

## NEAR COLLISIONS IN A COULOMB SYSTEM: QUANTUM TREATMENT

R. VILELA MENDES

*GTAE — Grupo Teórico de Altas Energias  
Av. Gama Pinto 2, P-1699 Lisboa Codex, Portugal*

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We discuss near collisions of equally charged particles in a quantum Coulomb many body system. Using the three-body dominance of near collisions at low energies, we may restrict the study to a system of two positively charged and one negatively charged particle in a box, with periodic boundary conditions. The main low energy collision states are found to be at the top of the negative energy bands. This suggests a *hybrid fusion* method where deuterons absorbed into a metal lattice would be resonantly excited to collision states by electromagnetic radiation in the ultraviolet range.

### 1. Introduction

Hydrogen and its isotopes (deuterium and tritium) are easily absorbed into metals like palladium or titanium, forming an interstitial solid solution.<sup>1</sup> The hydrogen isotopes occupy the free spaces between the atoms of the metal lattice. In static conditions and when the number of deuterons is smaller or equal to the number of palladium nuclei, the closest distance between the deuterons is about twice the internuclear distance in an ordinary deuterium gas molecule. For higher concentrations, even when two deuterons are contained in one of the octahedral cages of the fcc lattice, the equilibrium distance is estimated to be at least 30% larger than in the gas molecule.<sup>2</sup> Furthermore, first principle calculations show that at short distances there is virtually no *d* electron screening.<sup>3</sup> The conclusion is that in equilibrium conditions there is no special enhancement of the Coulomb barrier penetration factor and therefore, except maybe for occasional and irreproducible bursts<sup>4</sup> corresponding to improbable large deviations from the equilibrium configurations, cold fusion reactions of deuterium are extremely unlikely.

Transition metals can absorb hydrogen (and its isotopes) even beyond the density of the solid phase of H<sub>2</sub>. Comparing the relative ease with which hydrogen is confined in a metal lattice as compared to the difficulty of confining it in a hot plasma, it is tempting to speculate whether it might be possible to create conditions in the metal-deuterium solution which would effectively reduce the deuteron internuclear distances. From the discussion above it is clear that such conditions, if they were to exist, would have to be nonequilibrium conditions and the following

questions arise:

- (i) Are there nonequilibrium situations where the distance between the deuteron nuclei in a metal lattice is substantially reduced to near collision distances sufficient to initiate fusion reactions?
- (ii) Can such nonequilibrium conditions be created in a reproducible way, without destroying the metal lattice, thus leading to steady energy production?

To rely on thermal excitations to bring the deuterons into collision would require high temperatures that would melt the lattice, therefore subtler effects must be explored. In two previous papers<sup>5,6</sup> I have addressed question (i) in a classical mechanics context. The main conclusions that were obtained are the following:

- (a) The most unbiased nonequilibrium setting consists in assuming that the many-body deuterons–electrons system covers ergodically each energy surface in phase space. Under this hypothesis one finds that, at low energy, the instances of close proximity of two deuterons are dominated by three-body processes of the (DeD) type.
- (b) Concentrating in the three-body system of two deuterons and one electron, with periodic boundary conditions in a box of lattice size, one finds that in the microcanonical sense, there is a non-negligible probability for near collision of two deuterons. For fully ergodic motion on the energy surface (at zero energy), the probability for (DeD) near collisions is orders of magnitude above the probability for tunneling through the Coulomb barrier in a (DeD)<sup>+</sup> bound state. An event where two deuterons come to a distance  $\varepsilon$  is called an  $\varepsilon$  collision. For sufficiently small  $\varepsilon$ , the rate  $n_\varepsilon$  of  $\varepsilon$  collisions of positively charged particles of mass  $M$  is estimated to be

$$n_\varepsilon = \frac{C\varepsilon^\alpha}{b^3 + \alpha\mu_r}, \quad (1.1)$$

where  $\mu_r = \sqrt{Mb^3}/e$ ,  $b$  is the lattice spacing (size of the box),  $e$  is the electron charge,  $C \simeq 154$ , and  $\alpha \simeq 2.7$ . For a high concentration of deuterons in the metal lattice, this ergodic rate, if it could be realized, would lead to high fusion yields, although we should notice that for each individual process the rate is smaller than in the muon-catalyzed fusion.

The second important point to be answered is whether it is possible or likely to realize ergodic conditions in the metal–deuteron system. The results obtained in the classical mechanics setting<sup>6</sup> are not very encouraging. Deuterons trapped in interstitial positions cover a tiny area of its energy surface. Even if one increases the hopping probability by raising the temperature and increasing the concentration, the amount of the available phase space that is effectively explored by the system is severely limited by conservation laws and KAM tori or Mather cantori. Even without the trapping effect of the lattice, conservation laws lead to large deviations from the ergodic estimates. For example, in numerical simulations,<sup>6</sup> one finds consistently a rate of near collisions much smaller than the phase space estimates. The main reason is that near collisions at low energies are concentrated in a narrow

region near the zero angular momentum and, for a finite number of different initial conditions chosen at random, it is improbable to fall in this region.

In this paper the near collision problem is reanalyzed in a quantum setting. Due to the three-body dominance of near collisions we may again concentrate on a three-body (DeD) system, with periodic boundary conditions on a box to account for the lattice environment in which the system is immersed. The situation appears to be rather different from the classical one. Rather than having motion on an energy surface with a phase space region corresponding to near collisions, one has a splitting into energy bands with the states at the bottom of the bands being deuteron-separated states and the states at the top of the bands being near collision states. In this sense the quantum situation is more favorable, because one might be able to excite directly the near collision states by resonant excitation with the appropriate bandwidth energy. The three-body Hamiltonian to be considered is

$$\mathcal{H} = -\frac{\hbar^2}{2M_1}\Delta_{X_1} - \frac{\hbar^2}{2M_2}\Delta_{X_2} - \frac{\hbar^2}{2m}\Delta_Y + e^2 \left( \frac{1}{|X_1 - X_2|} - \frac{1}{|X_1 - Y|} - \frac{1}{|X_2 - Y|} \right). \quad (1.2)$$

It is convenient to choose a length scale to simplify the Hamiltonian (1.2). Writing

$$X_1^i = ax_1^i, \quad (1.3a)$$

$$X_2^i = ax_2^i, \quad (1.3b)$$

$$Y^i = ay^i, \quad (1.3c)$$

with

$$a = \frac{\hbar^2}{2Me^2}, \quad (1.4)$$

one obtains

$$H = \frac{a}{e^2}\mathcal{H} = -\Delta_{x_1} - \Delta_{x_2} - \frac{1}{\gamma}\Delta_y + \left( \frac{1}{|x_1 - x_2|} - \frac{1}{|x_1 - y|} - \frac{1}{|x_2 - y|} \right), \quad (1.5)$$

where  $\gamma = m/M$ . If  $e$  is the electronic charge,  $m$  the electron mass, and  $M$  the deuteron mass, then  $\gamma = 2.7 \times 10^{-4}$  and  $a = 7.209 \times 10^{-13}$  cm. For deuterons in a palladium lattice, the typical average deuteron separations are of the order of one angstrom. Most of the calculations carried out in this paper assume a box with periodic boundary conditions and size  $L = 0.94 \times 10^{-8}$  cm, that is  $L = 13039$  in units of  $a$ .

## 2. A Toy One-Dimensional Model

As calculations are easier and a full analysis may be carried out, I will first consider a one-dimensional model. Once the nature of the states corresponding to quantum

near collisions is understood in this model, the overall mechanism is easily carried out to the three-dimensional Coulomb case. Consider the Hamiltonian

$$H_1 = -\partial_{x_1}^2 - \partial_{x_2}^2 - \frac{1}{\gamma} \partial^2 y + [U(|x_1 - x_2|) - U(|x_1 - y|) - U(|x_2 - y|)] \quad (2.1)$$

for two positively charged and one negatively charged particles living on a circle of perimeter  $L$ .  $U(x)$  is the piecewise linear periodic potential

$$U(x) = \frac{1}{L} S\left(\frac{x}{L}\right),$$

$S$  being the function shown in Fig. 1. The  $1/L$  factors are included to have energy expectation values close to the intensity of Coulomb effects. Furthermore one chooses  $V = 6$  which leads for  $S(x/L)$  on the interval  $[-1/2, 1/2]$  to the same expectation value as the scaled Coulomb potential  $1/|x/L|$  in a ball of radius  $1/2$ . For simplicity call deuterons the positively charged particles and electron the negatively charged one. These are only suggestive names, the actual numerical predictions for the physical particles being deferred to the Coulomb problem in Sec. 3.

Consider a basis of box-normalized free momentum eigenstates with periodic boundary conditions  $\frac{1}{\sqrt{L}} \exp(i2\pi kx)$ ,  $k = n/L$ ,  $n = 0, \pm 1, \pm 2, \pm 3, \dots$ . Denote by  $|n_1 n_2 p\rangle$  a state with deuteron momenta  $n_1/L$  and  $n_2/L$  and electron momentum  $p/L$ . The matrix elements of the Hamiltonian  $H_1$  in this basis are

$$\begin{aligned} \langle n'_1 n'_2 p' | H_1 | n_1 n_2 p \rangle &= \delta_{n'_1 n_1} \delta_{n'_2 n_2} \delta_{p' p} (2\pi)^2 \frac{1}{L^2} \left( n_1^2 + n_2^2 + \frac{p^2}{\gamma} \right) \\ &+ \frac{V}{L} \delta_{p' p} \delta(n_1 - n'_1 + n_2 - n'_2) g(n_1 - n'_1 - n_2 + n'_2) \\ &- \frac{V}{L} \delta_{n'_2 n_2} \delta(n_1 - n'_1 + p - p') g(n_1 - n'_1 - p + p') \\ &- \frac{V}{L} \delta_{n'_1 n_1} \delta(p - p' + n_2 - n'_2) g(p - p' - n_2 + n'_2), \end{aligned} \quad (2.2)$$

where  $g$  is the function

$$g(\alpha) = \frac{1}{\pi\alpha} \left[ \sin(\pi\alpha) - \frac{4}{\pi\alpha} \cos\left(\frac{\pi\alpha}{2}\right) + \frac{2}{\pi\alpha} + \frac{2}{\pi\alpha} \cos(\pi\alpha) \right]. \quad (2.3)$$

When the Hamiltonian  $H_1$  is diagonalized, the eigenvector wave functions are written as linear combinations of the momentum eigenstates:

$$\psi(x_1, x_2, y) = \frac{1}{L^{3/2}} \sum_{n_1 n_2 p} c_{n_1 n_2 p} e^{i\frac{2\pi}{L} n_1 x_1} e^{i\frac{2\pi}{L} n_2 x_2} e^{i\frac{2\pi}{L} p y}. \quad (2.4)$$

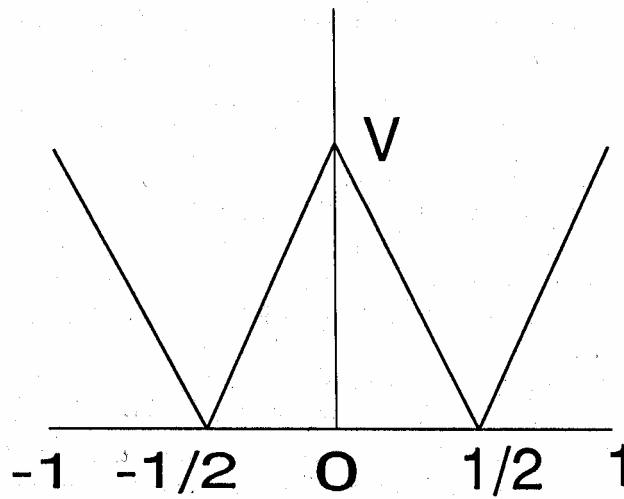


Fig. 1. One-dimensional piecewise linear periodic potential.

The center of mass motion is separated by changing coordinates to

$$R = \frac{1}{2 + \gamma}(x_1 + x_2 + \gamma y), \quad (2.5a)$$

$$r = x_1 - x_2, \quad (2.5b)$$

$$\eta = y - \frac{x_1 + x_2}{2}, \quad (2.5c)$$

and integrating over  $R$  one obtains  $\psi(r, \eta)$  which is displayed below for some of the relevant states. Of particular interest is the probability to find the (one-dimensional) deuterons at a distance  $|x_1 - x_2|$ . Integrating  $|\psi(x_1, x_2, y)|^2$  over all the other variables and summing over both signs of  $x_1 - x_2$ , one obtains

$$\begin{aligned} \rho(|x_1 - x_2|) &= |\psi(|x_1 - x_2|)|^2 \\ &= \frac{2}{L} \sum'_{\substack{n_1 n'_1 \\ n_2 n'_2 p}} \cos\left(\pi(n_1 - n'_1 - n_2 + n'_2) \frac{|x_1 - x_2|}{L}\right) c_{n_1 n_2 p} c_{n'_1 n'_2 p}^* \end{aligned} \quad (2.6)$$

where  $\sum'$  means that the sum is restricted to  $n_1 - n'_1 + n_2 - n'_2 = 0$ . The value of  $\rho(|x_1 - x_2|)$  in the neighborhood of  $|x_1 - x_2| = 0$  characterizes the near collision probability.

For the discussion below the parameters were fixed at values of physical interest for the deuteron-electron system, namely  $V = 6$ ,  $L = 13039$ , and  $\gamma = 2.7 \times 10^{-4}$ . Being interested in deuteron collision states at low energies we look for the structure of the negative energy states. This structure is easily understood in general grounds.

Due to the large values of  $1/\gamma$ , negative energy states of zero total momentum are of the form

$$\sum_{n=-\infty}^{\infty} c_n |n - n 0\rangle$$

with  $c_n = c_{-n}$ , the exact values of the coefficients  $c_n$  depending on the potential. The electron being strongly delocalized is energetically favorable to separate the deuterons. Hence, in the ground state, the coefficients  $c_n$  must alternate in sign, otherwise the cosines would pile up at the origin ( $r = 0$ ). Conversely for the state at the top of the negative energy band all signs are equal and the wave function has a large value at the origin.

Using a basis with 729 states a numerical diagonalization of  $LH_1$  is performed in the zero total momentum subspace. In Fig. 2 are plotted the (un-normalized) values of  $\rho(|x_1 - x_2|) = |\psi(|x_1 - x_2|)|^2$  at the origin, from the ground state up to an energy value equal to 7. One sees that large  $\rho(0)$ 's are only found at the top of the negative energy band. The state with the largest  $\rho(0)$  is the one with the highest energy in the band. It appears at all degrees of resolution in the study of the band, that is for all finite numbers of basis states used in the diagonalization. Such states will be called the *primary collision states*. The number of other states with non-negligible  $\rho(0)$  changes with the degree of resolution, meaning that they correspond to sharp local peaks. Two of these states are seen in Fig. 2. Figures 3(a)–(c) display the wave functions of the ground state, an intermediate state with  $\rho(0) \neq 0$ , and the state at

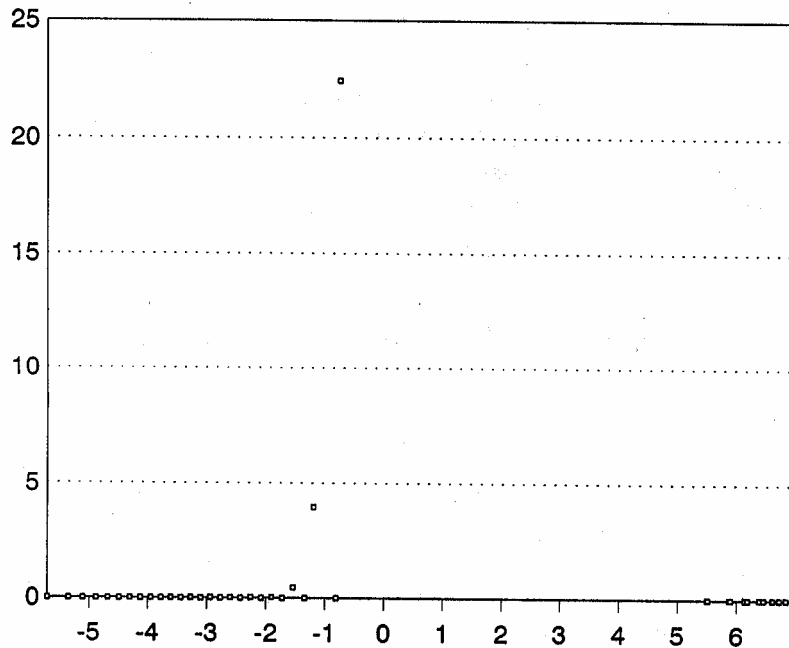


Fig. 2.  $|\psi(|x_1 - x_2|)|^2$  at the origin in the negative energy band for the zero momentum subspace.

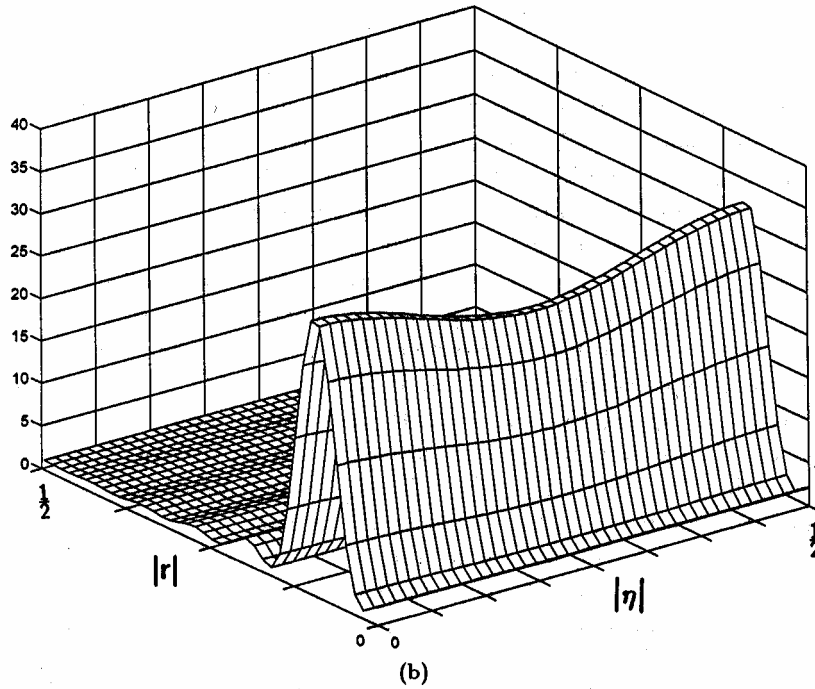
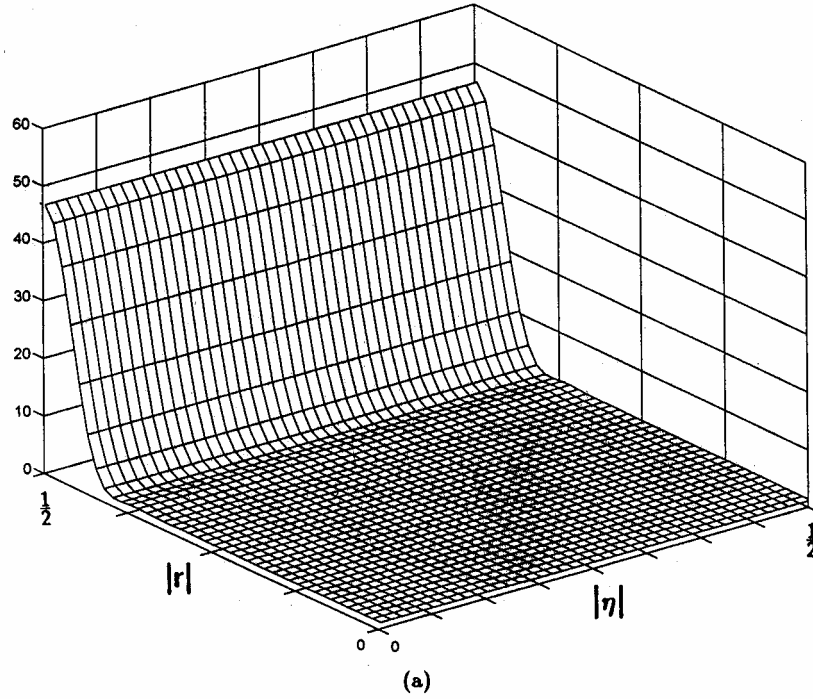


Fig. 3. Squared wave functions  $|\psi(|r|, |\eta|)|^2$  for the ground state (a), an intermediate state with  $\rho(0) \neq 0$  (b), and the state at the top of the negative energy band (c).

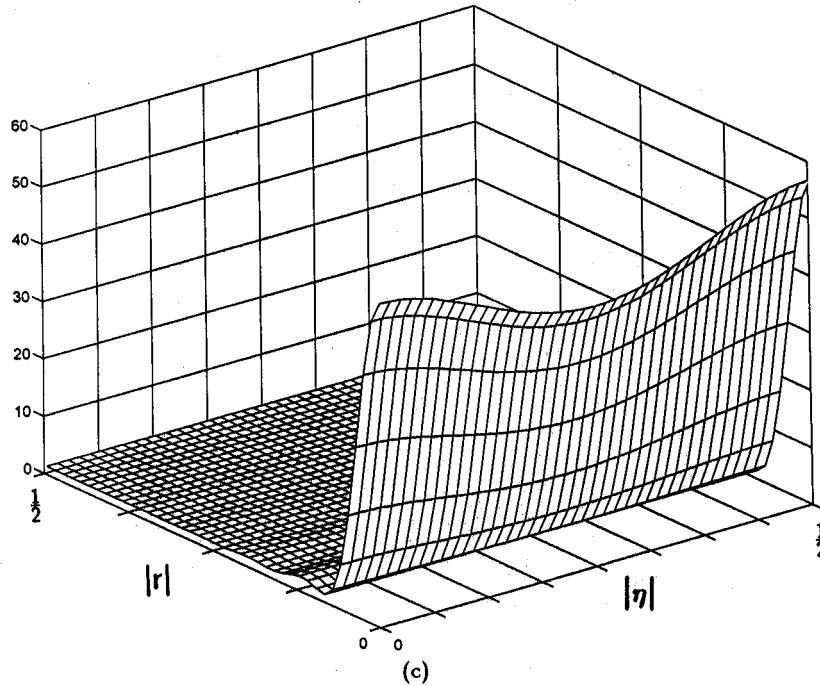


Fig. 3 (Continued)

the top of the negative energy band as functions of the relative deuteron distance and the distance of the electron to the deuterons center of mass,  $\psi(|r|, |\eta|)$ . Notice the relatively small value of  $\rho(0)$  for the intermediate state.

The first primary collision state at the top of the band is still a negative energy state, but is separated from the ground state by an energy of order  $5e^2/aL$ . This energy will be called *the near collision gap*. It is the energy needed to excite the system from the ground state to a configuration with high collision probability. Although this is merely a toy model, because parameters close to the Coulomb intensities were used, it is instructive to discuss the physical significance of the near collision energy gap. For the parameters that were used  $5e^2/aL \simeq 12.25 \cdot 10^{-11}$  erg. To bridge this energy gap by thermal excitations would require temperatures on the order of  $10^5$  K. However, this energy corresponds to an electromagnetic radiation of wavelength  $162 \text{ \AA}$ . Hence the near collision quantum states might be excited by resonant excitation using light in the ultraviolet range.

To excite the state with zero momentum at the top of the negative energy band would require a fine tuning of the excitation energy. However, if the zero total momentum restriction is lifted, the situation is more favorable because there are more collision states. This is shown in Fig. 4 where  $\rho(0)$  is plotted for (a finite basis approximation of) the negative energy band using 729 basis states without restrictions on the total momentum.



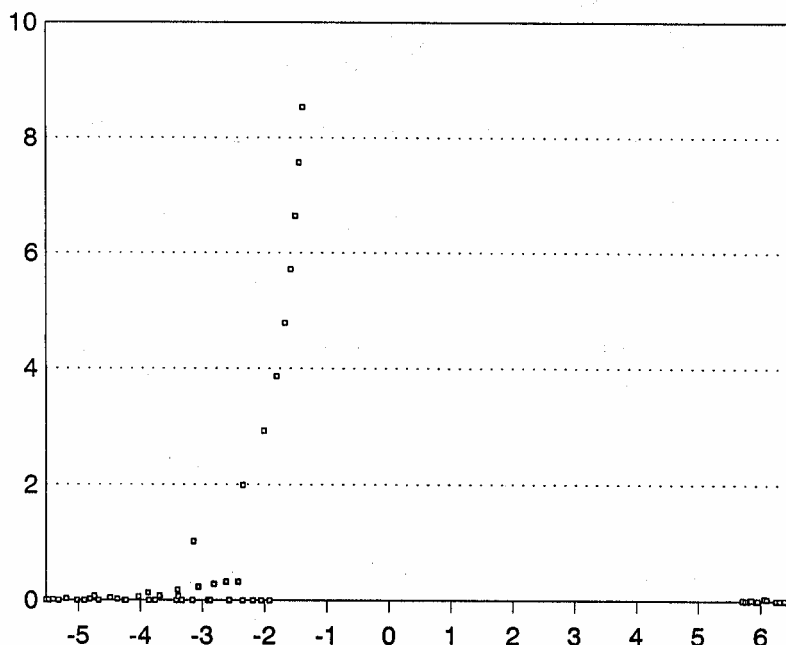


Fig. 4.  $|\psi(|x_1 - x_2|)|^2$  at the origin in the negative energy band.

### 3. Three-Dimensional Case

For the three-dimensional case, consider two positively charged particles of mass  $M$  and a negatively charged one of mass  $m$ , in a box of side  $L$  with periodic boundary conditions. The Hamiltonian is the Coulomb Hamiltonian of Eq. (1.5) with a periodicity condition on the potential to take into account the effect of the particles in the boxes that surround the box under study. As the Coulomb potential terms depend only on the radial variables  $r = |\mathbf{x}_1 - \mathbf{x}_2|$  or  $|\mathbf{x}_i - \mathbf{y}|$  one uses, for computational convenience, a mixed set of periodic boundary conditions. To compute the matrix elements integrate on a cube for all variables that do not appear explicitly in the potential. Then for  $\mathbf{r}$  integrate on a sphere with the same volume as the cube. Furthermore the potential is taken to be a periodic Coulomb potential. The effect of most concern in this paper is the near collisions of particles. Therefore it depends mostly on the Coulomb potential at short distances and must be relatively insensitive to the kind of periodic boundary conditions that are imposed. In any case the explicit consideration of a periodic Coulomb potential seemed the more appropriate one, to be consistent with the periodic boundary conditions.

On a basis of box-normalized momentum eigenstates  $(L)^{-3/2} \exp(i2\pi\mathbf{k} \cdot \mathbf{x})$  the matrix elements are

$$\begin{aligned} & \langle \mathbf{n}'_1 \mathbf{n}'_2 \mathbf{p}' | H | \mathbf{n}_1 \mathbf{n}_2 \mathbf{p} \rangle \\ &= \delta_{\mathbf{n}'_1 \mathbf{n}_1}^3 \delta_{\mathbf{n}'_2 \mathbf{n}_2}^3 \delta_{\mathbf{p}' \mathbf{p}}^3 (2\pi)^2 \frac{1}{L^2} \left( |\mathbf{n}_1|^2 + |\mathbf{n}_2|^2 + \frac{|\mathbf{p}|^2}{\gamma} \right) \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{L} \delta_{\mathbf{p}'\mathbf{p}}^3 \delta^3(\mathbf{n}_1 - \mathbf{n}'_1 + \mathbf{n}_2 - \mathbf{n}'_2) \frac{1}{\pi|\mathbf{n}_1 - \mathbf{n}'_1|^2} [1 - \cos(2\pi\rho|\mathbf{n}_1 - \mathbf{n}'_1|)] \\
& - \frac{1}{L} \delta_{\mathbf{n}'_2\mathbf{n}_2}^3 \delta^3(\mathbf{n}_1 - \mathbf{n}'_1 + \mathbf{p} - \mathbf{p}') \frac{1}{\pi|\mathbf{n}_1 - \mathbf{n}'_1|^2} [1 - \cos(2\pi\rho|\mathbf{n}_1 - \mathbf{n}'_1|)] \\
& - \frac{1}{L} \delta_{\mathbf{n}'_1\mathbf{n}_1}^3 \delta^3(\mathbf{p} - \mathbf{p}' + \mathbf{n}_2 - \mathbf{n}'_2) \frac{1}{\pi|\mathbf{n}_2 - \mathbf{n}'_2|^2} [1 - \cos(2\pi\rho|\mathbf{n}_2 - \mathbf{n}'_2|)],
\end{aligned} \tag{3.1}$$

where  $\rho = (\frac{3}{4\pi})^{1/3}$  and  $Ln_1$ ,  $Ln_2$ , and  $Lp$  are the deuterons and electron momenta.

For a wave function

$$\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{y}) = \left(\frac{1}{L^{3/2}}\right)^3 \sum_{\mathbf{n}_1\mathbf{n}_2\mathbf{p}} c_{\mathbf{n}_1\mathbf{n}_2\mathbf{p}} e^{i\frac{2\pi}{L}\mathbf{n}_1\cdot\mathbf{x}_1} e^{i\frac{2\pi}{L}\mathbf{n}_2\cdot\mathbf{x}_2} e^{i\frac{2\pi}{L}\mathbf{p}\cdot\mathbf{y}}, \tag{3.2}$$

the probability to find two deuterons at a distance  $|\mathbf{x}_1 - \mathbf{x}_2|$  is

$$\begin{aligned}
\rho(|\mathbf{x}_1 - \mathbf{x}_2|) &= |\psi(|\mathbf{x}_1 - \mathbf{x}_2|)|^2 \\
&= \frac{4\pi}{L^3} \sum'_{\substack{\mathbf{n}_1\mathbf{n}'_1 \\ \mathbf{n}_2\mathbf{n}'_2\mathbf{p}}} \frac{\sin\left(\pi|\mathbf{n}_1 - \mathbf{n}'_1 - \mathbf{n}_2 + \mathbf{n}'_2| \frac{|\mathbf{x}_1 - \mathbf{x}_2|}{L}\right)}{\pi|\mathbf{n}_1 - \mathbf{n}'_1 - \mathbf{n}_2 + \mathbf{n}'_2| \frac{|\mathbf{x}_1 - \mathbf{x}_2|}{L}} c_{\mathbf{n}_1\mathbf{n}_2\mathbf{p}} c_{\mathbf{n}'_1\mathbf{n}'_2\mathbf{p}}^*,
\end{aligned} \tag{3.3}$$

where  $\sum'$  means that the sum is restricted to  $\mathbf{n}_1 - \mathbf{n}'_1 + \mathbf{n}_2 - \mathbf{n}'_2 = 0$ .

When performing the numerical diagonalization of (3.1) one has now many more variables than in the one-dimensional model of Sec. 2 and it is not possible to include in the basis as many high momentum states as before. Therefore one expects that here only the primary collision states may be identified. For all practical purposes they are the more important anyway. Figure 5 shows the values of  $\rho(0)$  (for unnormalized wave functions) in the negative energy part of the spectrum, obtained from numerical diagonalization with a basis of 729 states at the zero total momentum. One now sees several negative energy bands, but the qualitative conclusions are similar to those of the one-dimensional model. The primary collision states are at or near the top of the bands. For the lowest negative energy band the near collision gap is  $\simeq 6.5e^2/aL$  which corresponds to a wavelength of 124 Å. For the numerical calculations I have been using  $L = 13039$  in  $a$  units which corresponds to  $L = 0.94$  Å. In Fig. 6 I have plotted the values of the near collision gap for the lowest negative energy band, computed for other values of  $L$ . Therefore for  $L$  in the range 0.94–3.7 Å the wavelengths required to bridge the first near collision gap are in the range 124–330 Å.

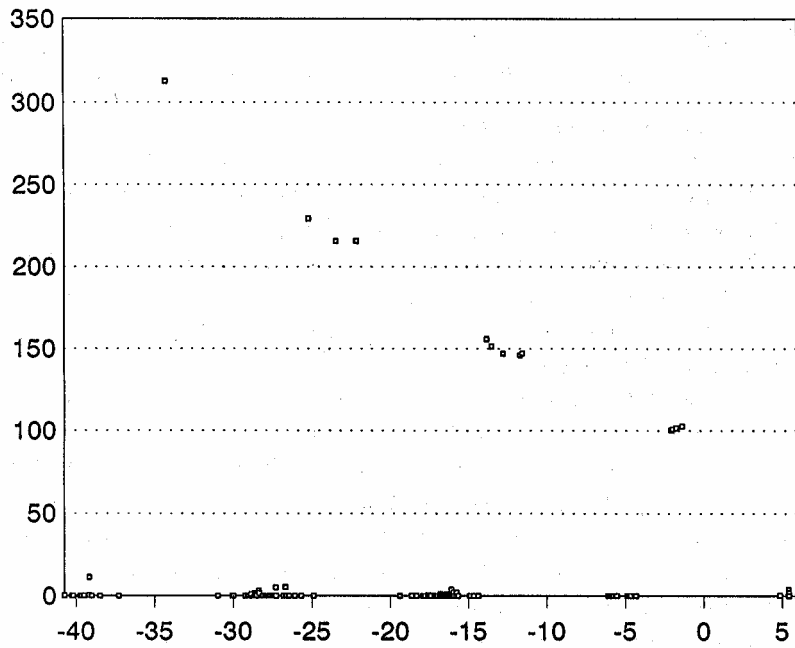


Fig. 5.  $|\psi(|x_1 - x_2|)|^2$  at the origin for the negative energy bands in the zero momentum subspace (three-dimensional problem).

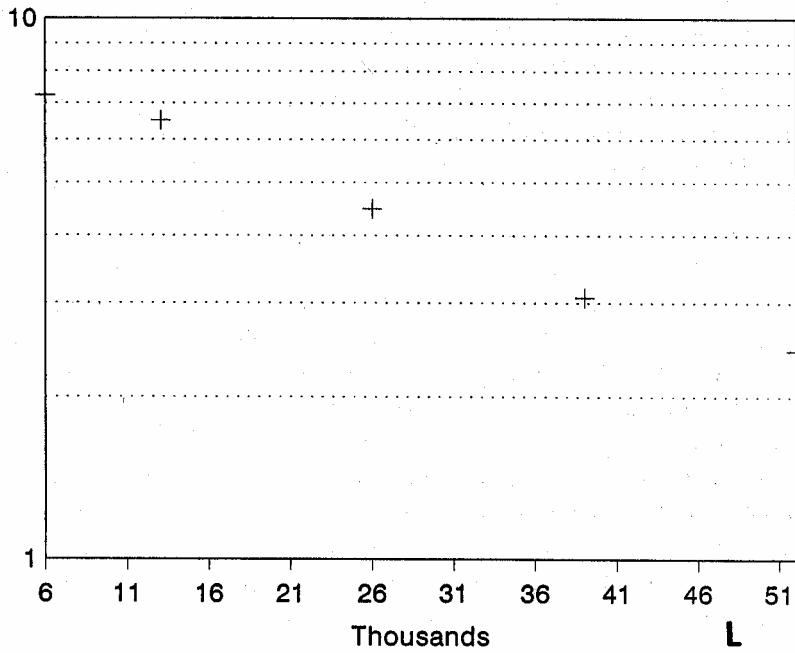


Fig. 6. Near collision gap (in  $e^2/aL$  units) in the lowest energy band.

#### 4. Conclusions

The situation concerning near collision states in a Coulomb system is the following:

- (a) Classically it is found that the low energy near collision events in the many body system have a small but non-negligible probability which is dominated by three-body (DeD) processes.<sup>5</sup> This probability is estimated from phase space volume considerations on the zero-energy surface. However, it is found that because of angular momentum conservation, even under ergodic motion conditions, the near collision region in phase space can only be accessed if one starts from very small initial angular momentum. Access to these configurations may also be hindered by the diffusion barriers of near integrable systems, that is KAM tori or Mather cantori. This explains why the near collision rates obtained in numerical simulations are substantially smaller than the phase space volume estimates.<sup>6</sup> In the classical mechanics setting near collisions have therefore the characteristic behavior of a large deviation effect with deviations towards smaller event rates in finite samples. Also, in the classical mechanics setting it is not clear how the situation might be changed, diffusion barriers and angular momenta being difficult to control at the microscopic level.
- (b) In quantum mechanics the situation looks different. This is no surprise because semiclassical considerations are not supposed to be reliable for the low energy levels that concern us here.<sup>7</sup> Instead of a constant energy surface with different types of behavior in it (foliated by conservation laws and approximate tori) we have a splitting of the negative energy levels into bands with the dominant near collision states staying at the top of the bands. The typical bandwidths are estimated to be too large to allow for excitation of the near collision states by random thermal excitations. This emphasizes, once more, how unlikely it is to obtain spontaneous cold fusion. However, the near collision states might be accessed by resonant excitation with electromagnetic radiation in the ultraviolet range.
- (c) As I have stated before, it is tempting to think of profiting from the hydrogen isotope confining properties of some metallic lattices to obtain a fusion device, provided an additional excitation mechanism is found that is sufficiently soft to preserve the lattice. This mixed approach is what I have called the *hybrid fusion* approach.<sup>6</sup> The results of the quantum systems studied above suggest that such a mechanism might consist in the excitation of the quantum near collision states by electromagnetic radiation. The performance of this scheme will depend critically on a good tuning up of the excitation radiation. As the required excitation energies are of the order of the bandwidths in the negative energy region, they could be found from absorption experiments.
- (d) For the detection of fusion events in the above setting notice that the three-body nature of the process may tend to select the  $T+p$  channel as the preferred one.<sup>8</sup>

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