Generalised Kronig-Penney model for ultracold atomic quantum systems

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We study the properties of a quantum particle interacting with a one dimensional structure of equidistant scattering centres. We derive an analytical expression for the dispersion relation and for the Bloch functions in the presence of both even and odd scattering waves within the pseudopotential approximation. This generalises the well-known solid-state physics text-book result known as the Kronig-Penney model. Our generalised model can be used to describe systems such degenerate Fermi gases interacting with ions or with another neutral atomic species confined in an optical lattice, thus enabling the investigation of polaron or Kondo physics within a simple formalism. We focus our attention on the specific atom-ion system and compare our findings with quantum defect theory. Excellent agreement is obtained within the regime of validity of the pseudopotential approximation. This enables us to derive a Bose-Hubbard Hamiltonian for a degenerate quantum Bose gas in a linear chain of ions.

I. INTRODUCTION

The Kronig-Penney (KP) model is an analytically solvable model of a one-dimensional (1D) crystalline solid in which the electron-nuclei interactions are replaced by contact potentials of the Dirac-delta form [1]. It is often used in text-books of solid-state physics to help clarify the emergence of an electronic band structure [2]. Although mostly considered to be of academic and educational - rather than quantitative - interest, a number of laboratory systems have become available for which the KP-model provides a useful starting point. These experiments range from solid state and surface science where one-dimensional structures of atoms can be surface-deposited in scanning tunnelling microscopy [3–5] to cold atomic systems in periodic potentials [6]. In such model systems, a setup in which one species forms a lattice of atoms - or ions - through which a second, untrapped, species can move, would create a situation reminiscent of the KP-model. This is particularly so, since the interaction between the lattice of atoms - or ions - and the untrapped atoms could be accurately described by Fermi’s zero-range pseudopotential [7, 8] that is commonly employed in ultracold atomic physics. The considered system may be of significant interest in constructing a quantum simulator of crystalline solids [9–11]. In particular, the inherent quantum nature of the lattice potential, that may have spin or phononic degrees of freedom, sets the system apart from quantum simulators based exclusively on (classical) optical lattice potentials [12]. In this way, the structure of a natural solid is more accurately emulated, making it possible to simulate electron-phonon coupling or Kondo physics.

In this paper, we generalise the KP-model, where a series of equidistant Dirac’s deltas forms the periodic potential as shown in Fig. 1 by including the first derivative of that delta potential. This allows our model to be used in the physical relevant scenario in which both s-wave and p-wave scattering are present. As in the original Kronig-Penney model, our model results in easy-to-interpret analytical expressions. We compare the model to a full numerical calculation based on quantum defect theory (QDT) for the case in which the crystal is formed by ions and the untrapped species is formed by neutral atoms. Excellent agreement is achieved within the validity regime of the pseudopotential approximation. We derive the corresponding Bloch and Wannier functions and demonstrate that the low-energy limit of the system is described by a Bose-Hubbard (BH) Hamiltonian, where the coupling term depends on the relative spin-orientation of the atom and ion [13, 14]. Recent advances in experiments combining atomic and ionic species may put the hybrid atom-ion system within experimental reach [13], and our model is of relevance to approaches where the ions are replaced by a second neutral species as well [16–18].

FIG. 1. (Color online). We consider a 1D system of scattering centers with spin degrees of freedom through which particles can move.
The paper is organised as follows: In Sec. II we briefly review the derivation of the pseudopotentials for even- and odd-waves as discussed in Ref. [19]. In section III we present our generalised KP-model, while in Sec. IV we compare it to a quantum defect theory calculation for an atom in an ion chain. Thereafter, in Sec. V we obtain the corresponding Bloch and Wannier functions and in Sec. VI we apply the model to the hybrid atom-ion system in order to derive the BH Hamiltonian. We discuss our findings and outlooks in Sec. VII Finally, in the Appendix we provide details on the 1D asymptotic solutions of QDT for the hybrid atom-ion system, in the Appendix B on the derivation of the energy-dependent scattering lengths, and in the Appendix C on the computation of the Wannier-Kohn wavefunctions.

II. PSEUDOPOTENTIALS FOR EVEN- AND ODD-WAVES

The so-called zero-range pseudopotential [2, 8], first introduced by Enrico Fermi in order to describe the short-range interaction of quasi free Rydberg electrons [5], has proven to be very successful to describe the interaction between ultracold atoms [21, 22]. The peculiarity of this potential is that it relies on a single parameter, the so-called 3D s-wave scattering length, which enables the description of the scattering at distances larger than the effective range of the van der Waals interaction with very good accuracy.

Under particular circumstances, it is also possible to describe the collision between ultracold bosonic atoms in a waveguide, that is, in a 1D setting where a tight transverse confinement is given, by a pseudopotential [22]. Let us remind how this works: Assuming no trapping potential for the two colliding atoms along the longitudinal direction x, while transversally they experience a strong harmonic confinement, the asymptotic form of the wave function in relative coordinates reads [22]:

\[
\lim_{|x|\to\infty} \Psi(x, \rho) = \left\{ e^{ik_s x} + f_e e^{ik_e |x|} + \text{sign}(x) f_o e^{ik_o |x|} \right\} \phi_o(\rho),
\]

where \( \phi_o(\rho) \) is the ground state of the transverse harmonic trap and \( \text{sign}(x) \) is the sign function. Here the first term in the curly brackets represents the incident wave, the second and third terms give the even and odd scattered waves, respectively. Besides, \( f_e \) and \( f_o \) are the 1D scattering amplitudes for the even- and odd-waves, respectively.

In Ref. [22] it has been shown that while \( f_e \neq 0 \), the odd-wave scattering amplitude \( f_o \) vanishes. This is a consequence of the bosonic symmetry of the colliding atoms. Furthermore, the odd-wave scattering amplitude vanishes also for a 1D delta pseudopotential [22].

Now if we have a spin-1/2 polarized atomic Fermi gas, depending on the internal state of the fermions and because the total fermionic wave function must be antisymmetric, both even-wave and odd-wave scattering can occur. The same happens if we have distinguishable particles like an atom and an ion. In these cases, this implies that the 1D delta potential is not sufficient to describe the interaction of two fermions in a symmetric spin state or of two distinguishable particles. This is clear from Eq. (1), as in these cases we have to expand the general solution to the Schrödinger equation both on even and odd functions.

Almost a decade ago, however, Girardeau and Olshanii have derived the analytical expressions for the even-wave and odd-wave pseudopotentials for two interacting fermions [11]. We note, however, that they can be applied to distinguishable particle too. The actual potential in this scenario is given by \( \nu(x) = \nu_{1D}^e(x) + \nu_{1D}^o(x) \), where the even and odd (two-body) pseudopotentials are defined as [11]:

\[
\nu_{1D}^e(x) = g_{1D}^e \delta_{\pm}^e(x), \quad \nu_{1D}^o(x) = g_{1D}^o \delta_{\pm}^o(x) \hat{\partial}_{\pm}.
\]

Here \( g_{1D}^e = -\hbar^2 / \mu a_{1D}^e \) and \( g_{1D}^o = -\hbar^2 / \mu a_{1D}^o \), with \( \mu \) being the relative mass of the fermionic - or distinguishable - particles, and \( a_{1D}^e \) and \( a_{1D}^o \) are the 1D scattering lengths for even- and odd-waves, respectively. The apex ‘ denotes the spatial derivative. Besides, the action of the two operators appearing in Eq. (2) on a wave function \( \psi(x) \) is given by:

\[
2 \hat{\delta}_{\pm} \psi(x) = [\psi(0^+) + \psi(0^-)] \delta(x),
\]

\[
2 \hat{\partial}_{\pm} \psi(x) = [\psi'(0^+) + \psi'(0^-)],
\]

where \( \psi(0^\pm) = \lim_{x \to 0^\pm} \psi(x) \). We note that the derivative of the delta potential appearing in \( \nu_{1D}^o(x) \) is a direct consequence of the fact that the odd part of the wavefunction in Eq. (1) is not continuous in \( x = 0 \).

Given this, we have all ingredients to solve the problem for a periodic potential of even- and odd-wave interactions.

III. GENERALISATION OF THE KRONIG-PENNEY MODEL

The Kronig-Penney model describes a single particle moving in a one dimensional periodic potential of rectangular barriers of height \( U_0 \) and width \( b \) separated by a distance \( d \) (see Fig. 2).

Now, from a quantum mechanical scattering point of view, the periodic potential

\[
V(x) = \sum_k \nu_{1D}^e(x - x_k)
\]

corresponds to the situation for which the cores and the moving particle are bosons, and therefore only even-wave scattering occurs [22]. Our goal here is to solve the Schrödinger equation for the following periodic potential
Thus, we aim at the determination of the dispersion relation for the single particle Hamiltonian \( H \). The wave function must satisfy the identity \([19]\)

\[
\psi(0^+) - \psi(0^-) = -a_{1D}^0 [\psi'(0^+) + \psi'(0^-)].
\]

This identity implies that the wave function is discontinuous in the origin, namely at the contact point, as we already pointed out at the end of Sec. \( \text{III} \). This condition is different from the one of \( v_{1D}^1(x) \), that is,

\[
\psi'(0^+) - \psi'(0^-) = -(a_{1D}^e)^{-1} [\psi(0^+) + \psi(0^-)].
\]

for which the derivative of the wave function has a discontinuity at the contact point. While for the latter the wave function is assumed to be continuous, in the former case (odd-wave) we shall assume that the left and right limits of the first spatial derivative are equal, namely \( \psi'(0^+) = \psi'(0^-) \) (see also Ref. \( [24] \)). We note, however, that this does not mean that the wavefunction is a continuous function.

The second condition we shall apply to solve the Schrödinger equation is due to the Bloch theorem \([2]\) which states that the wave function in the nearby interval \((II)\) is given by \( \psi_{II}(x) = e^{iqd} \psi_I(x - d) \) \([23]\) (see also Fig. 2). Here \( q \) is the Bloch vector or quasi-momentum. Putting together the two conditions we have:

\[
\psi_{II}(d^+) - \psi_I(d^-) = -2a_{1D}^e \psi_I'(d^-),
\]

\[
\psi_{II}'(d^+) = \psi_I'(d^-) = e^{iqd} \psi_I'(0^-). \tag{9}
\]

Now we make the following Ansatz for the wave function in the interval \([0, d]\):

\[
\psi_I(x) = A \cos(kx) + B \sin(kx), \tag{10}
\]

where \( k = \sqrt{2mE/\hbar^2} \). This wave function clearly solves the Schrödinger equation for a free particle in the interval \([0, d]\). Now by replacing \([10]\) in Eq. \( 9 \) we obtain a matrix equation, \( \mathbf{M} \mathbf{C} = 0 \), where \( \mathbf{C} = (A, B)^T \) and \( \mathbf{M} \) is a 2 \times 2 matrix defined as:

\[
\mathbf{M} = \begin{pmatrix}
\cos(kd) + 2a_{1D}^e k \sin(kd) - e^{iqd} & \sin(kd) - 2a_{1D}^e k \cos(kd) \\
k \sin(kd) & k \cos(kd) - e^{iqd}
\end{pmatrix}.
\]

By imposing the condition \( \det(\mathbf{M}) = 0 \) we finally obtain the following dispersion relation:

\[
\cos(qd) = \cos(kd) + a_{1D}^e k \sin(kd). \tag{12}
\]

For the sake of completeness we provide here also the dispersion relation for the even-wave described by \( v_{1D}^o(x) \):

\[
\psi(0^+) - \psi(0^-) = -a_{1D}^o [\psi'(0^+) + \psi'(0^-)].
\]

FIG. 2. (Color online). Sketch of the periodic potential used in the original Kronig-Penney model.

\[
V(x) = \sum_k v_{1D}^o(x - x_k) + \sum_k v_{1D}^o(x - x_k). \tag{5}
\]
We note that the size of the energy gaps grows as the energy becomes large, like in the usual KP-model. This is different with respect to the case, for instance, of an optical lattice with finite amplitude, where the difference between energy levels becomes smaller and smaller as the energy of the band increases. We explain this by noting that the behaviour is very similar to the eigenenergies of a particle in a box with perfectly rigid walls which scale as $E_n \propto n^2$ ($n$ is the quantum number). For a particle in such a box potential the energy difference between the levels increases. Hence, when the separation between the lattice sites is rather large (i.e., the pseudopotential is applicable) and because at the lattice sites the potential is infinitely large, the band structure of a particle in such a periodic potential is strictly connected to the energy spectrum of a particle in a box with perfectly rigid walls.

B. Solution for both even- and odd-waves

Now we solve the general problem for which the periodic potential is given by Eq. (5). To this aim, we apply once again the Bloch theorem and impose the conditions (7) and (8). This turns out to be equivalent to the following conditions:

$$a_{1D}^o \left[ \psi_{I}^o(0^+) - \psi_{I}^o(d^-) e^{-i qd} \right] + \psi_{I}(0^+) + e^{-i qd} \psi_{I}(d^-) = 0,$$

$$a_{1D}^e \left[ \psi_{I}^e(0^+) + \psi_{I}^e(d^-) e^{-i qd} \right] + \psi_{I}(0^+) - e^{-i qd} \psi_{I}(d^-) = 0.$$  

(14)

As previously described, we use the Ansatz (10) for the wavefunction in the region $I$ (see also Fig. 2) and compute the determinant of the new matrix $M$, from which we obtain the new dispersion relation

$$\cos(qd) = \frac{(a_{1D}^o + a_{1D}^e) \cos(kd)}{a_{1D}^o - a_{1D}^e} + (k^2 a_{1D}^o a_{1D}^e - 1) \frac{\sin(kd)}{(a_{1D}^o - a_{1D}^e) k}.$$  

(15)

In the limit $a_{1D}^o \rightarrow 0$ we recover (12), whereas in the limit $a_{1D}^e \rightarrow \infty$ we recover (13).

In figure 4 we show a typical band structure calculation (red dashed lines), for which we assumed energy-independent scattering lengths (see also Sec. IV).
IV. COMPARISON WITH QUANTUM DEFECT THEORY

In this section we compare the solutions obtained for the even and odd pseudopotentials with the solutions obtained via numerical integration of the Schrödinger equation for the atom-ion interaction potential. This scenario would correspond to an ion chain with separation $d$ between the ions, where an ultracold atom is free to move within the lattice, as in our recent proposal for an atom-ion quantum simulator [12].

In such a system the interaction between the moving particle and the scattering centre is caused by the electric field generated by the charge of the ion and the induced dipole of the atom, which at large distances has the following form in 3D:

$$\lim_{r \to \infty} V_{\text{int}}(r) = -\frac{C_4}{r^4}. \quad (16)$$

For $r \to 0$, Eq. (16) does not hold anymore and the potential becomes strongly repulsive. The exact form of the potential in this regime depends on the electronic sub-structure of the atom and ion. This short-range dependence can be parametrised in the ultracold regime by a single parameter, the so-called short-range phase $\phi$ [20]. The natural energy and length scales for the atom-ion interaction [10] are $E^* = \hbar^2 / (4m^2C_4)$ and $R^* = \sqrt{2mC_4}/\hbar^2$, respectively. Here $m$ is the mass of the atom, $C_4 = e^2\alpha_p/2$ with $e$ the charge of the ion, and $\alpha_p$ the static atomic polarisability [27]. In these units the energy of a free particle and the corresponding wavevector are linked as: $E = k^2$.

The atom-ion interaction clearly has a three-dimensional character, but an effective 1D theory can be developed for systems that are tightly trapped in the transverse direction [20]. Hence, we make such assumption for the atom and we write the transverse potential, in $E^*$ and $R^*$ units, as $V_\perp(r) = \alpha_\perp r^2$ with $\alpha_\perp = (R^*/\ell_\perp)^4$ and $\ell_\perp = \sqrt{\hbar/2m\omega_\perp}$. On the other hand, in the axial direction, $x$, we assume that the atom experiences no external confinement. Following Ref. [20], we also introduce the length scale $R_\perp = \alpha_\perp^{-1/6}$ (in the above atom-ion units), which denotes the distance at which the atomic trapping potential $V_\perp$ equals the atom-ion interaction. Then, it can be shown that for large distances between the atom and the ion, that is, $x \gg R_1 \approx \max(R_\perp, \ell_\perp)$, the atom-ion interaction can be described effectively in 1D like $-C_4/x^4$ [20].

Given all this, the Schrödinger equation for a single atom interacting with a static ion located at $x_i = 0$ in $E^*$ and $R^*$ units is given by:

$$\left( \frac{d^2}{dx^2} + \frac{1}{x^2} + E \right) \psi(x) = 0. \quad (17)$$

For $x \to 0$, the energy $E$ can be neglected and the equation can be solved analytically:

$$\psi_e(x) = |x| \sin \left( \frac{1}{|x|} + \phi_e \right),$$

$$\psi_o(x) = x \sin \left( \frac{1}{|x|} + \phi_o \right), \quad (18)$$

where $\phi_{e,o}$ denote the even and odd short-range phases (we refer to the Appendix A for some more details on choice of the above outlined asymptotic solutions). These phases, also called quantum defect parameters, encapsulate the physical content of the short range for which the actual atom-ion interaction is unknown. The parameters are two because in 1D we can have solutions with even and odd parity. Furthermore, although in the following we will treat the two phases as independent parameters, we note that they are not fully independent, since they are related both to the transverse confinement (i.e., $\omega_\perp$) and to the so-called 3D short-range phase [28]. We refer to Ref. [20] for a more detailed discussion.

Now coming back to the single atom problem in a 1D ion chain, we note that within quantum defect theory an atomic energy eigenfunction is described by a superposition of the asymptotic solutions [18] in the vicinity of each ion, up to a sufficiently small distance $R^* \gg x_0 \gg \ell_\perp$. Outside $x_0$, the two solutions $\psi_e(x)$ and $\psi_o(x)$ are propagated numerically by means of a renormalised Numerov method [22] up to the border of the real space unit cell for a fixed set of $(E, \phi_e, \phi_o)$ with the initial conditions chosen to match the asymptotic solutions smoothly at $x_0$. Since the even and odd solutions span the corresponding Hilbert space, the Bloch state can be written as

$$\psi_q(x) = c_{\psi}^{(e)} \psi_e(x) + c_{\psi}^{(o)} \psi_o(x) \quad (19)$$

with coefficients $c_{\psi}^{(e)}$ and $c_{\psi}^{(o)}$ for the even and odd states, respectively. Furthermore, in accordance with the Bloch theorem, each Bloch state fulfills

$$\psi_q(x + d) = e^{iqd} \psi_q(x) \quad (20)$$

under spatial translation by a lattice distance $d$. Together, these conditions allow us to relate $E = E(k)$ to $q$ and thereby to determine the band structure, in exact analogy to the Kronig-Penney model solution.

Now, if $E$ does not lie within a band gap, the associated Bloch vector $q$ is defined by the constraint of both the wave function and its derivative being continuous at the edge of the unit cell. If the ion is chosen to lie in the middle of the unit cell at $x = 0$, symmetry implies $\psi_e(-d/2) = \psi_e(d/2)$, $\psi_o(-d/2) = -\psi_o(d/2)$, $\psi'_e(-d/2) = -\psi'_e(d/2)$, $\psi'_o(-d/2) = \psi'_o(d/2)$ and the matching conditions imply the linear relations

$$A(q) \begin{pmatrix} c_{\psi}^{(e)} \\ c_{\psi}^{(o)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad (21)$$
where

\[
A(q) = \begin{pmatrix}
(1 - e^{iqd})\psi_e(\frac{N}{4}) & (1 + e^{iqd})\psi_o(\frac{N}{4}) \\
(1 + e^{iqd})\psi'_e(\frac{N}{2}) & (1 - e^{iqd})\psi'_o(\frac{N}{2})
\end{pmatrix}.
\]  

(22)

We note that this equation relates the energy (which is now hidden in the wavefunctions) to the wavenumber \(q\).

For normalizable, non-trivial solutions of \(\phi^\dagger e\phi_c = 1\) to exist, the determinant of the coefficient matrix \(A(q)\) has to vanish. The quasi-momentum corresponding to the chosen energy \(E\) is then efficiently determined by using, for instance, the Nelder-Mead algorithm [30] on the determinant \(\text{det}(A(q))\).

An example of such a band structure calculation is illustrated in Fig. 4 where the thick solid lines represent the energy bands for \(\phi_o = -\phi_e = \pi/4\) and \(d = 15R^*\). In the low energy limit the 1D scattering lengths are related to the corresponding even and odd short-range phase as:

\[
a_{1D}^{e,o} = -\sqrt{\frac{\mu}{m}} R^* \cot \phi_c^{e,o}
\]

(23)

with \(\mu\) being the relative mass of the atom-ion system. By replacing these definitions in the dispersion relation \([14]\) we obtained the energy bands that are displayed in Fig. 4 with red dashed lines. As it is shown, the ion separation is sufficiently large such that the KP-model can reproduce very well the lowest energy band corresponding to scattering states (see upper panel in Fig. 4). However, the agreement is worse at higher energy bands, as expected, since the relations \([28]\) do not hold anymore. The agreement, however, can be improved by considering energy-dependent scattering lengths, as it will be discussed in the next section.

To give a feeling about typical numbers, we note that the situation in Fig. 4 would correspond, for instance, to \(^{171}\text{Yb}\) ions separated by 5.6 \(\mu\)m interacting with a \(^{87}\text{Rb}\) atom. In this case \(E^*/h = 411\) Hz resulting in band gaps of tens of hertz. For the combination \(^{171}\text{Yb}\)\(^{3+}\)/\(^{6}\text{Li}\), the ions would be 1.1 \(\mu\)m apart with \(E^*/h = 167\) kHz leading to band gaps in the 10 kHz range.

A. Energy-dependent 1D scattering lengths

In order to compute the energy dependent scattering lengths, we adapted the formalism developed in Ref. [31] to our 1D scenario which is summarised in the Appendix [33]. The formalism has been applied to the previous discussed example and the result of the band structure calculation is shown in Fig. 4 (black dash-dot lines). The energy dependence of the scattering lengths drastically improves the result of our generalised KP-model which is now in perfect agreement with the QDT calculation also to higher energy bands.

We have checked the validity of this model for some pairs of short-range phases. In particular, \(\phi_e, \phi_o\) = \((-\pi/4, \pi/4), (-\pi/4, \pi/3), (-\pi/4, -\pi/4 + \epsilon)\) with \(\epsilon = 10^{-4}\). In the last case, we added a small correction \(\epsilon\) in order to facilitate the convergence of the Numerov method. We have also checked to which extend the pseudopotential with respect to the ion separation \(d\) is applicable.

We found that for scattering states the agreement with QDT is still good even for separations close to \(d = 3R^*\).

V. BLOCH AND WANNIER FUNCTIONS

Now we determine the corresponding Bloch wave functions. To this end, we make the Ansatz [32]:

\[
\psi_q(x) = N_q(k) \{ \sin(kx) + e^{-iqd}\zeta_q(k) \sin[k(d - x)] \},
\]

(24)

where \(N_q(k)\) is a normalisation constant. By using, for instance, condition (8) we obtain:

\[
\zeta_q(k) = 1 + \frac{a_{1D}^o k(e^{2iqd} - 1)}{a_{1D}^e k + e^{iqd}[a_{1D}^o k \cos(kd) - \sin(kd)]}.
\]

(25)

Now by imposing the Born-von Karman periodic boundary conditions we obtain the following quantisation of the quasi-momentum Bloch vector: \(q_j = 2\pi j/dN_L\) with \(n = 0, \pm 1, \pm 2 \ldots \pm (N_L - 1)/2\). Here \(N_L\) denotes the number of lattice sites. Thus, we normalise the Bloch wave function within a unit cell as follows

\[
\int_0^d dx |\psi_q(x)|^2 = \frac{1}{N_L},
\]

(26)

from which we finally obtain

\[
\frac{1}{N_L^2(k)} = \frac{d}{2} \sin(2kd) \left(1 + |\zeta_q(k)|^2 \right) + |\zeta_q(k)| \cos(qd - \arg(\zeta_q(k))) \left[ \frac{\sin(kd)}{k} - d \cos(kd) \right].
\]

(27)

It is easy to check that with the above outlined definitions also the condition (7) is fulfilled. Finally, accordingly to the Bloch theorem, we define the Bloch functions in another interval (i.e., cell) as:

\[
\psi_{j,n,q}(x) = e^{iqd} \psi_{j,n,q}^{(0)}(x - jd) \quad j \in \mathbb{Z},
\]

(28)

where \(\psi_{j,n,q}^{(0)}(x) \equiv \psi_q(x)\) and the index \(n\) refers to the \(n\)-th band with \(E > 0\). With the above outlined definitions, the Bloch functions over \(N_L\) lattice sites form an orthonormal basis.

In Fig. 5 we compare the Bloch functions obtained within QDT to the ones of our generalised KP-model.
FIG. 5. (Color online). Upper panel: real and imaginary parts of the Bloch function corresponding to the lowest energy band of Fig 4. Lower panel: absolute value of the Bloch wave function. In both panels the solid lines correspond to the result of QDT, whereas the dashed lines to the result of the KP-model. The short-range phases are $\phi_o = -\phi_e = \pi/4$ and the ions are separated by $d = 15R^*$. For a better visualisation, we normalised the displayed Bloch functions on the unit cell.

for the lowest scattering energy band that is displayed in Fig. 4. Good agreement for the absolute value of the Bloch functions between QDT and the generalised KP-model is shown, except at the scattering centres, as expected given the nature of the pseudopotential. On the other hand, the disagreement between the real and imaginary parts is essentially due to the relative phase induced by the factor $\zeta_q(k)$ in our definition (24).

Finally, in Fig. 6 we shown an example of Wannier-Kohn function computed within QDT and for our generalised KP-model. We recall that the Wannier functions, in contrast to the Bloch functions, form a maximally localised set of orthonormal states in real space (see also Appendix C for more details). Also in this case, very good agreement is obtained between the two theories, although the result of the KP-model displays a less smooth behaviour at the maximum and minimum of the real part of the function. This is essentially due to the singular behaviour of the pseudopotential in correspondence to the ion locations.

VI. APPLICATION: THE BOSE-HUBBARD MODEL

In this section we are going to present an application of the above outlined formalism focusing again on the hybrid atom-ion system. Our goal is to show that a Bose-Hubbard-type Hamiltonian can be derived for an ultracold atomic ensemble of bosons immersed in an ion chain in a regime where our generalised KP-model can be applied. We will compute the hopping and interaction matrix elements and compare them with QDT calculations. We note, however, that the present approach can be easily generalised to other systems as well.

A. Hopping matrix elements

In order to compute the hopping matrix elements we note that we do not need to compute the Wannier functions. There is a direct connection between the dispersion relation and the hopping matrix elements (34):

$$J_{l,l'} = \frac{1}{N_L} \sum_{q_k} E_q^{(n)} e^{i\eta_k d(l-l')}.$$  (29)

Here again $N_L$ is the number of lattice sites (32), whereas $E_q^{(n)}$ denotes the corresponding $n$-th energy band as a function of the Bloch vector $q$. We note that Eq. (29) can be easily obtained by expanding the the single particle Hamiltonian of the periodic potential on the basis of the Bloch functions and then apply the definition of Wannier function (C1).

Figure 7 shows the hopping matrix elements as a function of the interionic separation $d$ for various neighbour distances $l - l'$. As it is shown, for increasing separation between the ions, the strength of the hopping matrix elements decays. Additionally, the nearest neighbour matrix element is the largest one. Again, the calculation has been performed for the lowest scattering band.

Finally, we also note that we have checked for $d = 15R^*$ that, by using the definition of $J_{k,k+1}$ with the Wannier functions given in Eq. (32), we obtain the same result. Indeed, for the pair of short-range phases $\phi_o = -\phi_e = \pi/4$, we obtain $|J_{k,k+1}| \simeq 5.8 \times 10^{-3} E^*$ for the Wannier functions computed with our KP-model, while the result of QDT accordingly to Eq. (29) yields $6.0 \times 10^{-3} E^*$. 


Kohn basis of the lowest scattering band, that is, $\hat{\varphi}$

\[ \sum_{x} H = \frac{1}{\hbar} \int dx \hat{\varphi}^\dagger (x) \hat{\varphi} \psi(x) \psi(x). \]  

(30)

Here $\hat{H}_{sp} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$ is the single particle Hamiltonian, and $V(x)$ is given by Eq. 4. Besides this, in Eq. 30 we have introduced the 1D atom-atom coupling constant $g_{1D} = 2\hbar \omega \frac{a_{1D}}{\sqrt{\hbar \omega}}$, where $\Lambda = (1 - 1.4603 a_{1D}^2 / \sqrt{\hbar \omega})^{-1}$ is the Olshanii correction \[22\] with $a_{1D}$ being the 3D $s$-wave scattering length. This implies that transversally the motion is frozen to the harmonic oscillator ground state. Now, by expanding the atomic quantum field operator $\hat{\psi}(x)$ onto the Wannier-Kohn basis of the lowest scattering band, that is, $\hat{\psi}(x) = \sum_{j} W_{0}(x-x_{j}) \hat{b}_{j}$ with $[\hat{b}_{j}, \hat{b}_{j}^\dagger] = 1$, the many-body Hamiltonian becomes

\[ \hat{H} = \sum_{k,\ell} J_{k,\ell} \hat{b}_{k}^\dagger \hat{b}_{\ell} + \frac{\hbar}{12} \sum_{k,k',\ell,\ell'} U_{k,k',\ell,\ell'} \hat{b}_{k}^\dagger \hat{b}_{k'} \hat{b}_{\ell} \hat{b}_{\ell'}, \]  

(31)

where

\[ J_{k,\ell} = -\int dx W^*(x-x_{k}) \hat{H}_{sp} W(x-x_{\ell}), \]

\[ U_{k,k',\ell,\ell'} = \int dx \prod_{j=k,\ell} W^*(x-x_{j}) \prod_{s=k',\ell'} W(x-x_{s}). \]  

(32)

As it has been previously shown, the relevant hopping matrix elements are $J \equiv J_{k,k+1}$. Similarly, we have checked that the most relevant interaction matrix elements are $U_{0} \equiv U_{k,k,k,k}$, and that the elements $U_{1} \equiv U_{k,k,k+1,k+2}$, $U_{2} \equiv U_{k,k,k+2,k+1}$ are negligible. Indeed, for $d = 15 R^*$ and $\phi_{0} = -\phi_{c} = \pi/4$ we obtain: $U_{0}^{\text{QDT}} \simeq 0.1013 E^*$, $U_{0}^{\text{KP}} \simeq 0.0979 E^*$, $U_{1}^{\text{QDT}} \simeq 0.0012 E^*$, $U_{1}^{\text{KP}} \simeq 0.0013 E^*$, $U_{2}^{\text{QDT}} \simeq 0.0004 E^*$, $U_{2}^{\text{KP}} \simeq 0.0004 E^*$, that is, the off-diagonal matrix elements are two orders of magnitude smaller than the onsite interact energy $U_{0}$, and therefore they can be safely neglected. This shows again the good agreement between the exact QDT calculation and the generalised KP-model.

Given this, we are left with the following Bose-Hubbard-type Hamiltonian

\[ \hat{H} = \sum_{k,\ell} J_{k,\ell} \hat{b}_{k}^\dagger \hat{b}_{\ell} + \frac{g_{1D}}{2} \sum_{k,k',\ell,\ell'} U_{k,k',\ell,\ell'} \hat{b}_{k}^\dagger \hat{b}_{k'} \hat{b}_{\ell} \hat{b}_{\ell'}, \]  

(31)

where

\[ J_{k,\ell} = -\int dx W^*(x-x_{k}) \hat{H}_{sp} W(x-x_{\ell}), \]

\[ U_{k,k',\ell,\ell'} = \int dx \prod_{j=k,\ell} W^*(x-x_{j}) \prod_{s=k',\ell'} W(x-x_{s}). \]  

(32)
where ˆKohn functions [36].

The contribution of the (shallow) axial confinement of the

tering lengths is chosen), as we have shown in Ref. [13],

because the interaction depends on the internal state of

atoms and ions can be engineered.

Finally, we note that the Hamiltonian [34] resembles

the one of an atomic ensemble in interaction with a

field cavity mode. Such an interaction enables cavity-

mediated long-range atom-atom interactions [37]. In

our system the quantum potential is provided by the

atom-ion interaction where the atomic back-action on the

quantum lattice potential may generate atom-ion entan-

glement via phonons [12, 13]. Furthermore, we note that

with our setup we can also study the analogue of a sin-

gle atom transistor [16], where one ion of the chain can

eventually suppress the atomic tunnelling via the state-

dependent atom-ion interaction.

VII. CONCLUSIONS

In this work we have presented the solution of a
generalised Kronig-Penney model where both s-wave and p-wave scattering are present. We derived analytical expressions for the dispersion relation and the Bloch functions in this model. We have compared the results of the KP-model with a quantum defect theory calculation for the hybrid atom-ion system and found very good agreement between the two theories. For describing the higher energy bands, the energy dependence of the 1D atom-ion scattering lengths needs to be taken into account. This also enabled us to derive the low-energy Bose-Hubbard Hamiltonian for such a hybrid system. We stress that our generalised KP-model can be used to describe other systems as well, such as atoms trapped in an optical lattice or one-dimensional structures. Furthermore, our generalised KP-model can be used to derive simple analytical formulae, for example, for the phonon-atom coupling and the underlying physics of the polaronic Fröhlich Hamiltonian of a recently proposed atom-ion quantum simulator [12]. Given recent advances in experimental atomic and solid-state quantum physics, the model we analysed
has not only an academic interest, but it is indeed applicable to systems that can be realised in current experiments, for instance, with ultracold atomic gases.

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Appendix A: Short-range asymptotic solutions

In Ref. [26], a 1D QDT for ultracold atom-ion collisions has been developed. There it has been shown that

\[ \dot{\psi}_e(x) = |x| \sin \left[ R^*/x + \phi_e(k) \right] \quad x \ll \sqrt{R/k} \]
\[ \dot{\psi}_o(x) = x \sin \left[ R^*/x + \phi_o(k) \right] \quad x \ll \sqrt{R/k} \]

(A1)

are the even and odd solutions of the Schrödinger equation

\[ \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + C_4 \frac{|x|}{|x|^4} \psi(x) = 0. \]  

(A2)

Here we would like to show that such solutions are the most general ones of the 1D scattering problem with the \( x^{-4} \) potential and that two independent quantum defect parameters, \( \phi_{e,o} \), are indeed necessary for a full description of the scattering process.

To begin with, we note that the following pair of even and odd functions

\[ \psi_e(x) = x \sin \left( R^*/x \right) \quad x \ll \sqrt{R/k} \]
\[ \psi_o(x) = x \cos \left( R^*/x \right) \quad x \ll \sqrt{R/k} \]

(A3)

are also solutions of the differential equation (A2). Thus, one would be attempted to conclude that the general solution is given by: \( \psi(x) = A \psi_e(x) + B \psi_o(x) \) with \( A,B \) constants. Given this, one could also conclude that the relative phase between the even and odd solutions is the only relevant parameter such that the short-range phases \( \phi_{e,o}(k) \) are not independent parameters. Nevertheless, we note that the functions \( \psi_{e,o}(x) \) cannot generate all possible solutions of Eq. (A2). More precisely, if we consider the function

\[ \psi(x) = |x| \cos(R^*/x) \]  

(A4)

which is solution of Eq. (A2), then it is easy to show that it cannot be generated by the pair \( \psi_{e,o}(x) \) given by Eq. (A3). This implies that such a pair of even and odd solutions cannot span functions that have a cusp in \( x = 0 \), which are nonetheless solutions of the Schrödinger equation. Hence, we actually need two independent quantum defect parameters for a 1D description of the atom-ion scattering process.

Appendix B: Determination of the energy-dependent scattering lengths

In order to obtain the \( k \)-dependence of \( a_{1D}^{e,o} \) we adapt the general 3D theory developed in Ref. [31] for the atom-ion scattering process in the absence of external confinement to our pure 1D scenario. First we note that the Schrödinger equation (17) is very similar to the radial equation of the 3D scattering problem. For the sake of completeness we provide that equation [31]:

\[ \frac{d^2 F(r)}{dr^2} + \left( E - \frac{\ell(\ell+1)}{r^2} + \frac{1}{r^4} \right) F(r) = 0 \quad r > 0. \]

(B1)

Here \( F(r) \) is the radial part of the 3D atomic wavefunction and \( \ell \) is the partial wave quantum number. For \( \ell = 0 \) Eq. (B1) reduces to precisely Eq. (17), and therefore we can apply the theory of Ref. [31] by setting \( \ell = 0 \) and by replacing the 3D short-range phase with \( \phi_{e,o} \), whenever needed.

For the sake of clarity, we illustrate the main steps which enables us to compute the energy-dependent scattering lengths

\[ a_{1D}^{e,o}(k) = -\frac{\tan \delta_{e,o}(k)}{k} \]  

(B2)

with \( k = \sqrt{E} \) (in \( E^* \) and \( R^* \) units). To this end, we need to compute the energy-dependent phase shifts \( \delta_{e,o}(k) \), which are defined as [31]:

\[ \tan \delta_{e,o}(k) = \frac{A_{-\nu}(\phi_{e,o}) m_{-\nu} \cos \eta - A_{\nu}(\phi_{e,o}) m_{\nu} \sin \eta}{A_{\nu}(\phi_{e,o}) m_{\nu} \cos \eta - A_{-\nu}(\phi_{e,o}) m_{-\nu} \sin \eta}, \]

(B3)

where \( A_{\nu}(\phi_{e,o}) = \sin(\phi_{e,o} - \nu \pi/2 + \pi/4)/\sin(\pi \nu), \eta = \frac{\pi}{2}(\nu - \frac{1}{2}), \) and \( m_{\nu} = (4/k)^{\nu} S(\nu). \) Here the function \( S(\nu) \) is defined as:
In this case, the localisation is an instance of a Wannier function calculated matrices. In our numerical simulations γ ready sufficient.

Now given the parameter \( x \) we can proceed by numerically solve the following equation \[ \Delta = \begin{vmatrix} \ddots & \ddots & \ddots & \ddots & \ddots \\ \ddots & 1 & \gamma_{-2} & 0 & 0 & \cdots \\ \ddots & \gamma_{-1} & 1 & \gamma_{-2} & 0 & \cdots \\ \vdots & 0 & \gamma_{0} & 1 & \gamma_{1} & \cdots \\ \vdots & 0 & 0 & \gamma_{1} & 1 & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{vmatrix} \] (B9)

with \( \gamma_{n} = k/(4n^2 - \alpha) \) and \( \alpha = 1/4 \). As pointed out in Ref. \[31\], \( \Delta \) converges rather quickly for relatively small matrices. In our numerical simulations \( N \sim 50 \) was already sufficient.

**Appendix C: Wannier-Kohn functions**

Since the Bloch vector on a finite lattice is quantised, the Wannier functions are defined as the discrete Fourier transform of the Bloch states within each band

\[ W_n(x - x_j) = \frac{1}{\sqrt{N_b}} \sum_{q_k} \psi_{n,q_k}(x)e^{-iq_kx_j}. \] (C1)

Here \( x_j = jd \) with \( j \in \mathbb{Z} \). Note that the Wannier functions obey the following orthonormality condition

\[ S(\nu) = \frac{b^+_{\infty}(\nu)}{b^-_{\infty}(\nu)} \times \frac{\Gamma\left(\frac{n}{4} + \frac{1}{2}\right)\Gamma\left(\frac{n}{4} - \frac{1}{2}\right)}{\Gamma\left(\frac{n}{4} + \frac{1}{2}\right)\Gamma\left(\frac{n}{4} - \frac{1}{2}\right)}, \] (B4)

where \( \Gamma(x) \) is the Euler-function, and

\[ h^\pm_n(\nu) = \lim_{n \to +\infty} b^\pm_n(\nu), \] (B5)

\[ b^\pm_n(\nu) = h^\pm_n(\nu)h^\pm_{n-1}(\nu)h^\pm_{n-2}(\nu)\cdots h^\pm_1(\nu), \] (B6)

\[ b^\pm_n(\nu) = \frac{1}{1 - \frac{\nu}{E}} h^\pm_{n+1}. \] (B7)

Now given the parameter \( \nu \) we will explain immediately how to determine it – we start by setting \( b^\pm_N = 1 \), for some sufficiently large \( N \), and we calculate \( b^\pm_1 \) by means of Eq. \[ \{B7\} \) up to \( n = 1 \). This enables us to compute \( b^\pm_n(\nu) \) and, for a large \( N \), also \( b^\pm_1(\nu) \).

Finally, in order to compute \( \nu \) we can proceed by numerically solve the following equation [31]

\[ \cos(\pi \nu) = 1 - \Delta[1 - \cos(\pi \sqrt{\alpha})], \] (B8)

which is a trivial consequence of the orthonormalisation of the Bloch functions.

In Fig. [8] an instance of a Wannier function calculated within QDT is illustrated. As it is shown, the function is clearly not localised around a unit cell. In order to overcome this issue, we have applied Kohn’s prescription [33], namely we multiplied the Bloch functions by a constant phase factor computed within QDT such that \( \Re[\psi_{0,q}(0)] = 0 \), whereas for our generalised KP-model it has been computed such that \( \Im[\psi_{0,q}(0)] = 0 \). The reason of the different factors between the two approaches is due to the fact that within QDT all Bloch functions are (in principle) zero for \( x = 0 \), while this is not the case for the functions of our generalised KP-model. The result of this transformed function is shown in Fig. [6] for the case of QDT, which shows a more localised Wannier function, even though a series of smaller peaks are observed at different lattice sites. To improve further the localisation, we have multiplied the Bloch functions of Bloch vector \( q_j \) obtained within QDT by \( e^{-iq_jd/2} \) and the result is shown in Fig. [6] (right panel). In this case, the localisation is even better.
FIG. 9. (Color online). Wannier-Kohn function of the lowest scattering band within QDT: the cyan (solid thick) line represents the real part of $W_0(x)$, the red (dashed) line its imaginary part, and the black (dash-dot) line the modulus of the function. The blue dots serve only to indicate the position of the ions. The short-range phases are $\phi_o = -\phi_e = \pi/4$, and the ions are separated by $d = 15R^*$. 

[1] R. de L. Kronig and W. G. Penney, Proc. R. Soc. Lond. A 130, 499 (1931).
[2] C. Kittel, Introduction to Solid State Physics, eighth edition ed. (John Wiley & Sons, Inc., New York, 2005).
[3] N. Nilius, T. M. Wallis, and W. Ho, Science 297, 1853 (2002).
[4] J. E. Ortega and F. J. Himpsel, Lect. Notes Phys. 715, 147 (2006).
[5] N. Oncel, J. Phys.: Condens. Matter 20, 393001 (2008).
[6] I. Bloch, Nature Physics 1, 23 (2005).
[7] K. Huang, Statistical mechanics, second edition ed. (John Wiley & Sons, Inc., New York, 1987).
[8] M. Olshanii, Phys. Rev. Lett. 81, 938 (1998).
[9] M. D. Girardeau and M. Olshanii, arXiv:cond-mat/0309396 (2003).
and an ion. However, our definition is better suited when the ion motions is neglected.

[28] We note, however, that the 1D scattering lengths can be tuned either by the frequency of the transverse trap $\omega_\perp$ or by means of Feshbach resonances.

[29] B. R. Johnson, J. Chem. Phys. 67, 4086 (1977).

[30] J. A. Nelder and R. Mead, Comput. J. 7, 308 (1967).

[31] Z. Idziaszek, A. Simoni, T. Calarco, and P. S. Julienne, New Journal of Physics 13, 083005 (2011).

[32] B.-B. Wei, S.-J. Gu, and H.-Q. Lin, Phys. Rev. A 79, 063627 (2009).

[33] W. Kohn, Phys. Rev. 115, 809 (1959).

[34] U. Bissbort, Stochastic Mean-Field Theory for the Disordered Bose-Hubbard Model, Diploma thesis, Goethe Universität Frankfurt am Main (Germany), available at www.itp.uni-frankfurt.de/cms/index.php?id=116 (2007).

[35] $N_L + 1$ is the number of equidistant grid points of the first Brillouin zone (BZ) $(-\pi/d, \pi/d)$.

[36] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. 81, 3108 (1998).

[37] C. Maschler and H. Ritsch, Phys. Rev. Lett. 95, 260401 (2005).