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Research Article

Overcoming the Coulomb Barrier in Cold Fusion

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Abstract

Schwinger pointed out that under some circumstances the Coulomb barrier between paired charged particles is replaced by a correlation factor in a two-body wave function. This paper shows how having two deuterons bound within a common volume having a multiplicity of potential wells can lead to an energy-minimized Schwinger form of wave equation with wave function overlap. Relevance to a situation in which a small number of deuterium atoms is forced into a fully loaded palladium deuteride (PdD) host is discussed.

Keywords: Bloch state ions, Catalytic nuclear fusion, Coherent partitioning, Cold fusion, Ion band state theory

1. Introduction

In conventional nuclear fusion [1], the presence of a Coulomb barrier between interacting nucleons has always prevented nuclear reactions, except at high collisional energy or in the presence of negative muons. Reaction rates between deuterons are calculated by use of the Gamow factor. When the Gamow factor is applied to deuterons at condensed matter temperatures, it forces reaction rates to be much too low to be observable. Nonetheless, Julian Schwinger believed that the Gamow factor models were wrongly applied to cold fusion experiments. He stated, "In the very low energy cold fusion, one deals essentially with a single state, described by a single-wave function, all parts of which are coherent. A separation into two independent, incoherent factors is not possible, and all considerations based on such a factorization are not relevant [2]".

Energy minimization quantum mechanics can be used to model a localized charged particle pair and its response to its internal Coulomb repulsion potential. This response is normally determined by the value of λ_m/a_m, where λ_m is the DeBroglie wavelength and a_m is the Bohr radius of a particle of mass m. When $\lambda_m/a_m << 1$ the energy-minimizing

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configuration is that of adjacent, mutually incoherent single-particle wave functions prevented from significant mutual overlap by a Gamow factor. At $\lambda_m/a_m > 1$, the particles are described by a coherent 2-body wave function in which the two particles occupy a common volume of space. The Coulomb repulsion is expressed by a correlation factor that reduces the magnitude of the 2-body wave function at the overlap "point". An example of such a correlated 2-body wave function is the wave function of the spin-paired electrons of the helium atom.

As described by Seitz, the Hylleraas second approximation wave function is

$$\Phi_s = \mathrm{e}^{-\alpha s}(1 + a_1 u + b_1 |\mathbf{r}_{12}|^2),$$

where $s = |\mathbf{r}_1| + |\mathbf{r}_2|$, $t = |\mathbf{r}_1| - |\mathbf{r}_2|$, and $u = |\mathbf{r}_{12}| = |\mathbf{r}_1 - \mathbf{r}_2|$, and α, a_1 and b_1 are the constants determined by energy minimization [3,4]. $\mathbf{r}_1$ and $\mathbf{r}_2$ are the configuration coordinate position vectors that locate the electrons relative to the helium atom center of mass. The $\mathrm{e}^{-\alpha s}$ dependence is spherically symmetric, like the charge distribution around the H atom. The second factor, involving parameters t and u, modulates the 2-electron wave function and produces a downward cusp at zero separation point where t and $\mathbf{r}_{12} \to 0$ can be rewritten as

$$\Phi_s(\mathbf{r}_{\mathrm{cm}}, \mathbf{r}_{12}) = \Psi(\mathbf{r}_{\mathrm{cm}})\, g(\mathbf{r}_{\mathrm{cm}}, \mathbf{r}_{12}),$$

where $\Psi(\mathbf{r}_{\mathrm{cm}}) = \mathrm{e}^{-2\alpha|\mathbf{r}_{\mathrm{cm}}|}$ and $g(\mathbf{r}_{\mathrm{cm}}, \mathbf{r}_{12}) = \sim 1 + a_1|\mathbf{r}_{12}| + b_1|\mathbf{r}_{12}|^2$.

The $g(\mathbf{r}_{\mathrm{cm}}, \mathbf{r}_{12})$ is a correlation function which describes the anti-correlation between electrons. The amplitude of $\Phi_s(\mathbf{r}_{\mathrm{cm}}, \mathbf{r}_{12})$ decreases where $\mathbf{r}_{12} \to 0$.

Ion band state theory considers systems in which delocalized D^+ ions are embedded in a metal lattice. The dimension scale of the lattice periodicity is set by the electron Bohr radius a_e. The deuteron λ_m is about 1/4000 λ_e, where λ_e is the electron DeBroglie wave length. Since λ_m / a_e is $\sim 1/4000 << 1$, the expectation is that the Gamow factor type wave function would apply. The Schwinger statement contradicts this expectation. He implies that a system supporting cold fusion has been specially prepared so as to make the correlation form of interaction applicable at $\lambda_m/a_m = \sim 1/4000$.

This paper describes how the imposition of lattice periodic order on a D^+ 2-body wave function describing deuterons in a periodic metal lattice can prepare a system so as to satisfy the Schwinger prescription.

2. Density distributions

Function $|\Phi_s|^2$ is the normalized-to-unity density distribution of the 2-electron pair of the ground state helium atom. It is the stationary state distribution referred to in chemistry as a closed-shell orbital. $2e|\Phi_s|^2$ is the charge distribution that neutralizes the nucleus of the helium atom. A more compact electron charge distribution $2e|\Phi_{\mathrm{e,Li}}|^2$ of the same type screens the nucleus of the Li atom. The screened nucleus charge of the lithium atom forms the potential well within which the valence electron is embedded. The Li nucleus screened by $2e|\Phi_{\mathrm{e,Li}}|^2$ is called a mean field distribution in the language of condensed matter physics. The valence electron is prevented from assuming the electron density distribution $|\Phi_{\mathrm{e,Li}}|^2$ by the Pauli exclusion principle.

Figure 1a shows the charge density distribution for the pair of mutually incoherent deuterons of the D_2 molecule. Figure 1b is a similar drawing showing the charge distribution for a pair of coherently connected Bloch function deuterons as envisioned by the Ion Band State Theory [5]. The spatial distribution of a Bloch particle is defined by $|\Psi(r)|^2$, where $|\Psi(r) + \mathbf{R}_j| = |\Psi(r)|$, where $\mathbf{R}_j$ is any of N_{cell} Bravais lattice vectors identifying equivalent locations in the N_{cell} unit cells making up the occupied coherent volume. The coherent deuterons are mixed by imposition of coordinate exchange symmetry. In Fig. 1b, the pictorial representation of the exchange-symmetrized single-particle Bloch deuterons that make up the Bloch D^+ pair are assumed to have identical single-particle wave functions. The charge distribution in Fig. 1b then also describes the charge distribution of each of the single-particle Bloch deuterons.

Figure 1b drawing depicts the density distribution of surface deuterons in contact with a metal surface. The deuterons occupy a volume 1 layer thick and conform to the 2-dimensional array symmetry of the underlying metal

surface. Alternatively, the drawing serves to illustrate the density distribution of Bloch ions occupying a set of interstitial potential wells within a bulk metal crystallite. In either case the volume of the coherently occupied array is finite and measured by counting the number of occupied unit cells N_{cell}. The stationary state single-particle charge density in each potential well is $e|\Psi(r)|^2/N_{\text{cell}}$, assuming one potential well per unit cell.

In this paper the Ion Band State Theory models low-density deuterium matter as delocalized ions embedded in a metal crystallite. It is the "ion" equivalent of the electron band state theory of a metal. The term "ion" is used loosely in that it is required that the ion and the metal's neutralizing electronic charge maintain charge neutrality over the volume of each unit cell of a metal crystallite. Neutralized ions of this type are said to be "dressed". Dressed ions are ions that are fully screened within the confines of a single unit cell volume by the mobile electron medium of the metal. Consider a bulk metal containing numbers of 3-dimensional crystallite volumes separated from each other by potential barriers or by regions of lower crystalline order. Examples of such isolated ordered regions are shown in electron microscope pictures of "atom clusters" by Fujita [7]. We model sets of coherent ions confined to a bounded small local region of relatively high crystalline order. The size of a host crystallites containing a set of ion band state occupations is measured by counting the number of unit cells N_{cell} making up the ion coherence volume.

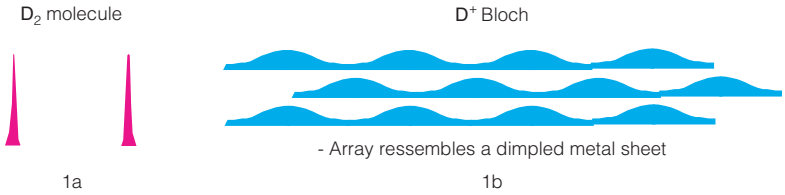

Figure 1. Toy Models: Part a shows the charge distribution of two D^+ in separated potential wells within a molecule's electron cloud. The deuterons are mutually incoherent. The Leggett and Baym modeling [6] has incoherence of this type. Part b shows a single Bloch D^+ in an array of potential wells provided by a metal crystal. Neutralization is provided by the metal's mobile electrons. Localized charge maxima are coherently coupled so that the sum over N_{cell} unit cells is a single delocalized deuteron. Part b can also depict the center-of-mass charge distribution of two Bloch D^+ ions coherently coupled by coordinate exchange, and also of a quasiparticle pairing of Bloch deuterons in a many-body D^+ Bloch system. The array of charge maxima is used to illustrate both a D^+ charge distribution having 3-dimensional periodic symmetry inside a metal, and a D^+ charge distribution inside an interface layer resting on metal surface having 2-dimensional periodic symmetry.

3. 2-Body Bloch function physics

The appropriateness of Fig. 2b Bloch function configuration is determined by energy minimization. Consider the effect of periodic symmetry on the behavior of a coherent many-body D^+ ion system in which a low number-density set of deuterons is subjected to an imposed periodic potential. Consider N_{D} deuterons inside a small crystal consisting of N_{cell} identical unit cells where $N_{\text{D}}/N_{\text{cell}} << 1$. An example would be 100 deuterons in a crystal made up 10^6 unit cells. Such a system is composed of bosons of mass m_{D} and charge e, where m_{D} is the deuteron mass and e is the deuteron charge. The N_{D} deuterons are indistinguishable particles described by single-particle Bloch wave functions $\Psi(\mathbf{r}, \mathbf{k})$ such that $|\Psi(\mathbf{r} + \mathbf{R}_n, \mathbf{k})| = |\Psi(\mathbf{r}, \mathbf{k})|$, where $\mathbf{k}$ is a wave vector quantum index and where the $\mathbf{R}_n$ is a set of N_{cell} distinct Bravais lattice vectors. Each of the set of $\Psi(\mathbf{r}, \mathbf{k})$ has a distribution within physical space $\{\mathbf{r}\}$ with an identical local density maximum in each of the N_{cell} identical unit cells. The energies of the $\Psi(\mathbf{r}, \mathbf{k})$ can be different, but because the D^+ are bosons, they can all be the same. Members of the Bloch D^+ set are allowed to have somewhat different spatial distributions.

The above system is described by a many-body wave function with coordinate exchange. Exchange replaces the N_D single-particle wave functions with N_D single-quasiparticle wave functions described by N_D Bloch functions. Because of exchange symmetry the quasiparticle states are coordinate-entangled. This means that the phase difference between a given pair of quasiparticles remains constant and independent of $\mathbf{r}$. In our treatment of the many-body description we consider only the set of 2-quasiparticle entanglements, one for each of the $N_b(N_b-1)/2$ distinct quasiparticle pairs. A full many-body treatment of the system would include the entanglements between sets of three quasiparticles, sets of four quasiparticles, etc. in addition to the set of paired quasiparticles considered here.

The standard protocol for constructing 2-particle wave functions is to start with a product of single-particle wave functions. This form of wave function gives the correct behavior for particle pairs with no self-interaction [8]. The single-particle wave functions are solutions of a Schrodinger equation. The solutions obtained customarily fit Born Von Karman periodic boundary conditions that do not properly match the box-like boundary that encloses a crystallite volume. In practice this procedure gives useful wave functions when applied to not-too-small lattice volumes. Finite cluster and thin-film calculations involving 3d and 4d metal atoms have shown that the resulting wave functions provide a good description of an embedded system provided that the host bulk-like crystal periodic environment has dimensions more that a few unit cells in depth.

For a periodic potential of the form $U(\mathbf{r}+\mathbf{R}_n)=U(\mathbf{r})$, the eigenstate wave functions are Bloch functions $\Psi(\mathbf{r})$ having "Bloch" symmetry as described by $|\Psi(\mathbf{r}+\mathbf{R}_n)|=|\Psi(\mathbf{r})|$. The simplest 2-body wave function $\Psi(\mathbf{r}_1,\mathbf{r}_2)$ is

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\Psi_1(\mathbf{r}_1)\Psi_2(\mathbf{r}_2), \tag{1}$$

where $\Psi_1(\mathbf{r}_1)$ and $\Psi_2(\mathbf{r}_2)$ are single-particle (or single-quasiparticle) Bloch functions and $\mathbf{r}_1$ and $\mathbf{r}_2$ are the physical positions of particles 1 and 2 in the metal lattice. The $\mathbf{r}_1$ and $\mathbf{r}_2$ are configuration coordinate vectors. Atomic physics has shown that this simple form of 2-body wave function is suitable only for modeling distinguishable, mutually incoherent particles 1 and 2. Neglecting the effects of spin, if the particles are indistinguishable and in the same state, the allowed 2-body wave function must have coordinate exchange symmetry, which is symmetric for bosons and suitably paired fermions, and is anti-symmetric for single fermions. Bosons and spin-paired fermions are symmetrized by applying the symmetric coordinate exchange symmetry constraint.

In the Ion Band State Theory, Ψ_1 and Ψ_2 are assumed to be independent Bloch functions and $\mathbf{r}_1$ and $\mathbf{r}_2$ refer to positions $\mathbf{r}$ in the lattice. Functions $\Psi_1(\mathbf{r})$ and $\Psi_2(\mathbf{r})$ have the symmetries:

$$|\Psi_1(\mathbf{r}_1+\mathbf{R}_{1_n})|=|\Psi_1(\mathbf{r}_2)| \quad \text{and} \quad |\Psi_2(\mathbf{r}_2+\mathbf{R}_{2_m})|=|\Psi_2(\mathbf{r}_2)|,$$

where $\mathbf{R}_{1_n}$ and $\mathbf{R}_{2_m}$ are independent Bravais lattice vectors. The 2-body wave function $\Psi(\mathbf{r}_1,\mathbf{r}_2)$ has the dual symmetry

$$|\Psi[(\mathbf{r}_1+\mathbf{R}_{1_n}),\mathbf{r}_2]|=|\Psi(\mathbf{r}_1,\mathbf{r}_2)| \quad \text{and} \quad |\Psi[\mathbf{r}_1,(\mathbf{r}_2+\mathbf{R}_{2_m})]|=|\Psi(\mathbf{r}_1,\mathbf{r}_2)|$$

for all positions $\mathbf{r}$ in the lattice, including the center-of-mass position $\mathbf{r}=\mathbf{r}_{cm}=(\mathbf{r}_1+\mathbf{r}_2)/2$.

4. The double Bloch function self-interaction picture

In order to quantify the point-particle aspect of the Coulombic self-interaction in a 2-body system, it is necessary to express the wave function in terms of center-of mass, separation coordinates, where $\mathbf{r}_{cm}=(\mathbf{r}_1+\mathbf{r}_2)/2$ and $\mathbf{r}_{12}=\mathbf{r}_1-\mathbf{r}_2$. One then seeks 2-body wave function solutions of the appropriate wave equation in terms of separable functions $\Psi(\mathbf{r}_{cm})$ and $g(\mathbf{r}_{12})$. Since $\Psi(\mathbf{r}_1,\mathbf{r}_2)$ is Bloch symmetric with respect to both $\mathbf{r}_1$ and $\mathbf{r}_2$, it is also Bloch symmetric in terms of $\mathbf{r}_{cm}$. The interesting question is the behavior of $\Psi(\mathbf{r}_1,\mathbf{r}_2)$ when $\mathbf{R}_{1_n}$ varies independently of $\mathbf{R}_{2_m}$. The assumption of independent lattice vectors means that $\mathbf{R}_{1_n}-\mathbf{R}_{2_m}=\mathbf{R}_{12_j}$ is also a Bravais lattice vector. This assumption makes $\Psi(\mathbf{r}_1,\mathbf{r}_2)$ Bloch symmetric with respect to both $\mathbf{r}_{12}$ and $\mathbf{r}_{cm}$.

The Schrodinger-like wave equation describing two interacting band state deuterons in a periodic lattice of N_{cell} unit cells is a six degree-of-freedom equation in center-of-mass,separation space. We examine solutions to Eq. (2) of the form

$$\Phi(\mathbf{r}_{\text{cm}}, \mathbf{r}_{12}) = \Psi(\mathbf{r}_{\text{cm}}) g(\mathbf{r}_{12}), \tag{2}$$

where $|\Psi(\mathbf{r}_{\text{cm}}+\mathbf{R}_{\text{cm}})| = |\Psi(\mathbf{r}_{\text{cm}})|$ with $\mathbf{R}_{\text{cm}} = (\mathbf{R}_{1_n}+\mathbf{R}_{2_m})/2$ and $|g(\mathbf{r}_{12}+\mathbf{R}_{12})| = |g(\mathbf{r}_{12})|$ with $\mathbf{R}_{12} = \mathbf{R}_{1_n}-\mathbf{R}_{2_m} \neq 0$ except in one unit cell.

Here $\mathbf{R}_{\text{cm}}$ is a Bravais lattice vector in physical space $\{\mathbf{r}_{\text{cm}}\}$ and $\mathbf{R}_{12}$ is a Bravais lattice vector in separation parameter space $\{\mathbf{r}_{12}\}$. This resulting symmetry is called "double Bloch symmetry". We determine the conditions for which this form of wave function minimizes system energy.

The 2-body wave equation can be separated into two wave equations:

$$\int^{\text{D}^+ \text{ Coherent Vol}} \Psi^*(\mathbf{r}_{\text{cm}}) \left\{ -\frac{\hbar^2}{4m_{\text{D}}} \nabla_{\text{cm}^2} + (2e) U_{\text{lattice}}(\mathbf{r}_{\text{cm}}) \right\} \Psi(\mathbf{r}_{\text{cm}})\, \text{d}^3\mathbf{r}_{\text{cm}} = E_{\text{ext}} \Psi(\mathbf{r}_{\text{cm}}) \tag{3}$$

and

$$\int^{\mathbf{r}_{12} \text{ lattice}} \left\{ -\frac{\hbar^2}{2m_{\text{D}}} \nabla_{12}^2 + \sum_{\substack{j=1 \\ \text{coherent} \\ \text{volume}}}^{N_{\text{cell}}} e^2/(N_{\text{cell}}|(\mathbf{r}_{12} + \mathbf{R}_{12_j})|) \right\} g(\mathbf{r}_{12})\, \text{d}^3\mathbf{r}_{12} = E_{\text{int}}\, g(\mathbf{r}_{12}). \tag{4}$$

The first term in Eq. (3) describes the center-of-mass kinetic energy density of a double deuteron, i.e., a mass-4, charge-2 exchange-symmetrized Bloch quasiparticle, coherently delocalized over N_{cell} unit cells of center-of-mass space. Center-of-mass space $\{\mathbf{r}_{\text{cm}}\}$ is also metal lattice space $\{\mathbf{r}\}$. The second term describes the potential energy of a mass-4, charge-2 exchange-symmetrized Bloch quasiparticle over N_{cell} unit cells of metal lattice space. This potential energy is periodic in physical space. The first term in Eq. (4) describes the kinetic energy density of internal motion of the double deuteron particle over the N_{cell} unit cells of separation space, which is an internal coordinate space associated with the difference in positions of two interacting deuterium nuclei. The second term in Eq. (4) is actually a sum over terms, as shown in Eq. (4). This sum of terms is a function that is well-defined near its singular points, where it describes the $e^2/|r_{12}|$ singular potential of the partitioned double-deuteron's dressed Coulombic self-interaction. Position vector $\mathbf{r}_{\text{cm}}$ ranges over N_{cell} unit cells of $\{\mathbf{r}_{\text{cm}}\}$, and separation vector $\mathbf{r}_{12}$ ranges over N_{cell} unit cells of $\{\mathbf{r}_{12}\}$. $\mathbf{R}_{12_j}$ is a set of N_{cell} Bravais lattice vectors locating equivalent points in $\{\mathbf{r}_{12}\}$.

Figure 2 shows a sketch of a possible $\Psi(\mathbf{r}_{\text{cm}}, \mathbf{r}_{12})$. Wave function factor $\Psi(\mathbf{r}_{\text{cm}})$ shows a density maximum within each of N_{cell} equivalent potential wells provided by lattice potential U_{lattice}. Wave function factor $g(\mathbf{r}_{12})$ causes $|\Psi(\mathbf{r}_{\text{cm}}, \mathbf{r}_{12})|$ to have a local minimum at each $\mathbf{r}_{12} + \mathbf{R}_{12_j} = 0$ point in separation space (i.e., at $\mathbf{r}_{12} = 0$ modulo $\mathbf{R}_{12_j}$). The functional form of $g(\mathbf{r}_{12})$ is that of a near constant amplitude function reduced periodically by a set of N_{cell} cusps. At each cusp point in wave equation (4), a singularity in the partitioned Coulomb self-interaction is cancelled by a singularity in the internal kinetic energy established by a discontinuity in the momentum $(i\hbar/m)\nabla_{12}\, g(\mathbf{r}_{12})$. If the mean value of $g(\mathbf{r}_{12})$ is a and the cusp depth is b, then $(a - b)/a$ is a measure of the degree of D^+D^+ wave function overlap.

5. Energy-minimization

Equation (2) describes band state ions in a metal lattice where a fermi sea of electrons is present that provides ion screening sufficient to guarantee charge neutrality in each unit cell. The electron screening requirement means that the

$e^2/|r_{12}|$ form of the Coulombic interaction shown in Eq. (4) is valid only well inside a screening volume V_{sc}, which is smaller than the volume of the unit cell.

We examine an energy-minimized form of $\Phi(\mathbf{r}_{cm}, \mathbf{r}_{12})$ at large N_{cell} with electron screening included. Energy minimization of Eqs. (3) and (4) proceeds independently. The energy minimized form of Eq. (3) is that of a charge-2, mass-4 double-deuteron in the lattice field $U_{lattice}(\mathbf{r})$. To obtain an energy minimized solution to Eq. (4), we start with a set of trial correlation functions $g(\mathbf{r}_{12})$. Here Hylleraas provides guidance in his approximate solutions for the 2-electron wave function of the helium ground state atom. In analogy to the simplest Hylleraas approximation, we choose a periodic form of Hylleraas-like trial functions $g(\mathbf{r}_{12})$ which meets the lattice requirement for periodic symmetry, namely

$$\begin{aligned} g(\mathbf{r}_{12}) &= A[1 + b\sin(\pi|\mathbf{r}_{12}|/4r_{sc})]/(1+b), && |\mathbf{r}_{12}| < 2r_{sc}, \\ g(\mathbf{r}_{12}) &= g(2r_{sc})A, && |\mathbf{r}_{12}| > 2r_{sc}, \end{aligned} \tag{5}$$

where A is a normalizing constant, b is the depth of the assumed cusp, and r_{sc} is a screening radius beyond which the Coulomb repulsion force between the coupled dressed deuterons is not felt. In the energy minimization process using Eq. (4), N_{cell} is kept fixed and various values of b are chosen so as to minimize the sum of internal potential energy E_{pot} and internal kinetic energy E_{ke}. The normalizing constant A for $g(\mathbf{r}_{12})$ is calculated to be

$$A = \{[1/(1-2b)]^{1/2}\}/(N_{cell}V_{cell}) + O(b^2, r_{sc}^3/V_{cell})$$

with b and r_{sc}^3/V_{cell} treated as small quantities.

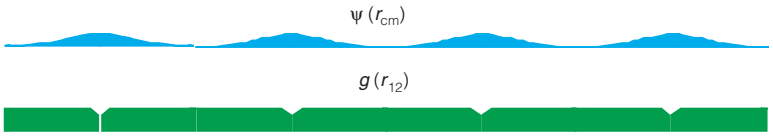

Figure 2. Toy Model. Factor $e|\Psi(\mathbf{r}_{cm})|^2$ measures the charge distribution of 2-D^+_{Bloch} in center-of-mass space $\{\mathbf{r}_{cm}\}$, which is also lattice space. The density distribution is the same array as differently depicted in Fig. 1 b. $g(\mathbf{r}_{12})$ is a Bloch wave function in separation space $\{\mathbf{r}_{12}\}$. It is normalized to a mean value = 1, so as to appear as a correlation function in the 2-body wave function $\Psi(\mathbf{r}_{cm}, \mathbf{r}_{12})$ describing a 2-D^+ Bloch pair. The deuterons are anti-correlated in the sense that the amplitude of $\Psi(\mathbf{r}_{cm}, \mathbf{r}_{12})$ decreases as $\mathbf{r}_{12} \to 0$ modulo $\mathbf{R}_{12_j}$, where $\mathbf{R}_{12_j}$ is a lattice vector in $\{\mathbf{r}_{12}\}$.

6. Cusp depth vs. N_{cell}

The above process determines the value of N_{cell} that minimizes system energy for suitable pre-selected values of b and r_{sc}. We are concerned with the behavior of E_{ke} and E_{pot} at large N_{cell}, for which the value of b that minimizes total energy is much less than 1. How are the $g(\mathbf{r}_{12})$ dependencies of E_{ke} and E_{pot} affected by N_{cell}? In the limit that $b \to 0$, one finds that $A \to 1/(N_{cell}V_{cell})$ and the integrand of the potential energy term $\to (1-2b)\{1+2b\sin(\pi|\mathbf{r}_{12}|/(4r_{sc}))\}$. Then, in the integration of $\mathbf{r}_{12}$ over the N_{cell} unit cells in $\{\mathbf{r}_{12}\}$, we find that

$$E_{ke}(g) = 2\pi(\pi^2/6 - 1)e^2 m_e a_e r_{sc} b^2/(m_D N_{cell} V_{cell}), \tag{6a}$$

where a_e is the electron Bohr radius. Similarly, we find, after integrating over $\mathbf{r}_{12}$, that

$$E_{pot}(g) = -(128/\pi)(\pi^2/8 - 1)r_{sc}\, e^2 b/(N_{cell}^2 V_{cell}). \tag{6b}$$

Evaluating Eq. (8) for an assumed test case, we take $V_{\text{cell}} = 16\,\text{Å}^3$ and $r_{sc} = 0.156\,\text{Å} = 0.1\times$ Wigner Seitz radius. Then

$$E_{\text{ke}}(g) = 0.82 \times 10^{-4} b^2/N_{\text{cell}}\,\text{eV},$$
$$E_{\text{pot}}(g) = -0.224 b/N_{\text{cell}}^2\,\text{eV}.$$

The energy minimizing condition $-\delta E_{\text{pot}}(g)/\delta b = \delta E_{\text{ke}}(g)/\delta b$, occurs at

$$N_{\text{cell}} = (m_{\text{D}}/m_{\text{e}})(r_{sc}/a_{\text{e}})32/\pi^2)[(\pi^2/8-1)/(\pi^2/6-1)](1/b) \quad (7)$$
$$= 0.59(m_{\text{D}}/m_{\text{e}})(r_{sc}/a_0)(1/b).$$

The energy minimizing condition is $N_{\text{cell}} = 6.83 \times 10^2/b$. More than ~90% dd overlap exists at $N_{\text{cell}} \geq 6.8 \times 10^3$, since $b < 0.1$.

Equation (7) shows how cusp amplitude b increases with decreasing N_{cell}. Figure 3 depicts $g(\mathbf{r}_{12})$ at three values of N_{cell}. When b becomes large enough that $g(\mathbf{r}_{12}) \to 0$ at $\mathbf{r}_{12} = 0$ modulo $\mathbf{R}_{12_j}$, the double Bloch wave function model becomes unphysical. Then $\Phi(\mathbf{r}_{\text{cm}}, \mathbf{r}_{12})$ reverts to the molecular form shown in Fig. 1a, and the two D^+ become mutually incoherent. The smallest N_{cell} supporting the Schwinger form of wave equation is designated $N_{\text{cell,critical}}$.

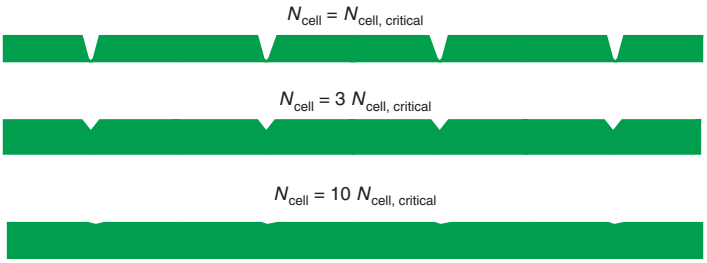

Figure 3. Toy Models. Correlation functions $g(\mathbf{r}_{12})$ are shown for three values of N_{cell}. The cusp depth becomes deeper with decreasing N_{cell}. At $N_{\text{cell,critical}}$ the values of $g(\mathbf{r}_{12}) \to 0$ at each $\mathbf{r}_{12} = 0$ modulo $\mathbf{R}_{12_j}$.

7. QM protocol, Wannier states, boundary conditions, and fluctuations

Wave equation,wave function quantum mechanics is a protocol that permits calculation of stationary states and associated energies for a defined environment. To match reality, various symmetry constraints must be applied so as to restrict the set of allowed wave functions. Many-body wave functions must comply with the Pauli exclusion principle and coordinate exchange symmetry. If the self-interaction between members of a coherent pair is to be modeled, the protocol must make use of a transformation from configuration coordinates to center-of-mass,separation coordinates. There has been an ambiguity in the rules governing this transformation. This paper tests the case where that the transformation expresses double Bloch symmetry.

The assumption that Double Bloch symmetry applies is supported by arguments based on using a Wannier states representation of a stationary state Bloch function [9]. A single-particle Bloch state is expressed as a sum over transiently occupied Wannier states, in each of which a whole particle occupies a single potential well for an unspecified time. A single Wannier state is not a stationary state and breaks periodic symmetry. The Bloch stationary state equals the symmetric sum over all the single-particle Bloch states, in accord with Anderson's symmetry principle [10]. When

two deuterons occupy a set of Wannier states, each deuteron is randomly placed in one of the N_{cell} unit cells. There is a $1/N_{\text{cell}}$ chance that both deuterons will end up in the same unit cell. Since there is no contribution to the Coulomb repulsion potential when the dressed deuterons are in different cells, the effective strength of the Coulomb repulsion is $e^2/(|r_{12}|N_{\text{cell}})$, as deduced by summing over the N_{cell} unit cells. This repulsion potential is the same as calculated using a double Bloch symmetry 2-body wave function.

The time-independent correlation functions $g(\mathbf{r}_{12})$ shown in Fig. 2 have discontinuities in momentum at N_{cell} cusp points in $\{\mathbf{r}_{12}\}$. At each of these points, the kinetic energy $\rightarrow \infty$ at a rate that exactly cancels the singularity in potential energy $e^2/(|\mathbf{r}_{12}|N_{\text{cell}})$. The magnitude and number of momentum discontinuities at the N_{cell} discontinuities is a boundary condition imposed on the 2-body wave function. The boundary condition in $\{\mathbf{r}_{12}\}$ complements the boundary conditions in $\{\mathbf{r}_{\text{cm}}\}$, which define the deuteron containment volume and the multiplicity and shape of potential wells in $\{\mathbf{r}_{\text{cm}}\}$.

In the Bloch picture, the fraction of charge located within any single unit cell is not a precisely measurable quantity. It is subject to quantum fluctuations about an expectation value. This behavior is the same as that described by Greiner *et al.* [11] for a low density set of Bose atoms in an optical lattice. Coordinate-entangled dressed deuterons in a metal lattice may share some properties with Bose atom condensates in an optical lattice.

8. Relevance to cold fusion

It has been widely assumed that the conventional picture of a "Coulomb Barrier", as formulated in scattering theory, should be relevant to Pons and Fleischmann "Cold Fusion". However, we now know that the Pons and Fleischmann claims do not mimic conventional fusion. Cold fusion reactions are not a result of the kinetic collision between two deuterons, and do not involve asymptotic plane wave scattering theory, such as leads to Gamow factors [8]. Instead it involves perturbative interactions between nuclear states formed from protons, neutrons, and resonant groupings thereof, like alpha particles and di-neutrons, as modeled by Wheeler [12]. The interactions between these nuclear components involve continuous potentials that are defined over the full range of distance scales, from subnuclear, through nuclear, through atomic, through the macroscopic dimension scales of metal crystals. Although the nuclear force potentials are confined to nuclear dimension, the electromagnetic interaction potential extends over the full range of length scales where interaction can occur. Furthermore, wave function coherence, expressed as an ordering of wave function phases over macroscopic distances, must be applied to the wave functions of the interacting nuclei.

Cold fusion viewed as a variant of $D^+ + D^+ \rightarrow {}^4He^{++} + \gamma$ takes place without radiation. It occurs rarely because the initial state D's are required to "be prepared" and "entangled" in a particular way. When additional D atoms are forced into a fully loaded PdD lattice, appreciable $D^+ - D^+$ overlap can occur at many different locations, simultaneously, without appreciable D^+ charge accumulation at any particular location. [13] These delocalized deuterons are "Bloch state" deuterons. At large $\mathbf{r}$ their asymptotic form is a Bloch function and not a plane wave. Although this paper does not explicitly deal with problems associated with energy release and dissipation, the Bloch wave function form provides a useful picture for understanding how, in a periodic solid, the conventional "Coulomb Barrier" can be altered through long-range coherence in a way that potentially leads to nuclear reaction [13,14]. The model accomplishes this by replacing the problem of "Overcoming the Coulomb Barrier" with an alternative energy minimization problem.

References

[1] Footnote: The conventional dd fusion reactions (d + d $\rightarrow {}^3$H + p and d + d ^{3}He + n) are computed using Gamow factors.
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