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ELECTRON SCREENING IN METAL DEUTERIDES

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Introduction

Experimental evidence in support of anomalies in metal deuterides has accumulated during the past decade. These anomalies include neutron emission, fast (MeV) charged particle emission, excess power generation and correlated ^{4}He production, tritium production and induced radioactivity. As yet, there is no consensus on a theoretical explanation for these effects. Prior to the introduction of any new physics that pertain specifically to the anomalies, one would like to have a basic understanding of the deuteron-deuteron interaction at close range due to conventional solid state effects. In this work we examine the general issue of electron screening between deuterons in a metal deuteride.

Screening and Recent Accelerator Experiments

In the case of molecular D_2, the screening between the deuterons is a consequence of the change of the electronic energy due to modifications in the electronic orbitals as a function of the deuteron separation. Within the framework of the Born-Oppenheimer approximation, this effect can be included as an effective potential in addition to the Coulomb repulsion between the deuterons. For example, when a fast deuteron collides with a stationary deuteron, electron screening should occur in much the same way as in the D_2 molecule. This should produce an increase in the fusion probability over the theoretical ion-ion calculation (with an unscreened Coulomb barrier) that will be most noticeable at low incident energy. Experiments involving keV deuterons incident on molecular deuterium gas targets give an increase in the fusion rate at low energy over

the theoretical ion-ion calculation that is consistent with such a screening mechanism [1,2]. The experimental data are fit to a screening energy U_S, which for D_2 gas targets is found to be about 25 eV. The corresponding screening length D_S is related by

$$D_S = \frac{e^2}{U_S} \tag{1}$$

In this case, the associated screening length is on the order of a Bohr radius. Similarly, keV deuterons incident on TiD targets show a low energy behavior consistent with a screening that is weaker than for molecular targets. The associated screening energy is 19 eV (with a screening length $D_S = 0.75$ Å).

Experiments in other metal deuterides show a much stronger relative enhancement in the fusion yield at low energy, which has been conjectured to be indicative of a much stronger electron screening effect. For example, In YbD, the screening energy is 60 eV ($D_S = 0.24$ Å). In PdD, the experimental result is consistent with a screening energy of 250 eV ($D_S = 0.058$ Å). We note that a screening length that is less than 0.1 Å is extremely small. It is hard to understand theoretically what physical mechanism could be responsible for such strong screening.

As PdD has been involved in experiments yielding anomalies such as neutron emission and excess heat, it would be natural to imagine that there might exist some physical mechanism that is capable of producing anomalously large screening in PdD. A recent computation by Ichimaru has indicated that large screening effects should be present in PdD near room temperature [3]. Consequently, we have been motivated to examine the issue of screening in metal deuterides, in order to understand whether there can exist a greatly enhanced screening effect.

A Naive Approach to Screening

In the simplest possible picture, the screening between two deuterons in a metal deuteride depends primarily on local electrons that are bound (in a local molecular sense), and somewhat less on more distant electrons through a polarization effect. In a naive view, one might postulate that the interaction between the deuterons at short range was of the form

$$V_{ij} \sim \frac{q_i q_j}{\epsilon} \frac{e^{-R/D_S}}{R} \tag{2}$$

At close range, the interaction is pure Coulombic; at longer distances the interaction is screened exponentially. The effect of polarization in this naive picture is taken into account through the introduction of a dielectric constant. In the computation of Ichimaru, polarization effects were accounted for through the introduction of a constant dielectric constant ϵ. Ichimaru estimated this dielectric constant to be on the order of 1.25 in PdD. Such a relatively high dielectric constant has a very large impact on the deuteron-deuteron overlap probability. There is reason to be concerned about the use of a constant dielectric constant in this application, as it is unlikely that there exists a uniform dielectric background medium when the two deuterons are closer together than the screening distance D_S.

An Improved Model

In order to include the effects of both local and distant electrons on the deuteron-deuteron interaction at short range, we are considering a model that seeks to include both effects explicitly. Local bound electrons can be modeled in the Born-Oppenheimer approximation through the use of an effective electronic potential. When the two deuterons are close, the local ground state electronic orbitals are compact and mismatched in energy from the surrounding orbitals of the host metal. In this case, we expect the effective potential to be close to the equivalent molecular problem. The dielectric response of the electrons at all other sites can be included using a form of linear response theory. One deuteron produces an electrostatic field that polarizes nearby electronic orbitals. The induced electronic polarization then produces a field that effects the second deuteron. The overall effect of the polarization is to cause a screening; however, the strength of this screening is diluted to some degree since the orbitals are relatively distant. Such a model should account for polarization effects much better than using a local dielectric constant as described in the naive model above.

A Hamiltonian that implements this type of model can be written as [4]

$$
\begin{aligned}
H \;=\; & \frac{|\mathbf{P}_1|^2}{2M_1} + \frac{|\mathbf{P}_2|^2}{2M_2} + \frac{q_1 q_2}{|\mathbf{R}_1 - \mathbf{R}_2|} + E_e(|\mathbf{R}_1 - \mathbf{R}_2|) + V_{lat}(\mathbf{R}_1) + V_{lat}(\mathbf{R}_2) \\
& + \sum_m \left\langle \frac{q_1 e}{|\mathbf{R}_1 - \mathbf{r}_m|} \left[E - H_0 \right]^{-1} \frac{q_2 e}{|\mathbf{R}_2 - \mathbf{r}_m|} \right\rangle \\
& + \sum_m \left\langle \frac{q_2 e}{|\mathbf{R}_2 - \mathbf{r}_m|} \left[E - H_0 \right]^{-1} \frac{q_1 e}{|\mathbf{R}_1 - \mathbf{r}_m|} \right\rangle \qquad (3)
\end{aligned}
$$

The first line of this Hamiltonian includes essentially the molecular D_2 problem in the metal lattice environment. The second two lines includes polarization effects with electrons centered at neighboring atomic sites. The summation over index m includes the different electronic orbitals at those neighboring sites. The expectation value is taken over electronic states.

It is possible to apply this model systematically to the different metal deuterides in order to understand screening effects. Two features of the model are obvious that are nearly independent of the host metal deuteride. One is that when the two deuterons are close, the underlying model becomes very much like the molecular D_2 problem, independent of the metal. Another is that it is apparent that polarization effects due to relatively distant electronic orbitals will give rise to essentially no screening effect between deuterons at short range. This is in contrast to the model of Ichimaru.

Dependence of the Dielectric Response on Deuteron Separation

A major focus of the model is to understand the dielectric response of the metal deuteride under conditions when the two deuterons are close together. It is possible to use a Taylor series expansion based on the center of mass and relative coordinates

$$R_1 = R_{cm} - \frac{1}{2}\Delta R \tag{4}$$

$$R_2 = R_{cm} + \frac{1}{2}\Delta R \tag{5}$$

in order to understand the physical content of the polarization terms. Keeping terms to second order in the separation ΔR leads to an expression of the general form

$$V_{pol} = V_0 + \Delta R \cdot M \cdot \Delta R \tag{6}$$

The polarization potential is made up of a constant solution energy offset V_0 that depends on the center of mass position R_{cm}, and a term that is quadratic in the separation ΔR where M is a function of R_{cm}. The detailed evaluation of the terms that appear in this kind of analysis has been carried out and submitted for publication elsewhere[5].

Discussion

The simplest possible model for screening between deuterons in a metal deuteride must include local orbital effects and polarization effects. When the two deuterons are close together, the local electronic orbitals are essentially molecular D_2 orbitals. In TiD, one is tempted to conclude that the local molecular picture extends to distances on the order of a Bohr radius or more. Polarization effects are weak when the deuterons are close, independent of the host metal. In PdD, the outer electronic orbitals of the Pd atoms mix with the $1s$ orbitals of the D atoms when the deuterons are far apart due to a near resonance in the energies of the orbitals. While this complicates the picture, the relevant screening length associated with such mixed orbitals cannot differ by a factor of 10 as would be required to account for the apparent experimental results. The screening length due to such mixing may decrease by about a factor of 2 from the molecular case as has been estimated by Ichimaru and colleagues.

So we are left with an apparent dilemma in accounting for the experimental results in PdD, while TiD seems to be consistent with the general picture described here. The situation becomes further confused relative to the anomalies, as the deuterides of both titanium and palladium appear to give rise to anomalies. To sort out the various issues, we need to be somewhat more precise in our arguments. We must distinguish between the static problem and the collision problem as being potentially different fundamentally in principle. In the case of the static problem, we must also distinguish between three different local environments.

We first consider the collision problem, which gives an apparent screening effect that seems to be impossibly large. The presence of screening is deduced based on a relative increase in the fusion yield at low energy as compared to the theoretical ion-ion collision problem. Hubler (private communication) has suggested that the experimental measurements may be susceptible to an artifact involving a nonuniform deuterium concentration gradient near the surface. If the outer 100 Å of the target near the surface had a higher density of deuterium, then the yield would be larger for the lower beam energy since the range of the deuterons is much shorter at 3 keV than at 10 keV.

Such an effect would give an apparent increase in the low energy yield, but would not be a screening effect. Kasagi has indicated that he measures this profile, and thereby guards against such an artifact (private communication). Nevertheless, due to the theoretical implications of the result, some way needs to be found to be sure that experimental artifacts are not present. For example, in the unlikely event that the deuterons should somehow channel in the intersticies between the Pd atoms preferentially at low energy, then the apparent relative yield would increase at low energy. It is not believed at present that this can happen.

One possible route to accounting for the low energy enhancement might be to consider atomic recoil during the collision event. For example, suppose that the incident deuteron accelerated the stationary deuteron so that it moved much closer to a neighboring Pd nucleus. The screening length in this case could be very much shorter if a more strongly bound Pd orbital (for example, an M-shell orbital) were involved in the screening. In the absence of a detailed analysis of the effect, this appears to be the only way that a screening length less than 0.1 Å could possibly occur. If such a mechanism were the answer to the dilemma, it would not apply to the screening between two nearly static deuterons in the lattice since they would never be found together near an inner Pd electron orbital.

If we focus now on the static problem, we find immediately that there is a question as to what conditions lead to significant tunneling. Three different situations might occur. Two deuterons could be at neighboring sites, and perhaps meet half-way in between. Alternatively, a deuteron from one site could be thermally excited to go into a neighboring site that is already occupied. Finally, it may be that there is a nearby host metal vacancy, so that it becomes much easier for two deuterons to approach. The latter two cases produce the largest tunneling probabilities, and are consequently the most interesting in the consideration of anomalies. In both cases, the local center of mass will likely be near a local potential minimum, and the confining potential will be approximately quadratic. The molecular approximation with minor modifications ought to be a good first approximation in both cases. Deviations from this will be due to orbital mixing with the metal atoms, which is strongest when the orbital align in energy such as in the case of Pd or Ni.

Other Effects

The discussion above has focused on the screening problem assuming a static lattice model. We note that phonons are present, and that it is possible for the interaction between the phonons and the electrons to introduce further complications. Electron exchange between the deuteron orbitals in the molecular case is understood, but one wonders about the situation when strong mixing between the hydrogen orbitals and the metal orbitals occurs. We note also that anomalies in metal deuterides appear to be correlated with conditions under which either an electron current density or ion flux density is present. An electron current will entail a minor modification of the local electron orbitals. An ion flux will be associated with an increase in the optical phonon excitation, which will produce a larger overlap probability.

References

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