heavy to justify the harmonic approximation. Therefore, by changing from rubidium atoms to strontium ions, systems with acoustic phonons are accessible.

Interaction between the Rydberg states and phonons occurs where there are interactions terms between the dipole moments. For a system of cold Rydberg ions with small dipole moment, the interaction potential is \(V(R_i, R_j, r_i, r_j) = \frac{1}{R_{ij}} + \frac{(R_i - R_j) \cdot (r_i - r_j)}{R_{ij}^3} + \frac{r_i^2 - 3(n_{ij} \cdot r_i)^2 + r_j^2 - 3(n_{ij} \cdot r_j)^2}{2R_{ij}^3} + \frac{r_i \cdot r_j - 3(n_{ij} \cdot r_i)(n_{ij} \cdot r_j)}{R_{ij}^3}\). (25)

The system should be prepared in the state discussed at the beginning of section 2, which simplifies the interaction to,

\[V(R_i, R_j) = \frac{1}{R_{ij}} + \frac{\bar{\mu}^2}{R_{ij}^3}.\] (26)

The monopole ion–ion interaction is only responsible for the phonon modes and the effective dipole–dipole interaction is identical to the cold atoms case. Thus, beyond a change in the form of the phonons, the resultant exciton–phonon interaction is the same for atoms and ions. We note that a fully excited \(|nS\rangle\) ion moves in a different potential to an ion in a fully excited \(|nP\rangle\) state. Since the ions are dressed, they have only a very small admixture of the Rydberg states, so the motion of the ions is mainly determined by the ground state properties of the ions which are very similar for \(|g\rangle\) and \(|h\rangle\) states, and therefore it is safe to assume that all ions move in approximately the same potential.

4. Experimental considerations

So far we have discussed the Hamiltonian of the atomic/ionic system and its condensed matter analogues. Now we sketch the manner in which experiments may be performed.

In the case of atoms or ions, we assume that each lattice site is occupied by a single atom/ion, and each site may be addressed individually in such a way as to allow the preparation of the initial simulator state \(|g\rangle\) or \(|h\rangle\) on each atom/ion. We assume also that the state of each atom may be measured by use of a laser tuned close to resonance with a closed transition involving the ground state of interest. Thus, the state of each atom/ion is detected in fluorescence.

In the case of atoms, the system may be prepared from a Mott insulator phase where a single atom occupies each lattice point. Alternatively, there exist proposals to obtain single occupancy in non-degenerate (and hence much lower density) atomic ensembles \([31]\). For ions
at low temperatures a suitable lattice is necessarily formed; it is possible to cool the motional states of the ion crystal using finely tuned lasers [32].

First, we discuss the Rydberg states which cause the atom–atom interaction in our SSH model. We couple our two hyperfine ground states \(|g\rangle, |h\rangle\) to the \(|nS\rangle\) and \(|nP\rangle\) Rydberg state, respectively. In the following we discuss the atom Rb\(^{87}\). These particular Rydberg states interact according to the dipole–dipole Hamiltonian in equation (9). In detail, this takes the form:

\[
V = \frac{1}{4\pi \epsilon_0} \sqrt{\frac{8\pi}{3}} \frac{(d_{nS,nP})^2}{R^3} \frac{1}{m} (-1)^m \langle 1, m; 1, m'| 2, m - m' \rangle Y_{2,m-m'}(\mathbf{R}),
\]

where the vector connecting the two atoms is \(\mathbf{R}\), \(d_{nS,nP}\) the dipole matrix element between the states \(|nS\rangle\) and \(|nP\rangle\) and \(Y_{2,m-m'}(\mathbf{R})\) is a spherical harmonic. The lasers select only the \(m = 0\) and \(m' = 0\) magnetic sublevels. In general, the dipole–dipole interaction scales with \(n^4/R^3\) and the lifetime of the Rydberg states scales with \(n^3\), which together mean that choosing the highest energy Rydberg state possible leads to the best possible properties of the atoms and ions for the simulator. However, experimentally we stress that for a given laser intensity, the Rabi frequency of the dressing laser scales with \(n^{-3/2}\), and the shift of the \(|nS\rangle\) atoms due to their mutual interaction (the ‘blockade shift’) scales with \(n^{11}/R^6\). Thus one cannot go to arbitrarily high \(n\) without shifting the \(|nS\rangle\) states too far from the dressing laser, or by making unreasonable demands on the laser intensity. We choose the \(n = 48\) states for which the laser power required to drive the \(|g\rangle \rightarrow |nS\rangle\) and \(|h\rangle \rightarrow |nP\rangle\) transition should be reasonable (the Rabi frequency for these transitions scales with \(n^{-3/2}\)), but where the 48S–48P interaction is 1252 MHz/\(\mu\)m\(^3\); large enough for our purposes. The lifetimes of these states are: \(\tau_{48S} = 106 \mu\)s and \(\tau_{48P} = 117 \mu\)s, but the effective lifetime of the dressed states are lengthened by a factor \(\alpha_s^{-2}\) and \(\alpha_p^{-2}\). Using this expression for \(V\) and reasonable values for the Rabi frequencies \(\Omega_s = \Omega_p = 100\) MHz and detunings \(\Delta_s = \Delta_p = 100\) MHz we calculate the nearest-neighbour exciton hopping rate \(\tilde{V}_{ij}\) for a separation of 2.5 \(\mu\)m to be 0.19 KHz, and a dressed state lifetime of 48 ms \(\approx 54\) exciton hopping times. We note that for these choices of \(\Delta_s, \Delta_p\) and \(\Omega_s, \Omega_p, \tilde{V}_{ij}\) diverges below a separation of about 2.2 \(\mu\)m, which sets an additional constraint on the types of experiments we can perform. We also know that the \(|nS\rangle\) atoms will interact with each other due to the van der Waals interaction \(V_{vdw} = C_6/R_{ij}^6\), where \(C_6\) is the appropriate van der Waals coefficient. For our 48S states, \(C_6 \approx 1050\) MHz \(\mu\)m\(^{-6}\).

Now we turn to considering some of the experimental values required for modelling an SSH Hamiltonian. We have in mind two set-ups which illustrate the utility of the model and some of the experimental issues that must be addressed. In the first case, a linear chain of atoms (of mass M) is confined by a far-detuned optical lattice formed from a pair of intersecting laser beams with wavelength \(\lambda\). As mentioned above, we stipulate that there be a single atom per lattice site. With counter-propagating lasers, such a system is characterized by the recoil energy \(E_r = 2\pi\hbar^2/M\lambda\) and the potential depth \(V_0\), which depends on the laser intensity. Assuming that the atoms are trapped near the potential minima, the phonon frequency will be \(\omega_0 = 2E_r\sqrt{V_0/E_r}/\hbar\), the atomic hopping energy \(J = (4/\sqrt{\pi})E_r(V_0/E_r)^{3/4} e^{V_0/E_r}\), and we estimate the on-site atomic repulsion energy as \(U = \sqrt{8/\pi} (a_s/a_0) E_r(V_0/E_r)^{3/4}\), with \(a_s\) the \(s\)-wave scattering length for the atoms—5.3 nm for Rb\(^{87}\)—and \(a_0\) the length of the ground state wavefunction. In order to initialize the system, it is necessary that the atoms be individually addressable, which determines the minimum lattice wavelength to be around 1 \(\mu\)m, however we adopt the more conservative 2.25 \(\mu\)m lattice wavelength considered above. In order that atomic tunneling rate \(J\) is suppressed, we require that \(V_0 \gg 20E_r = 4.53\) KHz; for the 2.25 \(\mu\)m
lattice spacing, \( \tilde{V}_{ij} = 1.43 \text{ kHz} \) and \( \omega_0 = 2.03 \text{ kHz} \). We then have \( J \approx 0.001 \text{ kHz} \), \( U = 2.3 \text{ kHz} \), increasing the localization further. We note that this phonon frequency is a large fraction of the site depth \( V_0 \). Also, for atomic spacings of 2.5 microns and upwards, \( V_{vdW} < 24 \text{ MHz} \), smaller than, but comparable to, the detunings \( \Delta_S \) and \( \Delta_P \) we have chosen for our example.

The tunability of the cold atom system in an optical lattice where the atomic potential \( V_{\text{lat}} = V_0 \sin^2(kx) \), \( V_0 = 20E_r \), is illustrated in figure 5 as a function of the lattice wavelength. The figure shows the relative energies associated with the trap depth, the phonons, the nearest-neighbour exciton–phonon coupling and the exciton hopping. Using realistic parameters, the phonon energy and coupling energy can be swapped. The resulting SSH model is in the weak-coupling, high-phonon frequency regime.

In the next experimental scenario we consider how a far more tunable system can be constructed by using painted potentials [33]. In this system the lattice potential is an array of Gaussian laser spots, with power \( P \) and focused to a waist \( w_0 \), in which case the traps have a potential \( V_{\text{trap}} = V_0 \exp(-2r/w_0^2) \) where the trap depth is \( V_0 = 2P/\pi w_0^2 \) and the phonon frequency is \( \omega_0 = (1/w_0)\sqrt{V_0/M} \). The trap spacing, \( d \), may be chosen such that tunneling is negligible by choosing \( d > w_0 \), and the phonon frequencies may then be determined by the laser power \( P \). In this case, we need to choose higher Rabi frequencies and detunings \( \Omega_{S,P} = 20 \text{ MHz} \) and \( \Delta_{S,P} = 100 \text{ MHz} \), respectively. For these parameters, and with the larger atomic separations (> 4\( \mu \)m), we calculate that the dressed state lifetimes are \( \approx 12 \text{ ms} \), which is about 85\( \tau_{\text{hop}} \), and that the blockade shift of the \( nS \) states is less than 2 MHz. We plot the the parameters associated with this potential in figure 6. Here, all hierarchies of phonon energy, coupling constant and exciton hopping can be achieved. A major advantage of the painted potentials is that much deeper potentials can be achieved, but phonon frequencies can be much smaller, putting the effective model in the physical regime of a condensed matter system. Also, rings of atoms can be created to explore periodic boundary conditions.

For modelling the SSH model using cold ions, we have not undertaken any detailed calculations to assess our simulator proposal, but we can make some points here. Ions trapped in an ion trap have phonon frequencies in the 100 kHz–2 MHz range, and spacing on the order

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**Figure 5.** Relative strength of on-site and near-neighbour energies in an optical lattice. \( \Omega = 10 \text{ MHz} \) and \( \Delta = 100 \text{ kHz} \). The polarons formed from weak coupling with high-energy phonons can be investigated.
of several $\mu$m. Thus, the phonons are very much higher in energy than the atomic case. Recent studies of Rydberg states of ions has shown that the interactions between the ions are very weak—additional complications involving RF dressing of the Rydberg atoms are required [34]. This means that implementation of the cold ion extension to simulate polarons formed from acoustic phonons in regimes relevant to condensed matter physics will be a major experimental challenge.

We end by describing an experiment to explore the self-trapping regime of the SSH model, which is a subject of current interest [14]. We consider studying the phenomenon of
self-trapping in the SSH model on a circular array of Gaussian spots—that is, a ring of traps. A particular lattice point is chosen for the location of a single excitation, and then the dressing fields are rapidly switched on. Since this impulse contains multiple momenta, the localized exciton state will expand into the lattice. The result of the simulation may be obtained by extracting the location of the excitation as a function of time. This may be achieved by rapidly switching off the dressing potentials, and then measuring the state of the atoms/ions at each lattice point. In the self-trapped regime, the exciton hopping will be suppressed, which will be observed as a narrowed distribution of final exciton locations. The hopping leads to a quantum random walk [35] so the mass can be extracted from the spatial distribution of an ensemble of measurements. Note that there are significant differences between the distributions arising from classical and quantum random walks.

5. Summary and outlook

In this paper, we have shown how systems of cold Rydberg atoms and ions can be used as a simulator for electron–phonon interactions, and derived the mapping onto a SSH model, which is used to simulate strongly deformable materials. We have also discussed how readout of physically relevant properties could be carried out. Further, we have discussed the parameters of the model that can be achieved, showing that rubidium atoms in painted potentials can be used to access physically relevant couplings, phonon frequencies and exciton hoppings.

It is relevant to discuss scalability here. A drawback of the current approach is that the excitations are bosons rather than fermions. It may be possible to simulate full fermion–phonon interactions using a more complicated two layer 2D optical lattice with dressed Rydberg atoms in the lower layer and an incomplete layer of Rydberg atoms in the upper layer. The Rydberg atoms in the upper layer will interact with those in the lower layer through the dipole–dipole interaction, leading to a Hubbard–Fröhlich model, but with the caveat that the system is much more complicated [36]. We note that much has been learnt by simulating Bose–Hubbard models with cold atoms, so we consider that the lack of fermionic excitations is currently a minor drawback. We hope that the proposed system will stimulate experimental work in the area, and encourage the development of quantum simulators for electron–phonon interactions which work with fermionic excitations. In the case of polymer physics, the quantum simulations are relevant as they may shed light on ongoing debates about self-trapping phenomena [14].

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References


[12] Landau L D 1933 Phys. Z. Sowjetunion 3 664
[22] Li W and Lesanovsky I 2011 arXiv:1108.3591