A cold atom quantum simulator for pairing, condensation and pseudogaps in extended Hubbard–Holstein models

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We describe a quantum simulator for the Hubbard–Holstein model (HHM), consisting of a single layer containing two dressed Rydberg atom (DRA) species held in independent painted potentials, predicting that boson-mediated fermion pairing, pseudogaps and Berezinskii–Kosterlitz–Thouless (BKT) transition temperatures are experimentally accessible. The HHM is important because it contains the essential physics of unconventional superconductors. Experimentally realizable quantum simulators for HHMs are needed: (1) since HHMs are very challenging to solve numerically and analytically (2) to understand pairing in unconventional superconductors where electron-phonon interactions (EPI) and strong Coulomb repulsion compete (3) to understand the role of boson-mediated local pairing in pseudogaps and fermion condensation. We propose and study a quantum simulator for the HHM using optical lattices, painted using zeros in the AC stark shift, to control two Rydberg atom species independently within a monolayer. We predict that interactions are sufficiently tuneable to probe: (1) both HHMs and highly unconventional phonon-mediated repulsions, (2) the competition between intermediate strength phonon and Coulomb mediated interactions, (3) how boson-mediated pairing of fermions leads to pseudogaps and BKT transition. Thus, the quantum simulator is suitable for investigating boson-mediated pairing and condensation of fermions in unconventional superconductors.

Boson-mediated pairing of fermions has not yet been observed in cold atom experiments. Cold atom quantum simulators have been very successful for simulating Hubbard models. The Mott metal-insulator and superfluid-insulator transitions have both been observed [1, 2]. The Feshbach resonance can be tuned into an attractive regime, allowing local pairing in attractive Hubbard models (AHMs) to be observed directly using gas microscopy [3]. In solid state systems AHMs are the effective Hamiltonian arising from boson-mediated interactions, so it would be of significant interest to probe such interactions directly.

Probing boson-mediated pairing in a quantum simulator is technically demanding, but potentially highly rewarding as this pairing reflects the mechanism of many superconductors. The recent discovery of hydrogen based superconductivity at ambient temperatures makes boson-mediated superconductivity particularly pertinent [4, 5].

Unconventional superconductors often contain significant Coulomb repulsions and boson-mediated interactions (such as EPIs) [6–11]. Furthermore, recent exact numerics provide strong upper bounds on superconductivity in the popular Hubbard model [12], identifying the need to include additional interactions alongside this model to explain superconductivity in such materials.

The HHM and its extensions [13, 14] contain the essence of these interactions, but the HHM is challenging to solve numerically and analytically. A tunable quantum simulator would allow this model to be explored without the complications of competing interactions and phases in unconventional superconductors. Moreover, interesting physics, e.g. BCS to BEC crossover, could be observed directly by tuning the interaction strength without the limitations of stoichiometry and pressure.

The innovations within the quantum simulator for the HHM proposed here are: (1) exploitation of zeros in the AC stark shift to generate bipartite lattices within a single optical pancake to reduce experimental complexity, (2) use of Rydberg mediated interactions to tune EPI and Coulomb repulsion independently, (3) the possibility to investigate highly unconventional repulsive interactions mediated via phonons, (4) the possibility to explore boson-mediated pairing, (5) the existence of a pseudogap, (6) the potential to investigate the BKT transition.

Two atom species, a fermion representing electrons and a boson representing phonons, can be trapped in different, but coexisting, lattices by exploiting state dependence in the AC stark shift [15, 16]. We consider bosonic 87Rb and fermionic 40K, trapped by linear polarized lasers of wavelength $\lambda_{ph} = 768.97\,\text{nm}$ and $\lambda_{f} = 790.07\,\text{nm}$ respectively. Wavelengths are chosen because the atom-light interaction at a wavelength between the D1 and D2 transition lines for the specified species cancels due to zeros in the AC stark shift. Thus species dependent potentials are realized. Lattice potentials are blue (red) detuned for 87Rb (40K), so bosonic atoms are trapped in an “inverse” lattice where absence of light leads to confinement. For convenience, we discuss attractive potentials for both species, but these can easily be painted from repulsive ones.

The optical lattice contains a single optical pancake with laser wavelength $\lambda_{pan}$ and width $w_{pan}$, within which potentials are painted using Gaussian beams [17]. The total lattice potential is $V(r) = \sum_{i} V_{\text{spot},i}(r - r_{i}) + V_{\text{pan}}(z)$, where $V_{\text{pan}}(z) = -V_{0,\text{pan}} \exp(-2z^{2}/w_{\text{pan}}^{2})$. $r$ is a vector that lies within the plane of the optical pancake.
and the z-axis is perpendicular to the pancake. The spot potential has the form, $V_{\text{spot}}(r) = -V_0 \exp(-2r^2/w^2)$. Fermion (boson) beams have waist, $w_1 (w_{ph})$.

Simulator properties are fixed by the pattern of optical lattice potentials. We investigate models generated by several spot configurations, shown in Fig. 1. The fermion lattice consists of single spots (red) and the phonon lattice multiple spots (green). Rotating phonon spot patterns with respect to the fermion lattice can change model properties. Deep phonon sites with filling $n=1$ in Mott insulator states are formed from multiple spots with a separation close to the Raleigh limit to make broad sites within which the atoms can oscillate. Shallow fermion sites are only partially filled.

The fermion hopping term is $H_{\text{hop}} = -t \sum_{i,j} c_i^{\dagger} c_j$, where $t \approx 4E_{\text{rec}}/V_0^{1/4}\exp(-2(V_0/E_{\text{rec}})^{1/2})/\sqrt{\pi}$. $a$ is lattice spacing. $E_{\text{rec}} = h^2 \pi^2/(2M_Ka^2)$. $c_i^{\dagger}$ creates a fermion on site $i$ with spin $\sigma$.

The phonon contribution to the Hamiltonian is $H_{\text{ph}} = \sum_{i,j} \varepsilon_{ij} d_i^{\dagger} d_j$, which is highly sensitive to the spot patterns, as shown in Fig. 4. We take the limit $r_c \ll a$ so that only near-neighbor (NN) and next-nearest-neighbor (NNN) terms are necessary in Eq. 5.

The conditions under which this reduces to a site-local HHM will now be determined. The form of the effective (retarded) interaction between DRAs in the (multi)polaron action [29],

$$\Phi_{ij'} = \sum_{j,i'} f_{ij,\nu} f_{ij',\nu},$$

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Repulsive interactions between NNN sites are a feature of the simulator. These arise when \( f_{ij} \propto \zeta_{ij,j} \cdot \hat{r}_{ij} \) changes sign due to reorientation of the sense of \( \hat{r}_{ij} \) relative to \( \zeta_{ij,j} \). Repulsive phonon-mediated interactions might seem surprising, since the EPI is commonly identified as attractive. However, repulsive EPI is predicted in condensed matter \([21]\).

A bipartite lattice with spot arrangements parallel to the lattice vectors (panel (B)) has an effective interaction displaying 4-fold symmetry and a small repulsive interaction on diagonal NNNs. A bipartite checkerboard pattern with no phonon site on alternate squares produces a very similar pattern (not shown).

Crosse patterns lead to effective interactions with square symmetry and the smallest off-site terms for centrally placed spots (panel (C)). Since the frequency and mass of the oscillators along the two directions are identical and the oscillators are independent, then the full \( \Phi \) is the sum of the \( \Phi \) for two parallel spot arrangements (panel (F)), rotated by 90° relative to each other [21]. The effective interactions are identical for 45° and 90° orientations of spots. A disadvantage is that multi-spot patterns are more complicated to paint.

By translating phonon spots so they approach an individual fermion site, \( f_{ij} \rightarrow \delta_{ij} \), leading to a better reproduction of the HHM (panels (D)-(F)). As \( b \) is decreased from 0.5\( a' \) (panel (D)) to 0.4\( a' \) (panel (D)), where \( a' = a\sqrt{2} \), the NNN repulsive terms reduce and for \( b = 0.3a' \), \(|\Phi_{\text{NNN}}|/|\Phi_{\text{OO}}| < 5 \times 10^{-4} \) (not shown). So reproduction of the HHM, with its local coupling, depends on the lattice spacing and temperature that can be achieved (since larger systems have lower energy scales relative to their condensed matter counterparts [20]). For comparison, panel (A) shows \( \Phi_{\text{FF}} \) for the Holstein model.

To assess the effects of phonon-mediated repulsive interactions on pairing we make a canonical Lang–Firsov transformation [22] to Eq. (4) to obtain an effective Hamiltonian,

\[
H_{\text{LF}} = -t' \sum_{(ij)} \bar{c}_i \bar{c}_j + \sum_{i\nu} n_{i\nu} W \Phi_{i\nu} \Phi_{00} + U_{\text{Fesh}} \sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{\nu \mu} \hbar \omega_{\nu \mu} d^\dagger_{\nu} d_{\mu}, \tag{6}
\]

where \( \lambda = \Phi_{00}/2W \hbar \omega_{\text{ph}}^2 \). When \( \hbar \omega_{\text{ph}} \gg t \) the effective hopping, \( t' = t \exp[-W\lambda(1-\Phi_{\text{NN}}/\Phi_{00})/\hbar \omega_{\text{ph}}] \).

If repulsive interactions are found on both diagonals (Fig. 2 (B) and (C)), solving the two-body Schrödinger equation for \( H_{\text{LF}} \) establishes the critical coupling,

\[
U_{\text{Fesh}}^{(C)} = -\frac{\gamma_1 t' V_1 V_2 + 4t^2 (V_1 + V_2)}{\gamma_1 V_1 V_2 + \frac{1}{2} t' V_1 + \gamma_2 t' V_2 + t^2} + 2W \lambda. \tag{7}
\]
We predict that BKT temperatures of $\sim 20nK$ can be achieved in experiments at small $V_0$ (Fig. 4(b)). BKT condensation would be identifiable via changes to the momentum distribution of the atoms, which can be measured using time of flight. No general expression exists for the BKT temperature, so we make estimates for low pair density $n_B = 0.01 \ll 1$ where $T_{\text{BKT}} = 4\pi \hbar^2 n_B a^2 k_B 2m^{**} \ln(4/n_B)$ [23, 24]. For strongly coupled onsite pairs, effective pair mass $m^{**} = \hbar^2/4W^2\lambda^2 + 2W^2/\ell^2a^2$ (see supplement).

The phase diagram at 20nK shown in Fig. 4(b) has four distinct regions. If $T_{\text{pair}} < T_{\text{BKT}}$ there is condensation at the BKT temperature. At $T_{\text{pair}} > T_{\text{BKT}}$, preformed pairs condense at $T_{\text{BKT}}$. We predict a pseudogap for $T_{\text{BKT}} < T < T_{\text{pair}}$. The normal state is at $T > T_{\text{pair}}$.

So we predict it is possible to transition between normal, pseudogap and BKT phases at $\sim 20nK$ by selecting $V_0 = 150nK$, $n_{\text{Ryd}} = 34$ and $\lambda < 0.09691$ to get $\lambda < 5$. For lower temperatures, this can be done at smaller $\lambda$. Thus the proposed simulator offers a route to the (as yet) unexplored physics of boson-mediated pairing and condensation of fermions in cold atom quantum simulators.

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