

The Ion Band State Theory

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Abstract

We have previously explained¹⁻³ how the occupation of ion band states by hydrogen (H) and deuterium (D) in palladium deuteride PdD and possibly Ni can result in radiationless fusion. The explanation includes a number of assumptions about the governing conditions associated with the process. As a consequence of these assumptions we predicted¹⁻³ important excess heat phenomena (loading requirements, by-products, etc.) of Cold Fusion (CF) that were subsequently observed^{4,5}. Although the governing ideas are based on mainstream solid state physics ideas, the underlying theory "seems" to have "evaded" a number of potential problems that have bothered many people concerning CF. As we have explained recently^{6,7}, as a result of these solid state physics effects, discontinuous changes in momentum and singularities in the effective kinetic energies associated with H or D that may occur through the occupation of ion band states provide a means for eliminating the phenomena that seemingly are omitted by the theory. In this paper we clarify the origin of these effects and their relationship to questions that have been raised associated with our treatment of the Coulomb barrier.

1. Introduction

The ion band state theory of radiationless fusion, which is based on mainstream many-body physics of the solid state, "seems" to have "evaded" a number of potential problems that have bothered many people concerning CF. An important reason for this is that the theory is based on the conventional assumption of solid state physics that all of the charged particles in the problem are forced to occupy a finite volume of space. As a consequence, the particles are bound to the solid, and the rules of bound (as opposed to unbound) state quantum mechanics apply. Important consequences of this fact include the possibility of discontinuous changes in momentum (through wave function cusps, for example) at points where electrostatic repulsion or attraction becomes infinite. Immediate consequences of this result include the possibility of large variations in deBroglie wavelength over small spatial domains (since the momentum may become discontinuous), significant particle-particle overlap at isolated locations by same charge charged particles, and the breakdown of the rules and underlying mathematics of conventional Gamow tunneling theory.

The paper explains, using a concrete example, the solid state physics rationale for dealing with the Coulomb barrier, based on energy minimization, in the particular context in which ion band state occupations may occur. Because in a realistic solid periodic symmetry plays an important role in defining kinetic energy in ion band states, and because electron screening requires that all ions be neutralized not only within each unit cell but effectively outside a small screening volume, in such a situation, in determining the

minimum energy of potentially interacting ion band state (IBS) deuterons (D^+), the Coulomb repulsion between two IBS D^+ 's is altered by the crystalline environment. In particular this repulsion is reduced by a factor $1/N_{\text{cell}}$, where N_{cell} = the total number of unit cells within the crystal.

A second important point brought out in the paper is that the underlying symmetry that results from periodic order, which is responsible for this dependence on crystal size, also plays a pivotal role in defining the potential avenues for reaction, once IBS D 's overlap. In particular, in any potential nuclear reaction, the potential stable channels for reaction are directly coupled to the requirement that periodic symmetry be maintained. This leads to the additional requirements that predominantly only ground state to ground state nuclear transitions be allowed in which the location of each initial or final state nucleus is described by an ion band state, and that potential reaction products be released in regions outside periodically ordered domains (for example at cracks, interfaces and surfaces of heat-producing crystals). These requirements also explain why high energy particles are not released and can be used in a self-consistent manner to explain a number of materials preparation procedures: e.g. the choice of host material, loading requirements, the choices of crystal size, and the role of temperature in the generation of excess heat.

2. Mainstream Physics

The ion band state theory of radiationless fusion is based on mainstream many-body physics. Experimental/theoretical support for the theory is provided by Puska et al.⁸ and Astaldi et al.⁹, where it is have shown that the excited surface states of H and D on Ni and Cu are ion band states. In *Nature* magazine Nieminen states that "What is good enough of electrons is good enough for protons, their chemical counterparts 2000 times more massive"¹⁰. Cassella¹¹ invokes 3-dimensional band states to explain neutron scattering results in $NbH_{0.03}$.

There is a thermodynamics rationale¹² for populating ion band states in PdD_x as $x \rightarrow 1$. A major component of system chemical potential is lattice strain energy¹³. Ideally, when an ordered compound such as low temperature PdD is forced to take on additional D, the added D must either force a localized expansion of the lattice or go into a band state. Forcing a localized lattice expansion is a highly endothermic process. Thus ion band state occupation is thermodynamically favored over a range of δ in $PdD_{1+\delta}$ at low temperature. However, too large a value of δ increases the energy level of the band state, which can lead to a two phase PdD + $Pd_3(\text{vacancy})D_4$ superlattice¹⁴. At ambient temperature, occupation of ion band states can be expected at values of x somewhat less than 1.

3. How Band States Form

One experimental situation that leads to band state occupation in PdD_x is illustrated schematically in Fig. 1. Fig. 1 is a 1-dimensional pictorial representation of the Pd lattice in which the valleys represent the octahedral sites for interstitial D atoms and the hills are the saddle points separating the stable locations. The figure illustrates conditions presumed to exist after prolonged electrolysis has created a polarized surface passivation barrier through which D^+ ions have been plated so as to raise the D chemical potential of the electrode. The figure shows ~90% of the interstitial sites occupied by localized "chemical" D occupations. However, at the above-equilibrium chemical potential it is postulated that a small 10^{-6} - 10^{-4} fraction (= the value of δ in $PdD_{1+\delta}$) of the ions are excited to higher energy states that are able to rapidly tunnel through the saddle points that separate locally confining potential wells. The ions then see the lattice as a whole. The new boundary conditions enable the ions to assume lattice symmetry. They become band state ions. The

ion band state theory says that radiationless fusion involves only interactions between band state ions, i.e.. none of the chemical interstitials or lattice ions serve as nuclear reactants or products.

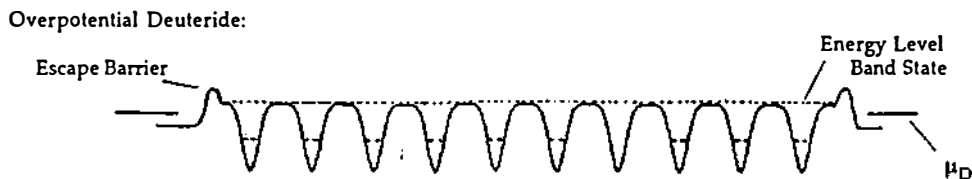


Fig. 1 Representation of PdD_x under conditions that enable D⁺ band state occupation.

4. Unbroken Lattice Symmetry

Why does being in a band state make a difference? One answer is found in the insights of P. W. Anderson¹⁵. Anderson presents a hierarchy of scientific disciplines, with each discipline distinguished by the physical laws or processes that play a major role within the discipline. In solid state, many-body physics, the important processes are dominated by a requirement of periodic order (unbroken lattice symmetry). In contrast, in all chemical processes within a solid, lattice symmetry is broken. Reactions between band state ions are governed by unbroken lattice symmetry. We now show how his principle when combined with electron screening leads to a reduced Coulomb barrier to fusion.

5: The Coulomb Barrier in Bound Systems

To understand how being in a band state can affect the Coulomb barrier, it is first necessary to understand how the Coulomb barrier is expressed in confined particle systems. By a confined-particle system we mean a system in which the particles are bound by having negative energy, i.e. they cannot escape to ∞ . Such systems are described by wave functions ψ such that $\psi \rightarrow 0$ as $r \rightarrow \infty$. The physics of the Coulomb barrier problem is contained in the 2-particle problem, as discussed below.

Consider the 2-ion-in-a-crystal problem. The stationary state wave equation is

$$\{-\hbar^2/2m [\nabla_1^2 + \nabla_2^2] + e^2/r_{12} + V_{\text{lattice}}(\mathbf{r}_1, \mathbf{r}_2)\} \Phi(\mathbf{r}_1, \mathbf{r}_2) = E \Phi(\mathbf{r}_1, \mathbf{r}_2) \quad (1)$$

where $\phi(\mathbf{r}_1, \mathbf{r}_2)$ is a 2-ion wave equation in 6 variables $x_1, y_1, z_1, x_2, y_2, z_2$, and the derived variable $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ = separation between ions. We have assumed no electron screening. To study the barrier problem it is necessary to change coordinates to $\mathbf{r}_{\text{cm}} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. When it is assumed that the electrostatic interaction between the lattice and the center of mass motion of each pair is very different than the comparable ion-ion electrostatic interaction $V_{\text{lattice}}(\mathbf{r}_1, \mathbf{r}_2) \approx V'_{\text{lattice}}((\mathbf{r}_1 + \mathbf{r}_2)/2)$. (For metals in which screening lengths are considerably less than the lattice spacing, this is a good approximation) Then, it is permissible to write $\phi(\mathbf{r}_1, \mathbf{r}_2) = \Psi(\mathbf{r}_{\text{cm}}) g(r_{12})$, and Eq. 1 becomes

$$\{-\hbar^2/2m [1/2 \nabla_{\mathbf{r}_{\text{cm}}}^2 + 2 \nabla_{r_{12}}^2] + e^2/r_{12} + V'_{\text{lattice}}\} \Psi(\mathbf{r}_{\text{cm}}) g(r_{12}) = E \Psi(\mathbf{r}_{\text{cm}}) g(r_{12}) \quad (2)$$

Here, $\Psi(\mathbf{r}_{cm})$ defines an amplitude at each point in the crystal and $g(r_{12})$ is a "dimming" function which decreases the amplitude of $\Psi(\mathbf{r}_{cm})$ as $r_{12} \rightarrow 0$. \mathbf{r}_{cm} and r_{12} are independent degrees of freedom. With suitable normalization $g(r_{12})$ can have values between 0 and 1. If $g(r_{12}) \rightarrow 0$ as $r_{12} \rightarrow 0$, there is a total Coulomb barrier against ion-ion overlap, which precludes nuclear reaction. If $g(r_{12})$ remains finite as $r_{12} \rightarrow 0$, then wave function overlap exists and fusion is allowed.

The role of the dimming function in determining overlap is illustrated by the well-known two-electron solution of the helium atom¹⁶. In Fig. 2 we show how the amplitude of the 2-electron wave function varies as $r_{12} \rightarrow 0$. Fig. 2 shows the case where both electrons are equidistant from the He nucleus. When the electrons are on opposite sides of the nucleus, $\Theta = 180^\circ$ or -180° and $g(r_{12}) = 1$. When the electrons are on top of each other, $\Theta = 0^\circ$ and $r_{12} = 0$. $g(r_{12})$ then has its minimum value. Since $g(r_{12}) \neq 0$, there is finite wave function overlap. If the electrons had the nuclear property of deuterons, they would fuse.

6. Cusp Condition

Fig 2 also illustrates an important property of charged point particles. The r_{12} dependency of the 2-particle wave function has a cusp at $r_{12} = 0$. The helium atom wave function (assuming infinite nuclear mass) is

$$\left\{ -\frac{\hbar^2}{2m_e} [\nabla_1^2 + \nabla_2^2] + \frac{e^2}{r_{12}} + V_{\text{central field}} \right\} \Phi(\mathbf{r}_1, \mathbf{r}_2) = E \Phi(\mathbf{r}_1, \mathbf{r}_2). \quad (3)$$

The singularity of e^2/r_{12} at $r_{12} = 0$ must be canceled by a singularity in the kinetic energy term if the equation is to be bounded, as required by the right hand side. This requires that

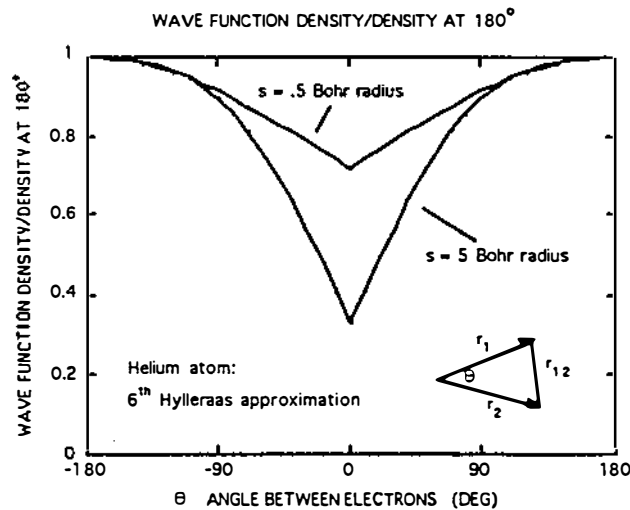


Fig. 2 Amplitude of helium ground state 2-electron wave function on the surfaces of 2 spheres for which $s = \text{constant}$. Values have been normalized with respect to the peak values, which occur when the 2 electrons are on opposite sides of the nucleus. Nature uses a cusp at $r_{12} = 0$ to compensate for the infinite electrostatic potential existing at this condition. The values at $\theta=0$ measure the degree of electron-electron overlap.

$d/dr_{12} \phi(r_1, r_2)$ must be discontinuous if non-zero, and the discontinuity in slope must have the proper value to cancel e^2/r_{12} . This condition is called the cusp condition. The amplitude b of the cusp shown in Fig. 2 is determined by system energy minimization. The variational method used by Hylleraas, which minimizes kinetic energy plus potential energy, determined the amplitude of b for the two cases shown in Fig. 2.

7. Principles Determining Wave Function Overlap

Two principles combine to effect a reduction in Coulomb barrier for band state ions. The first principle is that of unbroken lattice symmetry. The second principle is that of electron screening. The principle of unbroken lattice symmetry requires that each unit cell of a crystal must be equivalent, i.e. the 2-ion wave function must have the same amplitude distribution in each unit cell. Functions meeting this requirement are Bloch functions ψ such that $|\psi(\mathbf{r} + \mathbf{R}_{\text{Bravais}})| = |\psi(\mathbf{r})|$, where $\mathbf{R}_{\text{Bravais}}$ is any lattice vector \mathbf{R}_n . The Bravais lattice vectors locate sets of periodically equivalent points of the lattice. Electron screening is a property of metallic conductors. In metals there are itinerant electrons, which have much higher mobility than the ions. As a result, each ion present in the lattice is always surrounded by negative charge provided by the electrons, such that the ion's Coulomb field is always canceled outside a small partially screened volume. As a result, ions in different unit cells of a crystal do not repel each other.

The eigenstates of band state ions are spatially distributed wave functions which contribute a fractional charge e/N_{cell} to each unit cell of the host crystal, where N_{cell} is the number of unit cells in the crystal. It is, however, possible to expand Bloch wave functions in terms of a sum of virtual (i.e. short-lived) states called Wannier functions¹⁶. These virtual states can be viewed as snapshots of the system and show undivided ions located in randomly selected unit cells. The time independent eigenstate can be calculated as the average of all the virtual state snapshots. This procedure provides a picture of the effect of electron screening. Sometimes the snapshots show both ions in a single unit cell. Under these conditions the unit cell occupations are of the form

0 0 0 0 0 0 2 0 0 0 0 0 0 0 0 0 0

(Here, 0's represent "empty unit cells, while the "2" represents a doubly occupied site.) In this case the Coulomb repulsion potential between band state ions is e^2/r_{12} . However, most of the snapshots show the ions in different unit cells,

0 0 0 1 0 0 0 0 0 0 1 0 0 ... 0 0 0 0 0

In this second case the Coulombic repulsion potential is 0. The average-over-snapshots Coulombic repulsion potential is $e^2/(r_{12} N_{\text{cell}})$. This snapshot-averaged potential is that which applies to the electron-screened-ion-in-a-lattice problem.

8. The Eigenstate

We can now write the stationary state wave equation for 2 screened D^+ ions in a periodic lattice,

$$\{-\hbar^2/2m [\nabla_1^2 + \nabla_2^2] + e^2/(r_{12} N_{\text{cell}}) + V_{\text{lattice}}\} \Phi(r_1, r_2) = E \Phi(r_1, r_2) \quad (4)$$

This equation is consistent with unbroken lattice symmetry. The resulting wave function has both unbroken lattice symmetry and cusps at equivalent locations in each unit cell. Each point-particle interaction occurs simultaneously at periodically equivalent points. The solution is time-independent and describes the stationary state of the system.

We have carried out an energy minimizing variational analysis of a cusp-containing wave function describing the 2-ion case¹¹. The value of b that minimizes the sum of kinetic and potential energy at large N_{cell} is

$$b = 2/\pi (m_D/m_e) (r_{sc}/a_0) 1/N_{\text{cell}} \quad (5)$$

The analysis shows that the cusps have negligible amplitude at large N_{cell} ($N_{\text{cell}} = \sim 10^5$). As a result the $D^+_{\text{band}} + D^+_{\text{band}}$ interaction has no Coulomb barrier against fusion. a_0 is the Bohr radius.

9. Relation to QEDCM

The ion band state theory is consistent with the QEDCM¹⁷ picture of a non-perturbative ground state (NPGS). This idea, which also has been applied in the study of critical phenomena¹⁸, is based upon the notion that the ground state has preferential length scales associated with it which distinguish it from asymptotically free states (associated with higher energy) where preferential length scales are not present. In fact, the ion band state theory, as well as the more general problem associated with the physics of bound charged particles in a periodically ordered system, is governed by a self-consistent quantum field theory called Local Density Theory (LDT), in which the length scales and boundary conditions are all treated on an equal footing, governed by a single requirement: that energy be minimized, based upon the known rules of quantum mechanics.

In practice, the associated theory is also similar to the QEDCM picture in that the ground state does exhibit coherence at periodically equivalent points. However, the associated coherence does not result from the inference of the QEDCM plasma-like oscillations that result from variations in the zero of energy. In the ion band state theory, the coherence occurs as a natural consequence of unbroken lattice symmetry, particle exchange, and the properties of the many-body wave function. A fundamental difference is that the wave functions for the particles associated with the QEDCM plasma are described using the Gamow tunneling factors and formalism and do not incorporate particle-exchange, while the ion band state theory wave functions, which do incorporate particle-exchange, are derived by minimizing the energy in a situation that incorporates the boundary conditions of bound particles. As a consequence, the ion band state theory does allow for the possibility (through wave function cusps and other discontinuous changes in the momentum) of changes in kinetic energy that not only are not possible in the QEDCM plasma but which are dictated by the rules of Quantum Mechanics. A second important point is that the starting point of the ion band state theory, LDT, is a well-tested, self-consistent Quantum Field Theory that has been applied quite well for accounting for the electronic structure and dynamics of charge transport in transition metals and for PdD in particular, and that a key element in the success of this theory has been a treatment of kinetic energy that incorporates these kinds of discontinuous changes in momentum.

10. Reaction Possibilities: Guiding Principles

Band theory was invented to explain important anomalies associated with charge and heat transport in ordered, metallic solids. In particular, during the early days of quantum mechanics, it was discovered from conductivity measurements in these kinds of solids, that the effective mean free path of electrons between collisions is many orders of

magnitude larger than the one appropriate in classical, semi-classical, and even quantum mechanical (free electron approximation) modeling of conductivity. Beginning with Bloch, it was discovered that by including periodic order in the kinematics and statistics associated with quantum transport, these anomalies in mean free path not only could be explained, but that meaningful parameterizations of electronic structure, based on the notion of energy bands, could be applied to a large range of problems associated with ordered solids, in general, including insulators, semi-metals, and semi-conductors, as well as metals.

Beginning in the early 1960's, important computational and formal developments occurred, which have provided a means for relating macroscopic phenomena associated with charge and heat transport to a considerably more detailed, microscopic theory, from which these transport phenomena are deduced as a natural, semi-classical limit. In terms of understanding reaction possibilities in general in solids, and the associated implications for cold fusion, these facts have important implications: 1) the presence of periodic order may significantly alter the manner in which charge "moves" within a solid, 2) the locations of individual "particles" within a solid may be altered in manner in which the reaction site may appear (depending upon how the locations are measured) to be in a number of seemingly impossibly different locations at once, and 3) the kinetic energies and momenta of the "particles" may discontinuously change without altering their energies.

Beginning in the 1970's, through the use of LDT and modern computational methods, and by making comparisons of calculated results with application of modern experimental spectroscopic techniques (ultra-high-vacuum photo-emission, x-ray photoemission, etc.), we have obtained a quantitative understanding at a very fine level of detail of the underpinnings of the microscopic theory, and means for quantifying our knowledge of the role of kinetic energy in particular in the microscopic theory. Specifically, considerable progress has occurred in our understanding of most of the ordered metallic lattices, and in particular, in the study of PdD and Pd, and in the study of 3d and 4d transition metals. In the process of accomplishing this we have obtained an understanding of three important factors: 1) the rapid screening of charges in the local electrostatic environments present in these materials by electrons, 2) the presence of periodic order, and 3) (from a calculational viewpoint) the importance of obtaining self-consistent results. Extremely important points are that each of these factors plays an important role in determining the kinetic energy of the individual "particles", that the kinetic energies of "particles" that occupy band states are very different than the kinetic energies of non-band state "particles", and that when particles occupy band states, the reaction possibilities are strongly affected by kinetic energy.

An important assumption of our application of these ideas to the ion band state problem and the potential nuclear reaction possibilities, is that the associated situation is adequately described within this context. As a consequence, throughout, it is assumed that the dominant electrostatic problem is described using "self-consistent", single-particle theory, in a manner that does not invalidate the assumptions that govern the validity of this approach. As we have discussed elsewhere, the underlying dynamics of the many-body system is initialized by the single-particle band states. An important point is that from this starting point, the limitations of the single-particle representation provide constraints on the many-body physics. In particular, a form of "Born-Oppenheimer" separability is always required, in which the motion of the center of mass of each ion band state nucleus (either H, D, ^3H , or ^4He) is always constrained to be independent of the motions of the individual nucleons contained within each nucleus. In practice, this constraint restricts considerably the potential channels for nuclear reaction. However, not only is this requirement consistent with the underlying assumptions that the potential modes of interaction are the result of relatively "small" perturbations of the ground state, it also is consistent with a potentially more important result: in the crystal lattice, ion-band-state-mediated reactions occur in a manner in which it becomes impossible to identify either in the initial state or in

the final state the precise location where the center of mass of the reaction is located. A second important consequence is that potential nuclear reactions cannot significantly disrupt the underlying crystalline environment, either by destroying periodic order, or by requiring that energy be transferred to the solid in such a large amount locally that the underlying assumptions of the band theory and associated theory of transport phenomena become invalid. A final important point is that these assumptions not only can be quantified but also provide a rationale for understanding a number of results: 1) why ${}^4\text{He}$ is the predominant reaction product (which we predicted prior to measurements), 2) why the ${}^4\text{He}$ should be found at low-energy outside heat-producing crystals, 3) the role of loading and electronic structure in radiationless fusion, and 4) why no high energy particles are released in the phenomena. Elsewhere³, we have provided a detailed discussion of each of these predictions. It should be emphasized that each of these results follows from requirements that make the underlying picture valid, not as a consequence of theory. In other words, the assumption that ion-band-state-mediated reactions are at work requires that each of these effects be present, not the reverse.

In particular, implicit in the ion band state picture are the ideas of the "time-averaged" picture associated with the Bloch state picture and the occupation of Bloch states in a manner that minimizes energy. Important consequences of this are that: to minimize energy, a macroscopically small number (much less than N_{cell}) of ions occupy ion band states, and the resulting possibilities for nuclear reaction do not perturb the environment in a significant manner. When it is in fact impossible to determine the location of the center of mass of a particular nuclear reaction because the center of mass of each initial state and final state nucleus is in a band state, on the average, as we have previously discussed^{2,3}, each reaction occurs at all of the periodically equivalent locations in the solid. Heat release is then fractional: each $\text{D}+\text{D}\rightarrow{}^4\text{He}$ reaction releases an amount of energy $Q=23.8 \text{ MeV}/N_{\text{cell}}$ ($= 0.23 \text{ eV}$, for $N_{\text{cell}}=10^9$) in each unit cell. In the remainder of the paper, we will quantify a number of factors related to the point concerning the reasons that ${}^4\text{He}$ is found outside the crystals at low energy. To understand these factors, it is necessary to examine a number of points associated with ion band state transport.

11. Band Transport Theory

Modern Band State transport theory is based upon applying the Greens function methods derived by Kadanoff and Baym²⁰, which were extended by Langreth and Wilkins²¹ to the many-body physics associated with the single-particle, band state solutions that are appropriate in a solid. A fundamentally important point is that the relevant many-body physics of charge transport is converted through this procedure from a Greens function that describes the evolution of charge in the microscopic theory, to a semi-classical limit in which a Boltzmann transport equation such as

$$J_e(\mathbf{x}) = e/\hbar \sum_i g(\mathbf{x}, \mathbf{k}_i) \nabla_{\mathbf{k}} \epsilon(\mathbf{k})$$

can be used to quantify the relationship between the underlying microscopic dynamics and the macroscopic properties. Here $J_e(\mathbf{x})$ is the current density, \mathbf{x} is macroscopic position vector, which extends over the whole solid, $g(\mathbf{x}, \mathbf{k})$ is the Boltzmann "particle" distribution function, \mathbf{k} is the wave vector, and the $\epsilon(\mathbf{k})$ are the energy eigenvalues. To understand the role of periodic order in this process it is important to recognize its role in the underlying microscopic theory, as expressed in the solutions of the single-particle band state equations.

In modern band state theory, these solutions most often are derived based upon the single-particle LDT¹⁹ band theory. In practice these equations are derived as a subsidiary step in the problem of minimizing the total energy of the solid. In particular, in LDT, energy is minimized as part of a two step procedure in which, first, the charge distribution of all the electrons and nuclei is calculated self-consistently, based upon a prescribed choice of geometry, and then the geometry is varied until the minimum energy is obtained.

The single-particle (Kohn-Sham) band theory equations are used during the process of calculating the self-consistent charge density. Specifically, the initial charge density is used to construct a potential V_{lattice} based upon the trial geometry, which is defined by the spacing and orientation of the collection of periodically positioned nuclear centers. The band theory equations in turn are used to determine the density. With respect to the transport problem, important points are that V_{lattice} : 1) includes all of the electrostatic interactions from electrons and positive nuclear centers, and 2) is a periodic function of each of the Bravais lattice vectors \mathbf{R}_n , that separate any of the periodically positioned nuclear centers. Because V_{lattice} is periodic, $V_{\text{lattice}}(\mathbf{r} + \mathbf{R}_n) = V_{\text{lattice}}(\mathbf{r})$. Using this potential, the eigenstates (Ψ), and eigenvalues (ϵ) of an effective Schroedinger equation (the single-particle, Kohn-Sham equation) are constructed. In solving this problem, important simplifications are made possible by assuming that the geometry is periodic. The significance of this symmetry is that it means that each eigenstate Ψ may be selected as a Bloch state $\Psi_{\mathbf{k}}$, defined by the wave-vector \mathbf{k} and the Bloch condition

$$\Psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}_n) = e^{i\mathbf{k} \cdot \mathbf{R}_n} \Psi_{\mathbf{k}}(\mathbf{r}) \quad (6)$$

Each eigenvalue (also called a band energy) is also a function of the wave vector \mathbf{k} , namely, $\epsilon = \epsilon(\mathbf{k})$. This provides a method for solving the effective single-particle Schroedinger equation, which for electrons is

$$H_{\text{sp}}\Psi_{\mathbf{k}}(\mathbf{r}) = [-\hbar^2/2m_e \nabla^2 + V_{\text{lattice}}(\mathbf{r})] \Psi_{\mathbf{k}}(\mathbf{r}) = \epsilon(\mathbf{k}) \Psi_{\mathbf{k}}(\mathbf{r}) \quad (7)$$

Once these equations are solved, the density $\rho(\mathbf{r})$ is constructed¹⁹. It is important to note that because V_{lattice} is a periodic function of \mathbf{R}_n , its Fourier transform is defined by a discrete set of vectors (called reciprocal lattice vectors) \mathbf{G}_m , such that $\mathbf{R}_n \cdot \mathbf{G}_m$ is an integer multiple of 2π , for any values of m and n . As a consequence of this, $\epsilon(\mathbf{k}) = \epsilon(\mathbf{k} + \mathbf{G}_m)$, for any value of m . An important result of this fact is that during any interaction involving Bloch states, it is possible for discrete values of momentum, given by $\hbar\mathbf{G}_m$, to be transferred to and from the lattice without effecting the energy of the individual states, while preserving periodic order. These energy conserving processes in which momentum is changed, which are called UmKlapp processes, were first identified by Peierls²² as being important in the low temperature behavior of electrical conductivity. Because they provide a means for allowing a non-zero momentum-change interaction between different forms of quasi-particles that possess lattice symmetry (band state, phonons, etc.), at low temperature, they also provide a means for coupling surface phenomena with bulk phenomena in which minimal disruption of periodic order occurs.

Important points are: 1) the kinetic energy is treated in a manner consistent with the underlying boundary conditions, 2) the charge distribution and the lattice geometry are allowed to vary in a manner consistent with minimizing the energy, subject to the constraint that periodic order is maintained, and 3) exchange and correlation effects associated with the effects of occupying particular portions of the underlying many-body wave function are

treated in an approximate manner that becomes exact in the limit of small electron separation (a limit that applies quite well in transition metals).

Because the LDT energy is constrained to be stationary with respect to variations of the electron density, it follows that when small numbers of deuterium ions (and their electrons) are injected into any periodic host, the resulting energy may be constrained to be stationary with respect to variations in the densities of either injected ions or electrons provided both the ions and electrons occupy band states and variations in ion band state density are constrained to be independent of electron band state density, and provided the ion band states are derived using the negative of the Coulomb potential associated with Eq. 7 and the approximation that ion band state-ion band state exchange effects are negligible. The basis for the argument follows from continuity of the total energy with respect changes in density, and the fact that infinitesimal variations can occur when macroscopically small numbers of charged particles occupy band states.

We have previously summarized the underlying many-body physics that makes possible overlap between ion band states^{2,3}. The potential for overlap follows from the fact that the many-body state is constructed by forming the product of occupied single-particle band states, each of which has overlap (as a consequence of Eq. 5) with every equivalent lattice site in the crystal. An important point, however, is that overlap alone does not provide a means for understanding how reaction can occur. To understand how reaction might occur, it is important to understand how reactions occur within solids. Here, an extremely important point is associated with the manner in which charge and energy are transferred within a solid and the significance of the Kadanoff-Baym procedure.

In particular, Kadanoff and Baym (as shown by Langreth and Wilkins) observed that there exists a natural procedure for relating the angular frequency representation G_o of the single-particle Greens function associated with an arbitrary single-particle Hamiltonian H_{sp} and the comparable Greens function G to a macroscopic quantity, called the Wigner function, G_w , which, in the case of ordered solids, asymptotically approaches the solution of the Boltzmann equation that is used to describe charge and heat transport. In particular, G_o is directly related to solutions of the Kohn-Sham equations through the relationship

$$G_o(\mathbf{r}, \mathbf{r}', z) = \sum_{\mathbf{k}, \lambda} \frac{\Psi_{\mathbf{k}}(\mathbf{r}) \Psi_{\mathbf{k}}^*(\mathbf{r}')}{\hbar z - \epsilon_{\lambda}(\mathbf{k})} \quad , \quad (8)$$

where z is any complex frequency and the sum is over all wave vectors \mathbf{k} and all bands λ . The corresponding equation describing G_w is

$$\frac{\partial G_w}{\partial t} + \dot{\mathbf{k}} \cdot \nabla_{\mathbf{k}} G_w = 0 \quad , \quad (9)$$

where

$$\dot{\mathbf{k}} = -\nabla_{\mathbf{x}} \epsilon(\mathbf{k}) + \text{external forces} \quad . \quad (10)$$

Here, G_w may be interpreted as the probability of a charged particle occupying a band state with energy $\epsilon(\mathbf{k})$ at the position \mathbf{x} . In the general periodic solid case including disruptions in period order, \mathbf{x} is any integer multiple of any Bravais lattice vector. In the case of G_o , where order is assumed, the differentiation of $\epsilon(\mathbf{k})$ with respect to \mathbf{x} only alters the eigenvalue through changes in the wave function at the boundaries of the lattice where periodic order is lost. When additional effects (phonons, additional lattice imperfections,

and additional many-body effects) are included, the resulting expression for the single particle Greens function analog of G_0 solves a "Dyson's equation" in which time-dependent modifications, through collision processes, are required. These effects in turn can be related to a Boltzmann equation in which an additional term of the form

$$\dot{\mathbf{x}} \nabla_{\mathbf{x}} G$$

is added to the left side, where

$$\dot{\mathbf{x}} = \nabla_{\mathbf{k}} \epsilon(\mathbf{k}) \quad ,$$

and a complicated hierarchy of terms are included on the right side. The important point is that all of the many-body physics can be captured in G and G_0 .

A second important point, however, is that in the case of Eq. 9, an avenue exists through modifications of the eigenvalue at the boundary of the solid for changing the Greens function associated with a particular charged species (be it electrons or ions in band states) without significantly altering the underlying periodic order within the solid. A second important point is that the quantities $\dot{\mathbf{k}}$ and $\nabla_{\mathbf{x}} G$ may change discontinuously through Umklapp processes. These are processes in which the wave vector changes discontinuously by a reciprocal lattice vector, and physical momentum is transferred to the crystal as a whole.

We believe that a potentially dominant mode for reaction at low-moderate temperature involves the situation in which the energy release of $D_{\text{band}} + D_{\text{band}} \rightarrow {}^4\text{He}_{\text{band}}$ results in a shift of the electrostatic zero of the solid and an accompanying Umklapp-process-mediated momentum transfer (through lattice recoil), manifesting itself through a shift in the chemical potentials of ion band state ${}^4\text{He}$ and D . Because a constant shift of the potential is a periodic function and because all of the initial and final state contributions occupy band states, the densities of each are periodic and the perturbations to the electrostatic potential are all periodic functions, and are all small on a per unit cell basis. In such a situation, the dominant modes for interaction will be through effective neutralization of ${}^4\text{He}$ with boundary region electrons. These will manifest themselves through variations both in $\nabla_{\mathbf{x}} \epsilon(\mathbf{k})$ and in gradients of the chemical potential at the boundaries of the crystal through the quantities $\dot{\mathbf{k}}$ and $\nabla_{\mathbf{x}} G$.

12 WHY Cusps and Discontinuities in Momentum Invalidate Gamow Theory

In the 1-dimensional Gamow approximation the r_{12} dependence of the two particle wave function can be represented by $\phi(r_{12}) \propto \exp(i\phi(r_{12}))$, in which

$$\phi(r_{12}) = \int_{\infty}^{r_{12}} k(x) dx \quad , \quad \text{where} \quad k(x) = \sqrt{\frac{2m}{\hbar^2} (E - V(x))} \quad . \quad (11)$$

Away from the classical turning point (defined by $k(x)=0$) this formula is valid provided $|dk/dx| \ll |k(x)|^2$, while near the turning point a relationship between the second and first derivatives is used to identify the appropriate (connection formula) forms of the wave function that apply asymptotically far from the turning point, based on the premise that $k(x)^{1/2}$ is continuous and continuously differentiable on either side of the classical turning

point. When the first derivative of $\phi(r_{12})$ becomes discontinuous, $k(r_{12})$ is discontinuous so that $dk/dx \rightarrow \infty$. Then, Eq. 11 is not valid for any value of k . Also, because k is neither continuous nor continuously differentiable at a cusp, one cannot identify an appropriate form of the wave function that matches the Gamow function in the vicinity of the cusp, nor apply the conventional connection formula.

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