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On lattice confinement and hybrid fusion

R. Vilela Mendes

CMAFCIO, Universidade de Lisboa,
C6 - Campo Grande, 1749-016 Lisboa, Portugal
rvilela.mendes@gmail.com
rvmendes@fc.ul.pt

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Positive ions confined in a solid state lattice might be driven to low energy reactions by exploring, through quantum control, the 3-body wave function enhancements of the scar effect.

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In March 1989, Fleischmann and Pons[1] claimed to have obtained, at room temperature, nuclear fusion with deuterium atoms absorbed by electrolysis into a palladium electrode. Similar claims were made a few months later by another group.[2]

These claims were met with justified disbelief, if nothing else on grounds of the energy scales involved. How could a shielding effect in the solid-state environment, presumably on the order of a few eV's, be sufficient to overcome the Coulomb barrier? Furthermore the results could not be reproduced by experiments under carefully controlled conditions (Ref. 3 and references therein).

Most influential at the time was a theoretical paper by Leggett and Baym[4] which showed that, under equilibrium many-body conditions, the rate of tunneling to $r = 0$ separation of the deuterons was rigorously bounded above by the value calculated by the Born–Oppenheimer potential. Much too small to induce any meaningful fusion rates. In fact, if the effective repulsion at short distances of the deuterons were to be much reduced by the solid-state environment, then one would also expect a much increased binding affinity of α-particles to the metal, which is not observed. The work of Leggett and Baym definitely excludes any equilibrium, ground state or even low-lying effect.

Although unlikely at low temperatures, non-equilibrium effects require a different approach, namely, the study of the full dynamical n-body problem ($n \geq 3$). When computing the ground state or the low lying excited states of two positively charged particles surrounded by an electron cloud, the separation r of the particles is treated as a parameter to be fixed by minimizing the energy associated to each wave function. This provides for each state (ground or excited) the mean value of the parameter r. If however, one wants information on the near-collision probability of a 3-body system, the important issue is the value of the wave function at $r = 0$, with r treated as a dynamical variable.

A first approach to this question was to study the probability rate of near-collisions in a classical ergodic Coulomb system of two positive and one negative charge. A small, but non-vanishing rate, was found. In addition, if these 3-body collisions induce fusion reactions, the 3-body reaction seemed to favor a neutron suppressed channel. These results were summarized in two preprints[5,6] with an improved version published in Ref. 7. Of course, a classical ergodic system seemed very far from the lab conditions of the experiments. Perhaps it might provide corrections to the fusion rates in stellar models. On the other hand, if something of this kind could take place in the solid-state quantum environment, it would provide a simple explanation for the improbable, hardly reproducible nature of the phenomenon. Confining the positive ions in a molecular cell, rather than using magnetic fields, seemed an interesting prospect, as it is for some chemical reactions.[8] However, achieving the near-collisions, in a 3-body configuration, seemed too improbable to be of physical interest, at least as an energy-producing device. My interest in the subject died away. It was only resurrected by reading the papers by Heller[9] and Berry[10] on the scar effect.

The scar effect is a quantum phenomenon, a quantum scar being a wave function which displays a high intensity in the region of a classical unstable periodic orbit. Especially, relevant to the 3-body problem are the saddle scars which are related to the unstable harmonic motions along the stable manifold of a saddle point of the potential.[11,12] The scar effect may be used to reach and stabilize configurations which classically correspond to a zero measure set. In particular it might be used to induce reactions that are favored by unstable configurations. The question remained, of course, whether this might be relevant to the problem of low energy nuclear reactions in crystal lattices. It turns out that for a configuration of two positive charges inside an octahedral cage, with the vertices of the cage being occupied by atoms with a partially filled shell, although the ground states correspond to large separations, there are also relatively low-lying states with large collision probabilities.[13,14] Quantum triple-collision effects have also been found to be relevant in molecular physics.[15,16]

Here, this question will be revisited by studying the maximally symmetric states in a 3-body system of two positively charged particles of mass M and charge Ze and a negatively charged one of mass m and charge qe. The system has nine spatial degrees of freedom which for a maximally symmetric state may be reduced to two. Take one of the positively charged particles as the origin and use spherical coordinates for the other two particles. At this stage the Hilbert space measure is

$$d\mu = R^2 dR d\Omega_+ \rho^2 d\rho d(\cos\theta) d\varphi, \tag{1}$$

(R, Ω_+) being the coordinates of the second positively charged particle and (ρ, θ, φ) those of the negatively charged one. The Hamiltonian is

$$H = -\frac{\hbar^2}{2M}\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2 \frac{\partial}{\partial R}\right) - \frac{\hbar^2}{2m}\frac{1}{\rho^2}\frac{\partial}{\partial \rho}\left(\rho^2 \frac{\partial}{\partial \rho}\right) + V(R, \rho, \theta), \tag{2}$$

$$V(R, \rho, \theta) = \frac{Z^2 e^2}{4\pi\varepsilon_0}\frac{1}{R} - \frac{Zqe^2}{4\pi\varepsilon_0}\left\{\frac{1}{\rho} + \frac{1}{\sqrt{R^2 + \rho^2 - 2R\rho\cos\theta}}\right\}. \tag{3}$$

Let

$$\begin{aligned} \mu &= \frac{m}{M}, \\ G^2 &= \frac{Zme^2}{2\pi\varepsilon_0 \hbar^2} \end{aligned} \tag{4}$$

and redefine

$$\widetilde{R} = G^2 R; \quad \widetilde{\rho} = G^2 \rho; \quad \widetilde{H} = \frac{2m}{\hbar^2 G^4} H, \tag{5}$$

$\mu, \widetilde{R}, \widetilde{\rho}$ and $\widetilde{H}$ being dimensionless quantities, the results may easily be used both for molecular and nuclear environments. For a maximally symmetric state, one integrates over the angle variables obtaining

$$\begin{aligned} \widetilde{H} &= \frac{2m}{\hbar^2 G^4} H \\ &= -\mu \frac{1}{\widetilde{R}^2}\frac{\partial}{\partial \widetilde{R}}\left(\widetilde{R}^2 \frac{\partial}{\partial \widetilde{R}}\right) - \frac{1}{\widetilde{\rho}^2}\frac{\partial}{\partial \widetilde{\rho}}\left(\widetilde{\rho}^2 \frac{\partial}{\partial \widetilde{\rho}}\right) + \frac{Z}{\widetilde{R}} - \frac{q}{\widetilde{\rho}} \\ &\quad - q\left\{\frac{\mathcal{H}(\widetilde{R} - \widetilde{\rho})}{\widetilde{R}} + \frac{\mathcal{H}(\widetilde{\rho} - \widetilde{R})}{\widetilde{\rho}}\right\}, \end{aligned} \tag{6}$$

$\mathcal{H}$ being the Heaviside function. The maximally symmetric system is a two degrees of freedom system with integration measure

$$d\mu = \widetilde{R}^2 d\widetilde{R}^2 \widetilde{\rho}^2 d\widetilde{\rho}. \tag{7}$$

From (6) one sees that, in spite of the Coulomb barrier between the positive charges $(\frac{Z}{\widetilde{R}})$, the effective potential becomes attractive in the region $\widetilde{\rho} < \widetilde{R}$ if $\widetilde{\rho} < \frac{q}{Z-q}\widetilde{R}$. Given an eigenstate $\psi(R, \rho)$ of $\widetilde{H}$, the quantum probability for a two-body collision of the positively charged particles is proportional to

$$I_2 = \int d\rho \rho^2 |\psi(0, \rho)|^2 \tag{8}$$

and there is a quantum triple-collision if $\psi(0, 0) \neq 0$.

Because of the Coulomb barrier and the kinematical cost of localization it is to be expected that such states, if they exist, will be relatively high in the spectrum.

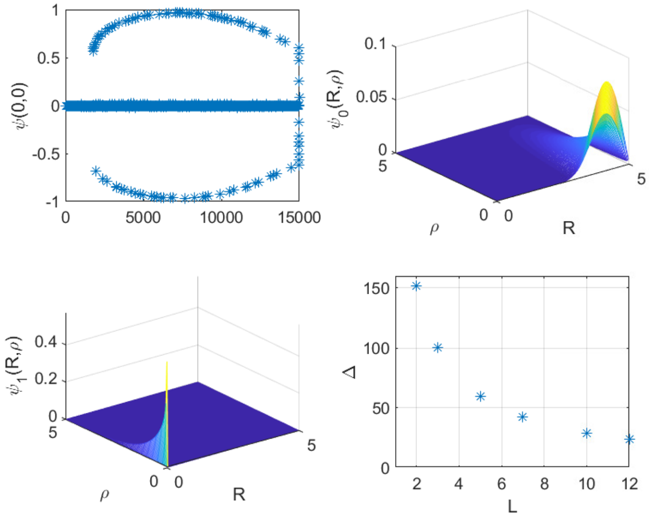

Fig. 1. (Color online) $\psi(0,0)$ (upper left), ground and first triple collision states (upper right and lower left) and L-dependence of the energy difference Δ.

Therefore to compute them one needs a method that involves very many basis states. A simple way to fulfill such a requirement is to represent the operator $\widetilde{H}$ in a fine grid of points in a box of size $[0, L]^2$[a] and diagonalize the resulting matrix. Figure 1 shows the results of such calculation. The upper left panel is the value of $\psi(0,0)$ along the spectrum. One sees that for all the lower part of the spectrum this is a vanishing value, although for high excitation values there are many triple collision states. The *energy difference* Δ between the ground state and the first quantum triple collision state (in $\widetilde{H}$ units) is plotted in the lower right panel for different values of L. The upper right and the lower left panels show the wave functions for the ground state and for the first triple collision state. The parameter μ is 2.7×10^{-4} in all cases and a grid of 15,000 points was used.

The conclusion is that confinement in a box may be an appropriate way to induce in a controlled way reactions that are hindered by the Coulomb barrier. The box, of course, is only a confining device, control of the reaction requires the accurate excitation of the system to the collisional states. Given the high placement of these states in the spectrum, spontaneous occurrence of quantum collisions is highly improbable. Computation of the required control energies needed, both for molecular and nuclear reactions, is obtained by converting the dimensional quantities to physical quantities through the conversion factors in Eqs. (4) and (5). As an example with $\mu = 2.7 \times 10^{-4}$, $Z = q = 1$, $m = 9.1 \times 10^{-31}$ Kg, $G^2 = 0.378 \times 10^{11}$ m^{-1}, $\frac{\hbar^2 G^4}{2m} = 54.42$ eV and $L \in [5, 10]$,[b] the energy differences Δ would be located in the

[a]Because one is using spherical coordinates this box size corresponds roughly to a lattice volume $\frac{4}{3}\pi L^3$.
[b][1.3,2.6] Å in physical units.

high ultraviolet–low X-ray range. This is only indicative, of course, because here the box only contains the three particles whether in a real situation of a solid state lattice many different electron orbitals are involved.

Could a solid state lattice used as a confining device and complemented by an external electromagnetic radiation tailored to excite the quantum triple collision states be used as a practical energy-producing *hybrid fusion* mechanism? It must be pointed out that given the scale of the excitation energies involved, this mechanism does not provide an explanation for any of the unexplained spontaneous "cold fusion" events. It is useful to remember that, also in magnetic confinement fusion, the magnetic fields only provide confinement and not the nuclear collisions needed for fusion. There the additional mechanism is microwave heating. For nuclei confined in a molecular cage, microwave heating is inappropriate as it might also destroy the confining cage. However a subtler quantum control mechanism exciting the triple collision (scar) states with electromagnetic radiation might be a possibility.

Repeating the original cold fusion experiments in better controlled conditions, as has been done recently,[3] may provide new insights in materials science and on improved measurement techniques at high pressures and temperatures. However no spontaneous meaningful energy production should be expected. What is needed is a careful experimental study of the energy spectrum of the many-body system associated to a pair of deuterons and of the quantum control mechanisms needed to excite the quantum triple collision states.

In short, there is in this paper no attempt to vindicate nor refute the eventual or hardly reproducible so-called cold fusion events. In fact, I think that all the noise about this phenomenon has had the unfortunate effect of neglecting the fact that confined quantum systems may display new interesting effects. It is my strong impression that unassisted cold fusion events, even if they exist, would be of little practical interest. Instead what I claim is the potential interest of exploring confined quantum systems where excited states are addressed by quantum control with laser pulses.

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