

LETTER TO THE EDITOR

Exact two-body bound states with Coulomb repulsion in a periodic potential

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Online at stacks.iop.org/JPhysA/39/L667**Abstract**

It is shown, through an elementary quantum mechanical calculation, that two particles interacting via a short range repulsive force in an external periodic potential can form a bound state. The two-particle wavefunction is labelled by a continuous centre-of-mass momentum. It is bounded and spatially localized in the centre-of-mass system; thus, the spatial wavefunction in the relative distance is square integrable and corresponds to a discrete energy. For instance, a combination of short-range (i.e. screened) binary Coulomb interactions and the periodic potential provided by the stationary ions, can create a two-electron bound state in a crystalline solid (Slater *et al* 1953 *Phys. Rev.* **91** 1323 and Hubbard 1963 *Proc. R. Soc. A* **276** 238). However, the phenomenon delineated here is universal in the sense that, under appropriate conditions, bound states are possible independent of the nature of the particles and/or the mechanism by which the external periodic potential is engineered. Our general wave mechanical result may explain experimental results presenting evidence of such bound pair states in solids (Gross *et al* 1971 *JETP Lett.* **13**) and photonic lattices (Winkler *et al* 2006 *Nature* **441** 853). It has many other potentially interesting consequences even for classical interacting wave systems (e.g. solitons) propagating in a periodic background. This result of wave mechanics and interference is remarkable in that two repulsively interacting particles cannot form a bound state when moving in vacuum. Two non-interacting particles moving in a periodic external potential can only ever form uncorrelated two-particle Bloch states and yet when both physical conditions are present they can move as a 'bound pair'.

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1. Introduction

The energy spectrum of free quantum particles (obeying the Schrödinger equation) in a periodic potential is disconnected, and consists of allowed and forbidden bands; the band

gaps arise due to Bragg reflections. The existence of the bound states for repelling particles can be qualitatively explained by the fact that the Bloch spectrum of a particle moving in a periodic potential implies negative effective masses for certain wave numbers (close to zone boundaries) and such particles subject to repulsive forces can form bound states. A deeper explanation may lie in the fact that Bragg reflection actually constrains two electrons to be close even though they repel each other, provided they both have energies close to a zone boundary.

This result, a characteristic of the wave nature of matter, does not apply to classical particles. Classical waves, on the other hand, do indeed duplicate this remarkable behaviour of quantum particles; well-defined bound states (called ‘Gap modes’) of the Alfvén waves emerge in an effective repulsive potential embedded in a periodic potential created by the toroidal magnetic field geometry in tokamak plasmas [5]. Nonlinearly interacting wave motions in a periodic external background (due to magnetic geometries or rotation) are also of great interest in plasmas (drift waves) and fluids (Rossby waves). [6].

In this paper, we provide a simple (and interestingly, in principle, exact) quantum mechanical calculation demonstrating that two particles (electrons, atoms, etc.), interacting through a short-range binary repulsion, can indeed form a bound state in a given periodic potential (this work is based on an earlier unpublished report of the authors [7]). The calculation is readily seen to apply to *any pair of repelling particles*—not necessarily identical—in any external periodic potential such as those created, for example, by suitable laser fields in cold-ion traps [2]. In principle, the effect can also be expected to apply, under suitable conditions, to solitons moving in a periodic external potential provided their mutual interaction can be represented by a short-range repulsion.

Since the repulsive potential in most cases of interest will be short range (i.e., ‘Debye-screened’) Coulomb, we will call the bound state derived in this paper a ‘Coulomb pair’. We will show, that unlike phonon-mediated Cooper pairing in wave-number space, the wavefunction of the ‘Coulomb pair’ (in the centre-of-mass frame) tends to be strongly localized in position space.

Consider two particles a, b interacting with each other via a repulsive potential $V_r(|x_a - x_b|)$ in the presence of an external periodic potential $V_p(x + d) = V_p(x)$. The time-independent Schrödinger equation, describing their motion is,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x_a^2} - \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x_b^2} + [V_p(x_a) + V_p(x_b) + V_r(|x_a - x_b|)]\Psi = E\Psi(x_a, x_b). \quad (1)$$

In the absence of either V_p or V_r , this equation may be solved to yield non-square integrable solutions corresponding respectively to ‘Bloch states’ ($V_r = 0$) or ‘scattering states’ ($V_p = 0$). Thus, when the particles are non-interacting (i.e., $V_r = 0$) but moving in the periodic ‘lattice potential’, the two particle states will have—by virtue of the Bloch/Floquet theorem—a characteristic Bloch structure in the centre-of-mass coordinate $X = (x_a + x_b)/2$ and a crystal momentum wave-number K . In the relative coordinate $|x_a - x_b|$, it will essentially be a scattering state (and therefore not square integrable and having a continuum eigenvalue structure) which will be finite at infinity. When the interaction potential is repulsive, this continuum eigenfunction structure will persist even if the external periodic potential is removed and the particles move in a vacuum. In the case when the repulsive interaction and the periodic potential are simultaneously present, we demonstrate the existence of eigen solutions of the two-body Schrodinger equation with square-integrable bound states in the relative coordinate (which therefore tend to zero as $|x_a - x_b| \rightarrow \infty$ unlike scattering states) and discrete eigen values, whilst the Bloch structure persists in the centre-of mass-coordinate, as required by the periodicity of the full two-body Hamiltonian.

2. Analysis of the two-body problem in periodic potentials

For a short-ranged (e.g., screened Coulomb) repulsive potential V_r , we find that equation (1) admits solutions that are Bloch-like $\simeq e^{iKx}W(x, y)$ in the centre-of-mass coordinate $x = (x_a + x_b)/2$ [$W(x, y)$ is periodic in x with the lattice period d], and localized in the relative coordinate $y = x_a - x_b$. These eigensolutions are nondegenerate and are labelled by K , the centre-of-mass ‘wavenumber’. Thus the wavefunction $\Psi(x_a, x_b, K)$ has a characteristic energy $E(K)$. The proof applies *mutatis mutandis* to any reasonable periodic potential and to any purely repulsive potential which is sufficiently short-ranged.

In the following, $\epsilon(k, n)$ is the eigen energy. For transparency of notation we use the reduced zone scheme in which k is the reduced zone wavenumber $-\pi/d \leq k \leq \pi/d$, and n is the band index. In the rest of this paper we will use ξ as a composite symbol for k and n with $\int_{\xi} \equiv \sum_{n=1}^{\infty} \int_{-\pi/d}^{\pi/d} (dk/2\pi)$ denoting integration over the allowed bands. The total (spin plus orbital) wavefunction must be antisymmetric. Since the potentials (by assumption) are independent of spin, we may look for spin zero (singlets) or spin one (triplet) solutions. For simplicity, we discuss the singlet case, corresponding to spatially *symmetric* wavefunctions. Unless otherwise stated, in the following the label Ψ refers to the symmetric spatial orbital. This orbital wavefunction is expanded in terms of symmetrized products of one-electron Bloch states, $e^{ikx}U_k(x)$ and satisfies, when substituted in equation (1), an integral equation for the amplitude $\hat{\Psi}$.

The solution is of the form $\Psi(\hat{\xi}_a, \hat{\xi}_b) = \delta(K - k_a - k_b)F(k_a, K - k_a, n_a, n_b)$ with F satisfying

$$[E - \epsilon(\hat{\xi}_a) - \epsilon(\hat{\xi}_b)] F(k_a, n_a, n_b) = (2\pi d)^{-1} \sum_{n'_a n'_b} \int \hat{P} F(k'_a, n'_a, n'_b) dk'_a. \quad (2)$$

These spatially symmetric solutions are even in $y \equiv x_a - x_b$. The kernel \hat{P} of the equation is obtained by transforming to the centre-of-mass x and the relative coordinate y [$x_a = x + y/2$, $x_b = x - y/2$, $dx_a dx_b \equiv dx dy$], exploiting the periodicity of the Bloch functions, and using the standard identity $\sum_{n=-\infty}^{n=+\infty} \exp[in\theta] = 2\pi \delta(\theta)$ for $-\pi \leq \theta \leq \pi$:

$$P = (2\pi/d)\delta(k'_a + k'_b - k_a - k_b) \int dy V_r(|y|) \exp[-iy(k'_a - k_a)] \\ \times \int_{-d/2}^{d/2} dx \Delta(x + y/2) \Delta(x - y/2), \quad (3)$$

where $\Delta_{a(b)} \equiv [U'_k(x)U_k^*(x)]_{a(b)}$ are periodic in $x_{a(b)}$, and the double integral constitutes \hat{P} .

We simplify equation (3) (essentially equivalent to equation (1)) to elucidate the basic physics of Coulomb pair-formation by putting Bloch functions equal to unity, by modelling the repulsive potential by $V_r = V_0 d \delta(y)$ leading to $\hat{P} = V_0 d^2$, and by restricting the k integration only to the two relevant bands $n = 1, 2$. Defining new dimensionless variables $k = kd/2\pi$, $K = Kd/2\pi$ ($-1/2 \leq k, K < 1/2$), $u = k - K/2$, and remembering the constraints on k'_a integration, equation (3) leads to the integral equation/dispersion relation,

$$\frac{1}{2V_0} = \sum_{i,j} \int_0^{(1-K)/2} \frac{du}{E - \epsilon_i(u - K/2) - \epsilon_j(u + K/2)}. \quad (4)$$

This equation is clearly a generalization of Hubbard’s [2]. Given the single-particle energy spectrum (i.e. $\epsilon(k)$) and the interaction potential V_0 , this equation is readily solved

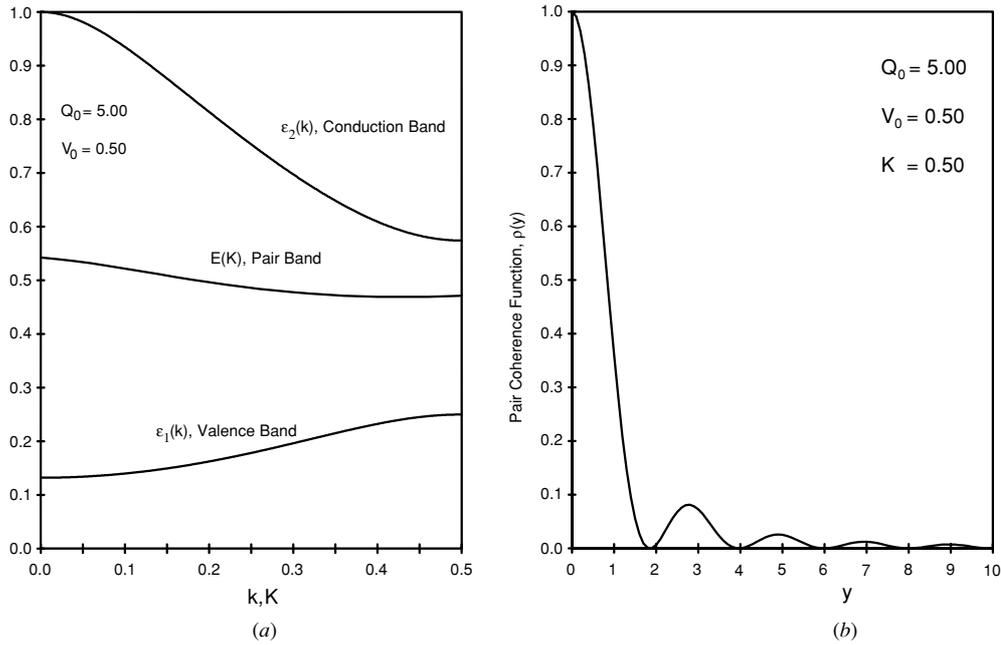


Figure 1. (a) Pair energy $E(K)$ and the Bloch energy bands for the Kronig–Penney potential, (b) Pair coherence function $\rho(y)$, see text for details.

numerically to give the energy $E(K)$ and the two-particle wavefunction in terms of the relative coordinate y . It admits, of course, various ‘scattering states’ which are not square integrable in y . We shall be more interested in the bound states. Even without solving equation (4), it is evident from the nature of the energy denominators that when E lies in the two-particle gaps caused by non overlapping Bloch band energies, the equation has nontrivial solutions which correspond to the two-particle bound states. It can be seen from elementary arguments that the pair wavefunction in this case is localized in y (i.e., $\int_{-\infty}^{+\infty} |\Psi(x, y)|^2 dy < |C|^2$).

We present as an explicit example, numerical solutions based on the one-particle dispersion relation $\cos 2\pi\epsilon^{1/2} + (\sin 2\pi\epsilon^{1/2}/2\pi\epsilon^{1/2})Q_0 = \cos 2\pi k$ corresponding to the well-known Kronig–Penney potential $V_p(x) = Q_0(\hbar^2/md) \sum_{n=-\infty}^{+\infty} \delta(x - nd)$, $Q_0 = (md/\hbar^2)Qb$, where $Q(b)$ is the strength (range) of the potential. Here we show a typical strong potential ($Q_0 = 5$) example for which the gap size is comparable to the band width. In figure 1(a), we plot the functions $\epsilon_1(k)$ (single-particle ‘valence’ band), $\epsilon_2(k)$ (single-particle ‘conduction’ band) and $E(K)$ for $V_0 = 0.5$ (a typical value when the screened Coulomb potential is approximated by a delta function). The precise location of the energy eigenvalue $E(K)$ will depend on the strength of the repulsive potential V_0 . The plot of $E(K)$ as a function of K shows: (1) that the minimum pair energy occurs at $K = 1/2$, and (2) that the pair energy for the chosen parameters has a slow K variation (high effective mass). In figure 1(b) we display a plot of the relative probability density $|\Psi(x, y)|^2/|\Psi(x, 0)|^2 = \rho(y)$ as a function of y (measured in d) for the most tightly bound $K = 1/2$ state. The probability density falls off rapidly implying a short coherence length $\xi \simeq d$, the lattice period. The pair size remains between $1 - 10d$ for all reasonable values of Q_0 and V_0 . Thus, the present pairing mechanism can operate essentially independently of any other (for example, the lattice-phonon mediated, long-range Cooper pairing for electrons in a crystalline lattice).

3. Discussion and conclusions

The main results of the preceding calculation can now be summarized: (1) in a periodic external potential, two electrons (or indeed any pair of like-charged particles, identical or otherwise) interacting through a short-ranged repulsive potential can be 'bound' to form a spin zero compound boson with a spatial extent of the order of a lattice length. For electrons in a solid lattice it will have a charge of $-2e$. This result is remarkable since neither of the two potentials can, by itself, yield states localized in the *relative* coordinate (but Bloch-like in the centre-of-mass coordinate). (2) An essential requirement for solutions of this type to exist is the disconnected nature of the single-particle energy spectrum (i.e. the existence of distinct band gaps). (3) Typically, the two-particle energy $E(K)$ is a continuous function of the lattice momentum K of the pair, and forms a band with higher energies than would be the case if both constituents had energies in the valence (i.e. lower) band. Thus these pair states possess higher energies and are 'excited' relative to the ground state of the two-particle system. This is perfectly understandable since the repulsive interaction can only ever increase the energy of a pair relative to the unperturbed system.

We believe that our calculation, firmly based as it is on wave mechanics, can provide a theoretical framework for a detailed understanding of the recent experiments of [2]. It shows that the correlation of repulsively interacting particles in periodic potentials is a characteristic of interacting waves, having little to do with spins, complicated many-body effects, second-quantization (thus the particles need not both be bosons or fermions) etc. Perhaps the simplest physical manifestation of the phenomenon under discussion is provided by the delocalized motions of paired electrons in a benzene ring structure. The predicted energy of the bound state, as well as its spatial shape and extent, could be readily compared with the experiment. It would also be of interest to consider the case of two interacting solitons in a periodic potential. This problem could be attacked numerically (and indeed experimentally) and would have interesting consequences for nonlinear optics and wave motion generally. The proof-of-principle calculation presented here suggests, and this remains to be verified by detailed numerical simulations and possibly also by experiments, that under suitable conditions, bound pairs of solitons can exist in stable (or meta stable) states and propagate together in the environment of an external periodic potential.

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