Emulating Solid-State Physics with a Hybrid System of Ultracold Ions and Atoms

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We propose and theoretically investigate a hybrid system composed of a crystal of trapped ions coupled to a cloud of ultracold fermions. The ions form a periodic lattice and induce a band structure in the atoms. This system combines the advantages of high fidelity operations and detection offered by trapped ion systems with ultracold atomic systems. It also features close analogies to natural solid-state systems, as the atomic degrees of freedom couple to phonons of the ion lattice, thereby emulating a solid-state system. Starting from the microscopic many-body Hamiltonian, we derive the low energy Hamiltonian, including the atomic band structure, and give an expression for the atom-phonon coupling. We discuss possible experimental implementations such as a Peierls-like transition into a period-doubled dimerized state.

The study of quantum many-body systems through quantum simulators, as initially proposed by Feynman [1–3], is one of the major challenges of experimental quantum physics. Trapped ultracold quantum gases and ions in electromagnetic traps have proven to be among the most successful systems for this task [4,5]. Both systems are tunable throughout a wide range of parameters and have been used in seminal quantum simulations [4,5]. Neutral atomic systems, which can exhibit fermionic statistics naturally, have been very successful in analog simulation of solid-state systems. These setups are even able to simulate artificial gauge fields [6], and control over and detection of individual atoms is now within reach [7–9]. Trapped ionic systems, on the other hand, have exhibited a remarkable precise control of preparation and measurement of arbitrary system states and can be used to construct a universal digital quantum simulator [10]. Their scalability, however, remains an important issue and is currently under intense investigation [11,12].

In this Letter, we propose a setup to realize an analog quantum simulator, consisting of the combination of a trapped ion crystal interacting with a system of ultracold fermionic atoms [see Fig. 1(a)], combining the advantages of both systems [13–18]. Specifically, we focus on a 1D ion chain, but higher-dimensional structures could also be used. We envision fermionic atoms simulating electrons in a solid-state system with ions forming the lattice. A crucial component of solid-state systems, namely, the phonon-electron coupling, arises naturally in our scenario. This feature is absent in ultracold atoms trapped in optical lattices, where there is no significant backaction of the atoms on the lattice. Likewise, trapped ion systems do not naturally feature fermionic statistics, so that the quantum simulation of coupled fermion-phonon systems would add significant experimental complexity [19]. The proposed simulator may be used to study models of electron-phonon coupling, such as the Fröhlich model, Peierls transitions, and the emergence of phonon-mediated interactions.

Alternative proposals for investigating phonon couplings include self-assembled lattices of ultracold dipolar molecules [20] and optically trapped nanoparticles [21], whereas backcoupling to cavity photons has also been demonstrated [22]. Our proposal is complementary to these approaches and offers advantages in the precise control of the couplings and configuration of the system.

The interaction between an atom and an ion is caused by an induced dipole moment in the atom and for sufficiently large distances is given by $V_{AI}(r) = -(C_{4}/r^4)$, where $r$ denotes the atom-ion separation. This defines both a natural length scale $R^* = \sqrt{2m_{A}C_{4}/\hbar^2}$, typically in the 100 nm regime [23], and an energy scale $E^{*} = \hbar^4/(4m_{A}^2C_{4})$, where $m_{A}$ is the atomic mass [24]. The interionic Coulomb repulsion leads to phonon branches which also couple to the atoms. Interactions between the atoms are short range and can be tuned, e.g., by Feshbach resonances. In Table I, we list some typical energy and length scales of our proposed quantum simulator as compared to typical natural solid-state systems. One advantage of our proposal is the flexible mass ratio: a large ratio (e.g., $^{4}$Li atoms and $^{174}$Yb$^{+}$ ions) is reminiscent of solid-state systems, whereas equal masses (e.g., $^{40}$K and $^{48}$Ca$^{+}$) are also possible.

The outline of this Letter is as follows: we first derive the effective low energy Hamiltonian of the system of spinless ions and atoms and determine an explicit expression for the atom-phonon coupling. Thereafter, we demonstrate the use of our system as a quantum simulator by investigating a...
Peierls-like transition of a system of fermionic atoms. Finally, we discuss the experimental implementation and further possibilities in an outlook.

Derivation of the low energy model.—The system is microscopically described by three terms in the Hamiltonian \( \mathcal{H} = \mathcal{H}_I + \mathcal{H}_A + \mathcal{H}_{AI} \), where

\[
\mathcal{H}_I = \sum_{j=1}^{N_I} \left[ \frac{p_{j}^2}{2m_I} + V_I(\mathbf{R}_j) \right] + \frac{e^2}{4\pi\varepsilon_0} \sum_{i<j}^{N_I} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{1}
\]

describes \( N_I \) ions, each of mass \( m_I \) and charge \( +e \) trapped in a Paul trap represented by the single-particle potential \( V_I(\mathbf{R}_j) \), with pairwise Coulomb interactions. \( \mathbf{R}_j \) and \( p_j \) are the position and momentum operators of the \( n \)th ion, respectively. The \( N_A \) atoms are described by a Hamiltonian \( \mathcal{H}_A = \sum_{\alpha} \left[ \frac{p_{\alpha}^2}{2m_\alpha} + V_A(\mathbf{r}_\alpha) \right] \) that includes a tight transverse optical dipole (or magnetic) trap given by \( V_A(\mathbf{r}) \) which is orientated parallel to, and can be displaced by a distance \( \Delta_r \) from, the center of the Paul trap. In contrast to the case of ions [25], the fermionic quantum statistics of the atoms plays an essential role. The atom-ion interaction is described by the Hamiltonian \( \mathcal{H}_{AI} = \sum_{i,j} V_{n,n'}(\mathbf{r}_i, \mathbf{r}_j) \). For the theoretical description, we apply periodic boundary conditions. To derive a low energy effective Hamiltonian, we separately transform the ionic and atomic degrees of freedom into diagonal form and express the coupling between the systems in this basis.

The dominant energy scale is set by the interionic repulsion, which, in conjunction with the trapping potential \( V_I \) and a given axial ionic lattice spacing \( d \) (typically of the order 1–20 \( \mu \)m), defines the classical equilibrium position of the \( j \)th ion \( \mathbf{R}_j \). This classical configuration minimizing the electrostatic energy \( E_I^{(0)} \) corresponds to a linear string, planar zigzag, or structures of three-dimensional crystals [26]. As the fluctuations of quantum or thermal origin in the ion displacement are small, the ionic Hamiltonian is well suited to an expansion in terms of the position fluctuation operators \( \delta \mathbf{R}_j = \mathbf{R}_j - \mathbf{R}_j \). Hence, we write

\[
\mathcal{H}_I = E_I^{(0)} + \mathcal{H}_I^{(1)} + \mathcal{H}_I^{(2)} + \cdots
\]

where the first order terms vanish identically and the low energy spectrum and the dynamics are determined by

\[
\mathcal{H}_I^{(2)} = \sum_{n,l} \frac{p_{n,l}^2}{2m_I} + \frac{1}{2} \sum_{n,n'} V_{n,n'} \delta R_n \delta R_{n'} |_{0},
\]

where the combined label \( n = (j, D) \) designates the \( j \)th ion in spatial dimension \( D \), \( V_{n,n'} = \partial^2(V_I + V_A)/\partial \delta \mathbf{R}_n \partial \delta \mathbf{R}_{n'} \), and \( V_{AI} \) the interionic potential. After transforming into the basis of phonons with bosonic operators \( |\alpha_\alpha, \alpha_\beta \rangle = \delta_{\alpha_\alpha', \beta} \), where \( \alpha \) is a collective mode label [27], the Hamiltonian in units of \( \hbar = 1 \) takes on the form (see Supplemental Material [28], Sec. II)

\[
\mathcal{H}_I = E_I^{(0)} + \sum_{\alpha} \omega_{\alpha} \left( \alpha^{+} \alpha + \frac{1}{2} \right) + \frac{p_{\alpha}^2}{2m_I} + O(\alpha^3). \tag{2}
\]

The spectrum \( \omega_{\alpha} \) for a particular linear ion string is shown in Fig. 1(b).

In a similar fashion, an expansion in \( \delta \mathbf{R}_j \) is made for the atom-ion operator \( \mathcal{H}_{AI} = \mathcal{H}_{AI}^{(0)} + \mathcal{H}_{AI}^{(1)} + \cdots \), where

\[
\mathcal{H}_{AI}^{(0)} = \sum_{i,j} \frac{C_4}{|\mathbf{R}_i - \mathbf{R}_j|},
\]

\[
\mathcal{H}_{AI}^{(1)} = 4C_4 \sum_{i,j} \left( \frac{\mathbf{R}_i - \mathbf{R}_j}{|\mathbf{R}_i - \mathbf{R}_j|^6} \right) \cdot \delta \mathbf{R}_j.
\]

To lowest order \( \mathcal{H}_{AI}^{(0)} \), the atoms feel a periodic lattice of ions pinned to their classical equidistant positions, and the higher orders (\( \mathcal{H}_{AI}^{(1)}, \text{ etc.} \)) describe couplings to ionic phonon modes. The atomic eigenstates of \( \mathcal{H}_A + \mathcal{H}_{AI}^{(0)} \) are Bloch states \( \phi_{k,\alpha}(\mathbf{r}) \) with energy \( E_{k,\alpha} \) and characterized by a quasimomentum \( k \) and a band index \( \alpha \). The form of the

| TABLE I. Comparison between a typical natural solid-state system and the proposed quantum simulator. The characteristic length and energy scales for atom-ion interaction are defined in the text and correspond to the hydrogen electron for the solid-state system. The fermionic mass (electron or atom) and ionic core are denoted by \( m_f \) and \( m_I \), respectively. |
|---|---|---|
| Lattice spacing \( d \) (nm) | 0.3–0.6 | \( 10^{-3} \)–\( 10^{4} \) |
| Length scale \( R^* \) (nm) | 0.026 | 71 | 245 |
| Energy scale \( E^* \) (kHz) | \( 10^{13} \) | 167 | 2.1 |
| \( d/R^* \) | 10–20 | 14–140 | 4–40 |
| \( m_f/m_I \) | \( 10^{-1} \)–\( 10^{5} \) | 29 | 1.0 |
| Fermi energy (MHz) | \( 10^8 \) | 0.02 | 0.02 |
| Phonon energy (MHz) | \( 10^6 \) | 0.01–10 | 0.01–10 |
long-range atom-ion potential $V_{AI}(r)$ is unbounded from below, and the low-lying energy bands [see Fig. 1(c)] are essentially superpositions of local bound states of each ion with flat dispersions (bandwidth $\leq 20$ Hz for Yb$^+$--Li with $d = 1 \mu m$). Furthermore, they are energetically separated by a large gap [see Fig. 1(c)] and should not play a significant role if the atoms are moved into the ion string in an appropriate sequence [29]. On the other hand, the Bloch states with energies above the threshold [see the upper state in Fig. 1(c)] have a considerably larger bandwidth of typically a few kHz. We expect that adiabatic loading of the atoms into the ion system will populate the lowest of these scattering bands. As it is well separated in energy from other bands, we can work within a single-band approximation and henceforth omit the band index. Alternatively, the system may be prepared into this band by either cooling the atoms or the ions as long as the coupling to the molecular bands is low. When the atom and ion traps are separated by a large distance $\Delta_r$, the atomic band structure is bounded from below, and it is most relevant to consider the band with lowest energy.

The single-atom part of the Hamiltonian is $\mathcal{H}_A + \mathcal{H}_{AI}^{(0)} = \sum_k \epsilon_k c_k^\dagger c_k$, where $\epsilon_k = \int d^3 r \phi_k(r) \bar{\Psi}^\dagger(r)$ creates an atom in Bloch mode $k$. As the long-range atom-ion coupling diverges for small separations, an effective description of the short-range coupling is important. It is possible to determine the effective 1D Bloch states and the corresponding dispersion relation within quantum defect theory, as discussed in [28], Sec. I. For sufficiently strong transverse confinement, any low energy eigenstate will be well approximated by the form $\psi(z, \rho) = \psi_{1D}(z) \phi_\perp(\rho)$ in spatial regions between the ions, where the potential felt by the atoms is almost cylindrically symmetric. Here, $\phi_\perp(\rho)$ is the lowest 2D harmonic oscillator state of the optical dipole trap and the trap is oriented in the $\mathbf{e}_r$ direction. The effect of the ion can then be characterized by the odd and even 1D short-range phases $\varphi_o$ and $\varphi_e$ [23]. A typical dispersion relation and Bloch state are shown in Figs. 1(c) and 1(d), respectively. The effective 1D theory is valid only for atom-ion distances that are larger than the transverse wave packet size $l_\perp$. For Li and Yb$^+$, and assuming a transverse atomic trap frequency of $\omega_\perp = 2\pi \times 200$ kHz, we find $l_\perp \sim R^*$. Hence, for these parameters, the 1D description is applicable only for interion distances $d \gg R^*$ and energies $E < E^*$. For tighter atomic confinement or heavier atomic species, the description holds over larger parameter regimes. Obtaining the exact form of the atomic wave function closer to the ion would, however, require a 3D description.

The dominant term of the coupling Hamiltonian is

$$\mathcal{H}_{AI}^{(1)} = \sum_{k,k',n} \lambda_{k,k'}^{(s)} \alpha_n c_k^\dagger c_{k'} + \text{H.c.}$$

It is useful to define the potential $V_n(r) = (r - \mathbf{R}_j) \cdot \mathbf{e}_D/|r - \mathbf{R}_j|^6$, in terms of which the phonon coupling is given by

$$\lambda_{k,k'}^{(s)} = 4C_4 \sum_n \frac{u_{k}^{(s)} - u_{k'}^{(s)}}{\sqrt{2m_1 \Omega_n}} \int d^3 r V_n(r) \phi_k^*(r) \phi_{k'}(r),$$

where $u_{k}^{(s)}$ and $u_{k'}^{(s)}$ are the phonon mode coefficients and $\Omega_n$ is the bare angular frequency (see [28], Sec. II). Note that $\lambda_{k,k'}^{(s)}$ is only uniquely defined up to the (arbitrary) complex phases of the individual Bloch and phonon modes.

To calculate $\lambda_{k,k'}$, in the case of overlapping atom and ion traps, we require an accurate description of the Bloch states very close to the ions, which is unfortunately not available in the quantum defect calculation. Furthermore, the secular approximation for the ions neglecting ion micromotion may break down [30,31]. We note that a full quantum mechanical treatment of the effect of the time-dependent trapping potential will require a many-body quantum Floquet formalism [32] and is beyond the scope of the present Letter.

For an atomic cloud tightly confined in the transverse direction and transversally displaced from the ion string by $\Delta_r\mathbf{e}_r$, the low energy single-particle Bloch states are in the transverse ground state and of the form $\psi_{k,\perp}(r) = \psi_{1D}(z) \phi_{1\perp}(r)$. The 1D Bloch $\phi_{1\perp}(r)$ states in the potential $V_{1D}(z) = \sum_n V_{AI}(|z_\epsilon - \mathbf{R}_j|)$ can be calculated by diagonalizing the Hamiltonian in the plane wave basis. The atom-phonon coupling $\lambda_{k,k'}^{(s)}$, which vanishes unless $q = k - k'$, where $q$ is the quasimomentum corresponding to phonon index $s$ (see [28], Sec. III), is shown in Fig. 2. The transversal coupling features a pronounced peak at $q = |k - k'| = \pi/d$ as the system approaches the zigzag transition, discussed in the following.

Transverse Peierls-like transition.—As a demonstration of our quantum simulator, we investigate a Peierls-type transition [33] at $\Delta_r > 0$. It is energetically favorable for a 1D metallic crystal to undergo a transition to an insulating phase, the so-called Peierls transition, when cooled below a critical temperature, as a gap opens in the electronic band structure. For particular fermionic filling, this decrease in

![FIG. 2 (color online). The interaction between atoms and ions is expressed as an atom-phonon coupling $|\lambda_{k,k'}^{(s)}|^{q=k\rightarrow k',s}$ in the low energy limit. For atoms displaced by $\Delta_r = 0.75 R^*$ and tuning to a small $\omega_{q=k\rightarrow k',s} = 0.0093 \Omega_n$ (a) the longitudinal coupling is several orders of magnitude smaller than (b) the transverse coupling, and the latter may exceed the bandwidth while still being smaller than the band gap.](image317to560@560x258)
energy is enough to offset the increase due to the ion distortion. In our case, the energy that the linear ion string gains as it is distorted into a period-doubled zigzag configuration is offset by the lowering of the energy of the atomic system at half-filling [see Fig. 3(c)]. The structural phase transition from a linear to a zigzag configuration in trapped ions has previously been the subject of theoretical study, as it can be coupled to quantized fields [34,35]. The present proposal goes one step further by using a fermionic quantum field to induce the phase transition, thereby emulating the Peierls effect as observed in natural solid-state systems.

Fixing a separation $\Delta_r$ between the atom and ion traps, we treat the ion positions classically. The ions are perturbed from their equilibrium positions by an amount $\delta$ oriented along the trap separation such that $\mathbf{R}_i' = \mathbf{R}_i + (-1)^n \delta_i$, giving rise to an ionic energy increase $\Delta E_i = m_i \omega_{0}^2 \delta_i^2 + O(\delta^4)$, with $\delta = |\delta|$, associated with a zigzag mode frequency $\omega_k = \pi/d$. For $T \to 0$, zigzag order will always be preferred as the band gap scales linearly with $\delta$ and the energy of classical ion displacement increases with $\delta^2$, for small $\delta$. At finite temperature, the preferred configuration is determined by minimizing the free energy, calculated for the combined ion and noninteracting atomic system by parametrically varying $\delta$.

A sample band structure for noninteracting $^{40}\text{K}$ atoms near a $^{40}\text{Ca}^+$ ion string is shown in Fig. 3(c) where a zigzag mode frequency $\omega_k = \pi/d$, and atomic temperature $T_A = 15$ nK $= 0.15 E_r/k_B$. The phase diagram for noninteracting $^{40}\text{K}$ with $^{40}\text{Ca}^+$ is shown in Fig. 3(b) for varying temperature and atom-ion trap separation. Furthermore, while the largest critical temperatures occur for half-filling when $\Delta_r$ is large, the optimal critical temperature, shown in Fig. 3(d), occurs for larger fillings per ion $n$ as $\Delta_r \to 0$.

Implementation.—For the proposed quantum simulation, the interacting quantum systems can be prepared individually and their mutual coupling strength can be controlled by varying the distance $\Delta_r$ between ions and fermions. The ion crystal can be cooled to its ground state using resolved sideband cooling. The motional state of the ion crystal can be initialized and read out by laser-induced coupling to internal states of the ions which can be measured with standard fluorescence measurements [36]. Building on these techniques, interferometric methods have been proposed to probe ion crystals near structural phase transitions [37].

Precise control over small numbers of ultracold fermions in optical traps has recently been demonstrated [38]. The atomic density profile is accessible via absorption imaging in combination with time-of-flight analysis. For low densities, the atoms can be retrapped in an optical molasses trap to prevent them from leaving the imaging region during detection. While we have focused on fermionic atomic species in this Letter, it is also possible to trap bosonic species such as $^7\text{Li}$, where ion-controlled tunneling dynamics and Josephson physics may be investigated [39].

Hybrid ultracold atom-ion systems pose several challenges for experimental realization. Inelastic collisions—in particular, charge transfer and molecular ion formation—may limit the lifetime. It has been observed that for some species, the rates may be sufficiently small to study intricate setups, such as in a recent experiment where the spin relaxation of a single $^{174}\text{Yb}^+$ ion immersed in a bosonic Rb bath has been studied [18]. However, no experimental data are available for inelastic rates between ultracold K or Li with trapped ions. The use of polarized fermionic systems may reduce the effects of three-body recombination as binary atom collisions are suppressed in the ultracold regime [40]. In the geometry in which we studied the Peierls transition, ions and atoms are separated and inelastic collisions are suppressed. For the reduction of atomic heating effects due to ion micromotion, we rely on the largest experimentally feasible mass ratio between ions and atoms ($^{174}\text{Yb}^+$ and $^6\text{Li}$) [31] and prevent...
the atoms from approaching the ions too closely [30]. To further mitigate micromotion-induced heating, it may be feasible to use heavier molecular ions, which could be sympathetically cooled by suitable co-trapped ion species.

In conclusion, we have proposed an analog quantum simulator for lattice Hamiltonians that can be tuned into a regime of strong coupling to vibrational phonons. This allows for the simulation of complex many-body Hamiltonians that even go beyond seminal condensed matter models, such as the Fröhlich and Holstein models, known to be relevant for phenomena such as superconductivity. Future work will focus on solving the 3D many-body atom-ion problem, including short-range interactions, considering the time-dependent potential of the ions and the role of the spin degrees of freedom in order to engineer entanglement between the atoms and ions.

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[24] Note that the common definition of $R^*$ and $E^*$ makes use of the reduced mass of the two-body system of an atom and an ion. However, our definition is better suited to a many-body system.
[25] Because of the very strong interactions and large interparticle spacing, the ions have a very low phase space density.
[27] For instance, in the linear crystal regime, $s = (k, \gamma)$ and $\gamma$ denotes either the acoustic longitudinal or one of the two transverse modes.