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It is widely accepted that in molecular systems the nuclear interaction plays a negligible role, because of the strong Coulomb repulsion of the nuclei at small distances. We are going to show that this is not always true. The existence of an extended nuclear resonance may lead to considerably enhanced nuclear reaction rates in appropriately prepared molecules. Especially we point out that $p + p + {}^{16}\text{O}$, i.e., the constituents of water, can form a ${}^{18}\text{Ne}(1^-)$ threshold resonance which decays under energy release into ${}^{17}\text{F}$ and a proton.

In this note we consider the increase of the reaction probability of nuclei in molecules due to the existence of nuclear resonances. Appropriate candidates for such a mechanism are molecules in which the nuclei involved can form near-threshold resonances. The long tail of the corresponding wave functions is expected to lead to a noticeable overlap with the molecular functions, and hence to a measurable transition probability from the molecular to the nuclear states. For a two-atomic molecule it will be shown that an even exponential enhancement arises, instead of the usual reduction of nuclear cross sections due to Coulomb repulsion.

Let us discuss some examples of such threshold states. A typical case is the Boron isotope ${}^8\text{B}$. In its ground state the proton has a separation energy of only 0.13 MeV, being thus represented by a wave function with a long-ranged tail. The treatment [1] of the process $p + {}^7\text{Be} \rightarrow {}^8\text{B} + \gamma$, which is crucial in the solar neutrino problem [2], did in fact require integrations up to 300 fm.

Another example is the ${}^5\text{He}(3/2^+)$ resonance which plays a decisive role in muon catalyzed fusion of deuteron and triton in the $d\text{t}\mu$ molecule [3]. The presence of this near-threshold resonance (50 keV resonance energy, 60–70 keV width) enlarges the fusion probability at least by four orders of magnitude, as compared with nuclear reactions in molecules like $p\text{d}\mu$ or $dd\mu$ where no such resonances occur.

To achieve a similar enhancement of the fusion probability already in normal (electronic) molecules, we have to look for a nuclear resonance which lie much closer to the corresponding threshold energy. The excited 1^- state

of the Neon isotope ${}^{18}\text{Ne}$ satisfies this requirement. Its experimental energy [4] of 4.522 MeV coincides up to the given digits with the threshold energy of the three-body channel $p + p + {}^{16}\text{O}$. Vice versa, any $pp{}^{16}\text{O}$ system, being rotationally excited into a 1^- state, is energetically degenerate with this ${}^{18}\text{Ne}(1^-)$ resonance. In nature this system occurs in form of stable, chemically bound water molecules. These molecules, being rotationally excited, thus, contain always some ${}^{18}\text{Ne}(1^-)$ admixture. And this nuclear state can decay not only into the original $p + p + {}^{16}\text{O}$ channel, but also into a two-body channel like ${}^{17}\text{F} + p$, with an energy release of 0.6 MeV. Excited water molecules, thus, have a non-vanishing probability of “burning” into this final state.

In order to get some feeling for the corresponding transition probabilities, we consider as a more simple example the two-atomic $D{}^6\text{Li}$ molecule. There exists also in this case an excited nuclear state, the Beryllium resonance ${}^8\text{Be}(2^+)$, close to the $d + {}^6\text{Li}$ threshold¹. Indeed, according to [5] the resonance energy is $(22.2 + i 0.8)$ MeV, while the threshold, i.e., the energy needed to break up the ${}^8\text{Be}$ ground state into $d + {}^6\text{Li}$, lies at 22.2798 MeV. A noticeable interference between the nuclear and molecular wave functions, hence, is again to be expected.

For an estimate of the corresponding transition probability we use the following model. The resonance state $\psi_{\text{res}}(r)$ is simply chosen as an outgoing Coulomb s-wave,

$$\psi_{\text{res}}(r) = \frac{1}{N_{\text{res}}} \frac{e^{i\eta \ln \kappa r}}{r}, \quad (1)$$

with $\eta = Z_1 Z_2 \alpha \sqrt{\mu c^2 / 2E}$ being the Sommerfeld parameter. Here, α is the fine structure constant and E , the relative energy of the outgoing particles, $E = \frac{k^2}{2\mu}$. The

function (1) is assumed to be normalized to unity within the range of the nuclear interaction [6]. This choice of N_{res} reflects the nuclear origin of the outgoing particles, which move outside the nuclear volume exclusively under the influence of the repulsive Coulomb potential. The molecular wave function $\psi_{\text{mol}}(r)$, representing the motion of the nuclei d and ${}^6\text{Li}$ under the influence of an effective attractive potential with strong Coulomb repulsion at the origin, is chosen as a product of the regular

¹This resonance can decay into various channels, e.g., $n + {}^7\text{Be}$, $p + {}^7\text{Li}$, $\alpha + \alpha$, with noticeable energy yield [5].

Coulomb solution $F_0(\kappa, r)$ and an exponential decreasing function associated with size of the molecule,

$$\psi_{\text{mol}}(r) = \frac{1}{N_{\text{mol}}} \frac{F_0(\kappa, r)}{r} e^{-\kappa r}. \quad (2)$$

Within our model, the transition amplitude is given by

$$I = \int d^3r \psi_{\text{res}}(r) \psi_{\text{mol}}(r). \quad (3)$$

In order to calculate this overlap integral we use for the regular Coulomb function the representation

$$F_0(\kappa, r) = C_0(\eta) r e^{-ir} M(1 - i\eta, 2, 2ir), \quad (4)$$

with

$$M(a, b, z) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \int_0^1 e^{zt} t^{a-1} (1-t)^{b-a-1} dt, \quad (5)$$

and $C_0(\eta) = \exp(-\pi\eta/2)\Gamma(1+i\eta)/\Gamma(2)$. This integral representation allows us to perform the space-integration in (3) analytically. That is, the contributions of the wave functions to the transition amplitude are taken into account exactly from all distances,

$$I \propto 4\pi C_0(\eta) \frac{\Gamma(2)\Gamma(2+i\eta)}{|\Gamma(1+i\eta)|^2} \int_0^1 \left(\frac{1-t}{t}\right)^{i\eta} \times \quad (6)$$

$$\times \frac{dt}{[1-i(2t-1)]^{2+i\eta}}.$$

Since $\eta \gg 1$ near the threshold, the remaining integral can be evaluated by means of the saddle point method. The saddle point, from which the main contribution to the integral (6) stems, lies at

$$t_1 = 1 + \frac{1}{2} \left[\sqrt{\sqrt{2}+1} + i\sqrt{\sqrt{2}-1} \right]. \quad (7)$$

The leading term in (6), thus, looks like

$$I \propto \frac{C_0(\eta)}{\kappa} \frac{\Gamma(2+i\eta)}{|\Gamma(1+i\eta)|^2} \frac{e^{0.614\pi\eta}}{\sqrt{\eta}} \left[A + O\left(\frac{1}{\eta}\right) \right], \quad (8)$$

with an η -independent constant A . In other words, we obtain for the relevant transition amplitude

$$I \propto \eta^{3/2} \exp[(0.614 - 1/2)\pi\eta]. \quad (9)$$

Thus, opposite to the usual Coulomb barrier factor $\exp(-\pi\eta)$ which for increasing η decreases, we have now an increasing factor. Therefore, due to the fact that instead of a short-ranged bound state we deal with a resonance state of long range, the contributions to the overlap integral originate essentially from intermediate and large distance regions.

The present report aimed at pointing out the general property (9) valid in all situations of the type considered here. The specific features of any concrete example enter the problem via the reduced mass μ and the charge numbers Z_1, Z_2 in the Sommerfeld parameter η , and via the normalization factors N_{res} and N_{mol} . By adequately choosing these factors, fairly realistic values of the transition amplitudes (3) can be obtained for the present and all analogous cases. Multiplying the squares of these amplitudes by $\omega = |\epsilon_{\text{mol}}|/\hbar$, with ϵ_{mol} being the binding energy of the molecular state ψ_{mol} , one ends up with estimates of the corresponding reaction rates. All this will be the subject of practical applications of the above formalism to special cases, e.g., the $d + {}^6\text{Li}$ system.

As discussed at the beginning, the rotationally excited ($pp^{16}\text{O}$) state appears as a promising example for fusion reactions in normal (electronic) molecules. Qualitatively a similar behaviour as in the two-body case is to be expected also in this three-body case, a prediction confirmed by recent calculations based on estimates similar to the ones described above [7].

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