United Kingdom Atomic Energy Authority

UKAEA FUS 531

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August 2006

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

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July 17, 2006

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 wave function is labeled by a continuous centre of mass momentum. It is bounded and spatially localized in the centre of mass system. For instance, a combination of short-range (ie 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*[3] and *Hubbard* [4]). However, the phenomenon delineated here is quite 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 ([1]) and photonic lattices([2]). It has many other potentially interesting consequences even for classical interacting wave systems (e.g. solitons) propagating in a periodic background.

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, then, 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 particles with negative effective masses 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 behavior 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 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 Coulomb, we will call the bound state derived in this paper as a "Coulomb pair". We will show, that unlike phonon-mediated Cooper pairing, the wave function of the "Coulomb pair" (in the centre-of-mass frame) tends to be strongly localised 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,

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

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' ($V_p = 0$). For a short-ranged (e.g., screened Coulomb) repulsive potential V_r, we find that Eq. (1) admits solutions that are Bloch-like $\simeq e^{iKx}\,W(x,y)$ in the center 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 center-of-mass 'wavenumber'. Thus the wave function $\Psi(x_a, x_b, K)$ 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* wave functions. Unless otherwise stated, in the following the label Ψ refers to the symmetric spatial orbital. This orbital wave function is expanded in terms of symmetrized products of one-electron Bloch states, $e^{ikx}U_k(x)$ and satisfies, when substituted in Eq. (1), an integral equation for the amplitude $\hat{\Psi}$.

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

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

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 center 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 $-\pi \leq \theta \leq \pi$:

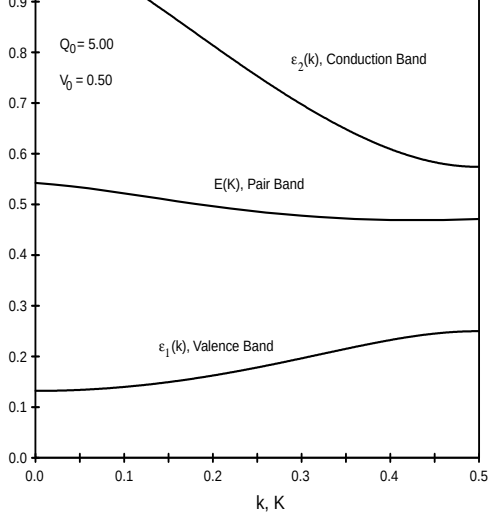
$$P = (2\pi/d)\delta(k'_a + k'_b - k_a - k_b) \int dy V_r(|y|) \exp[-iy(k'_a - k_a)] \int_{-d/2}^{d/2} dx\, \Delta(x+y/2)\Delta(x-y/2) \tag{3}$$

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 Eq.(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, Eq. (3) leads to the integral equation/dispersion relation,

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

This equation is clearly a generalisation of Hubbard's [2]. Given the single-particle energy spectrum (ie $\epsilon(k)$) and the interaction potential V_0, this equation is readily solved numerically to give the energy $E(K)$ and the two-particle wave function 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 Eq.(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 wave function in this case is localized in y (ie,$\int_{-\infty}^{+\infty} |\Psi(x, y)|^2 dy < |C|^2$).



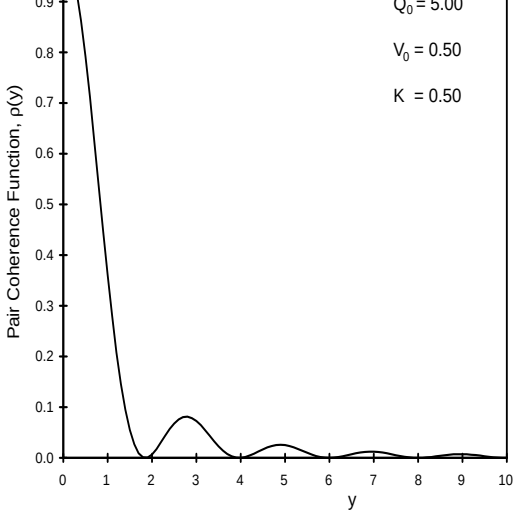


Fig. 1a: Pair energy $E(K)$ and the Bloch energy bands for the Kronig-Penney potential, Fig. 1b: Pair coherence function $\rho(y)$, see text for details.

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 $V_p(x) = Q_0(\hbar^2/md)\sum_{n=-\infty}^{n=\infty}\delta(x-nd)$, $Q_0 = (md/\hbar^2)Qb$, 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 Fig. 1a, 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 Fig. 1b 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)

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 (ie 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 and also possibly in the molecular dynamical theory of defect propagation in materials. We hypothesize 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.

Acknowledgement: One of the authors (AT) is funded by the United Kingdom Engineering and Physical Research Council (EPSRC).

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