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CLUSTER–IMPACT FUSION: BRIDGE BETWEEN HOT AND COLD FUSION?*

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ABSTRACT

Beams of D_2O clusters with $10 \sim 1000$ eV per deuterium yield unexpectedly high fusion rates. This is an energy range intermediate between hot and cold fusion, and as such may serve as a link bridging the two regimes. We present a theoretical model capable of explaining apparently conflicting experimental results with beams of D_2O clusters in which fusion rates higher than expected were observed, and beams of D_2 clusters in which no fusion was observed. Calculated results indicate that total deuterium–deuterium fusion rates can be enhanced by many orders of magnitude by the use of deuterium–heavy atom cluster beams. A set of experimental tests is proposed.

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ABSTRACT

Beams of D_2O clusters with $10 \sim 1000$ eV per deuterium yield unexpectedly high fusion rates. This is an energy range intermediate between hot and cold fusion, and as such may serve as a link bridging the two regimes. We present a theoretical model capable of explaining apparently conflicting experimental results with beams of D_2O clusters in which fusion rates higher than expected were observed, and beams of D_2 clusters in which no fusion was observed. Calculated results indicate that total deuterium-deuterium fusion rates can be enhanced by many orders of magnitude by the use of deuterium-heavy atom cluster beams. A set of experimental tests is proposed.

I. INTRODUCTION

Beuhler *et al.*[1,2] (BFF)[1] report cluster-impact fusion rates $\sim 10^{25}$ times higher than expected[3,4] from single deuterium-deuterium $(D-D)$ collisions at center of mass (CM) energies of 150 eV/D, and $\sim 10^{100}$ times higher at 15 eV/D. This is reminiscent of the unexpectedly high fusion rates reported for cold fusion.[5,6] The deuterium energy range for cluster-impact fusion is intermediate between hot and cold fusion, and as such may serve as a link bridging the two regimes. Several theoretical models[7-9] have been proposed to explain the discrepancy but fail to reproduce the observed fusion rates[1] by many orders of magnitude.[10] In a previous paper,[3] one of us demonstrated that the factor of 10^{25} could not be accounted for by compression and electron screening alone which could at most account for only a factor of $\sim 10^{10}$. This left an unaccounted discrepancy of 10^{15}.

Beuhler *et al.*[1,2] measured $D-D$ fusion rates in a series of experiments in which singly charged clusters of D_2O molecules ($(D_2O)_n^+$, $n = 25 - 1300$) accelerated to 200 to 325 keV (with a beam current of $\sim 1\ nA$) were incident on TiD, $(C_2D_4)_n$ and $ZrD_{1.65}$ targets. The unexpected results of these experiments with D_2O clusters which correspond to fusion rates $\sim 10^{-1}s^{-1}/D-D$ appear to be contradicted by Fallavier *et al.*[11] (FKPRT) who carried out similar experiments using pure deuterium clusters ($D_{200}^+ \sim D_{300}^+$) with kinetic energies of 100 - 150 keV in the same range of incident CM energy per deuteron (200 eV $\sim$ 375 eV) and observed no $D-D$ fusion events. Their upper limit[11] for the fusion rate is more than one order of magnitude below the observed value of BFF.[1]

In this paper, we describe in greater detail our recently proposed cluster–transport impact–fusion mechanism[12] to describe both these positive[1,2] and negative [11] results from the cluster–beam fusion experiments.[1,2,11] We show that heavy atoms such as O in the cluster, and Ti, Zr, or C in the target are essential for obtaining high fusion rates by Rutherford double–backscattering and energy reflection enhancement of the D's for the experiments as conducted, and thus we can reconcile the conflicting results. We also predict the conditions required for comparable yields from D and D_2O clusters. As previously suggested by one of us,[4] a resonance cross–section is proposed as an explanation for the behavior of the very low–energy data as the number of molecules in a cluster increases to $n \approx 400 \sim 1000$, or as the energy per D decreases to 15 eV in the CM system.

II. OUR THEORETICAL MODEL AND ANALYSIS

In our model, molecular clusters $(D_\alpha X_\beta)_n^+$, of ~ 10 Å size disintegrate into $(\alpha+\beta)n$ atoms upon impact with the target during $\Delta t \sim 10^{-14}s$ for a cluster velocity of $\sim 10^7 cm/s$. During Δt, we assume that a local Maxwell-Boltzmann (M–B) distribution $f(\vec{r},\vec{v},t)$ is developed for the $(\alpha+\beta)n$ atoms due to a local thermalization using a fraction of the total kinetic energy E_t. Although the total number of atoms per cluster is limited to $(\alpha+\beta)n$, the total number N_t of atoms involved with a cluster–beam with an intensity of $\sim 1\ nA$ is large, $N_t = 0.625 \times 10^{10}(\alpha+\beta)n/s$ ($\approx 2 \times 10^{12}/s$ for $(D_2O)_{100}$), and hence can be regarded as a reasonable statistical system moving with the total kinetic energy E_t. Recent molecular–dynamics simulations by both Carraro *et al.*[7] and Shapiro and Tombrello[13] indicate that the high energy tail of the energy distribution decays approximately exponentially like the M–B distribution as produced in the early stages of the collisional cascade initiated by cluster impacts.

II.A. Energy Enhancement by Rutherford Double–Backscattering

The enhancement of the $D-D$ fusion rate over the conventional estimate is expected for the case of the $(D_2O)_n^+$ beam[1] but not for the case of the $(D)_n^+$ beam[11] because deuteron thermalization mainly occurs due to multiple scatterings between incident deuterons, heavy target atoms (e.g., Ti), and oxygen atoms in the clusters after the breakup of the D_2O atoms. For example, if an incident deuteron with an initial (cluster) velocity v_i in the leading edge of the cluster backscatters first from a target titanium atom and then again from an incoming oxygen atom, the deuteron can be accelerated to a final maximum velocity of $v_f = [((M_{Ti}-m)/(M_{Ti}+m))((M_0-m)/(M_0+m)) + 2M_0/(M_0+m)]v_i \approx 2.49\ v_i$; i.e., the kinetic energy of the incident deuteron can increase by a factor of $(v_f/v_i)^2 \approx 6.2$. In contrast, for the case of a pure deuterium $(D)_n^+$

beam, similar double backscatterings of an incident deuteron from a target titanium atom and then from another incoming deuterium atom cannot increase the deuteron kinetic energy since the final maximum deuteron velocity is given by $v_f = [((M_{Ti} - m)/(M_{Ti} + m))((m - m)/(m + m)) + 2m/(m + m)]v_i \approx v_i$. Therefore, the presence of heavy atoms in the $(D_2O)_n^+$ cluster efficiently populates the high energy tail of the deuteron M–B distribution via multiple collisions that lead to substantial thermalization during the impact time period of $\Delta t \approx 10^{-14}$ seconds, and hence to enhanced reaction rates. The pure deuterium $(D)_n^+$ cluster beam will not achieve as high a degree of thermalization as the $(D_2O)_n^+$ clusters upon impact, and only inefficiently populates the high energy tail because of the absence of heavy atoms in the $(D)_n^+$ cluster; this means less enhanced (smaller) reaction rates.

One can now ask whether Rutherford double–backscattering can actually have a significant effect on the high–energy tail of the deuteron velocity distribution. We consider the specific case of the original BFF experiment. We define the fraction of deuterons which undergo backscattering as

$$F = Pt = \tilde{n}\sigma v t \tag{1}$$

where $P = \tilde{n}\sigma v$ is the probability per unit time for a single deuteron to backscatter from a layer of target atoms (titanium), $\tilde{n}$ is the density of the target at its surface layer, v is the incoming deuteron velocity, and σ is the backscattering cross–section

$$\sigma = \int_0^{2\pi} d\phi \int_{\pi/2}^{\pi} d\theta \sigma(\theta) \sin\theta \tag{2}$$

Here we take $\sigma(\theta)$ to be the Coulomb differential scattering cross–section:

$$\sigma(\theta) = \left(\frac{Z_d Z_t e^2}{2\tilde{\mu} v^2}\right)^2 \frac{1}{\sin^4 \frac{\theta}{2}} \tag{3}$$

where Z_d, Z_t are the atomic numbers for the deuteron and target atoms, respectively, and $\tilde{\mu}$ is the reduced mass. For the present case, $\tilde{\mu} \approx m_d$ is the deuteron mass. After inserting (3) into (2) and integrating, we find that

$$\sigma = \pi \left(\frac{Z_d Z_t e^2}{m_d v^2}\right)^2 = 1.63 \times 10^{-20} \left(\frac{Z_d Z_t}{E_d(\mathrm{keV})}\right)^2 cm^2 \tag{4}$$

where $E_d = m_d v^2/2$. In eq. (1), t is the time it takes a deuteron to penetrate the target layer, assuming a hard–sphere interaction. Therefore if one defines d to be approximately the target atomic or ionic diameter, then $t \approx d/v$ so that eq. (1) thus gives an approximate backscattering probability:

$$F = \tilde{n}\sigma d = 1.63 \times 10^{-20} cm^2 \tilde{n} d \left(\frac{Z_d Z_t}{E_d(\mathrm{keV})}\right)^2 \tag{5}$$

(for the maximum energy enhancements which we calculate below for double-backscattering, F calculated from eq. (5) is an overestimate, since maximum energy enhancement occurs when the scattering angle is $\theta \approx 180°$–eq. (5) describes the *total* backscattering probability of the deuteron anywhere into the backward hemisphere for any final deuteron kinetic energy). For the case of a 0.1 keV deuteron backscattering off a titanium lattice surface, we have $\tilde{n} = n_{Ti} \simeq 5.7 \times 10^{22} cm^{-3}$ and $d \approx 2 \times 10^{-8}$ cm ($\sim$ atomic diameter), so that $F = F_{DTi} \approx 0.90$. For the case of a $\sim$ 0.1 keV deuteron backscattering from an oxygen atom in the D_2O cluster, $\tilde{n} = n_{D_2O} \approx 3.0 \times 10^{22}$ cm^{-3} and $d \approx 3 \times 10^{-8}$ cm, so that $F = F_{DO} \approx 0.094$. Therefore, taking into account that a deuteron which backscatters from titanium loses very little energy, the probability that a 0.1 keV deuteron firsts backscatters from a titanium nucleus and then off an oxygen nucleus is $F_1 = F_{DTi}F_{DO} = (0.90)(0.094) = 0.085$, i.e., a 100 eV cluster deuteron has a 1 in 12 chance of undergoing a Rutherford double–backscatter and being accelerated to a kinetic energy as large as 620 eV. Note that F_1 is probably conservative, since the deuteron interacts electrodynamically with the heavy atoms well beyond the hard–sphere radius.

Observe that eq. (5) indicates that $F \propto E_d^{-2}$, so that if a 620 eV deuteron undergoes the double backscatter described above, it has a probability of $F_1 = 0.085/(6.2)^4 = 5.7 \times 10^{-5}$ of doing so. Therefore the probability that a 100 eV deuteron will undergo two double backscatterings will be $F_2 = F_1(.1 \text{ keV}) \times F_1(.62 \text{ keV}) = 4.9 \times 10^{-6}$, if the deuteron picks up maximum energy after it backscatters from an oxygen for the first time. The above value for F_2 is almost certainly a lower limit, given that the deuteron will generally not pick up the maximum energy available from the oxygen atoms, and given the conservative nature of F_1. Therefore, F_2 can easily be a few orders of magnitude larger, and we may conclude that for low energy ($\sim$ 100 eV) deuterons single double–backscattering most likely (and double double–backscattering possibly) contributes significantly to the thermalization process in cluster breakup. Note that F_1 and F_2 will be significantly higher for smaller E_d than for larger E_d (since $F_2 \propto E_d^{-4}$), so that large clusters with small E_d will be affected much more by this multi-scattering process than small clusters with large E_d. Therefore, this process may make a contribution to the slow drop off of yield with increase in cluster size as observed by BFF[1] (see below). It is also possible that for small E_d, atomic backscattering may have a larger cross–section than the higher–energy Rutherford backscattering, thus increasing the probability for energy enhancement by multiple backscattering at lower energies.

II.B. Low–Energy $D - D$ Fusion Cross Sections

For $D - D$ fusion, the two dominant channels are

$$D + D \rightarrow {}^3\text{H}(1.01 \text{ MeV}) + p \ (3.02 \text{ MeV}) \tag{6}$$

and

$$D + D \rightarrow ^3\text{He}(0.82\text{ MeV}) + n\ (2.45\text{ MeV})\ . \qquad (7)$$

Experimental values of the cross–section, $\sigma(E)$, for (6) and (7) can be parameterized as[14]

$$\sigma(E) = \frac{S(E)}{E}\, e^{-(E_G/E)^{1/2}} \qquad (8)$$

where E_G is the "Gamow energy" given by $E_G = (2\pi\alpha Z_p Z_D)^2\mu c^2/2$ or $E_G^{1/2} = 31.39\ (\text{keV})^{1/2}$ for the deuteron reduced mass $\mu \approx m/2$. E is in units of keV in the CM reference frame. The astrophysical factor, $S(E)$, is extracted from the experimentally measured values[14] of the cross–section, $\sigma(E)$, for $E \gtrsim 4$ keV and is nearly constant[14] ($S(E) \approx 52.9$ keV $- b$) for both reactions (6) and (7) in the energy range of interest here, $E \lesssim 1$ keV, assuming an equal branching ratio. However, if $\sigma(E)$ happens to have resonant behavior at low energies as previously suggested by one of us,[4] the extrapolation method may yield erroneous values for $\sigma(E)$ or $S(E)$ at low energies, since the non-resonant relation, eq. (8), is not applicable to cases involving resonant reactions.[4,14]

For the case of possible low–energy resonances,[4] the cross–section for reactions (6) or (7) is given by ($(\alpha) = (6)$ or (7))

$$\sigma^{(\alpha)}(E) = \sigma(E) + \sigma_R^{(\alpha)}(E) + \text{interference terms} \qquad (9)$$

where the resonance cross–section is parameterized as[14]

$$\sigma_R^{(\alpha)}(E) = \frac{\pi\hbar^2}{M_D E}\, \frac{\omega^{(\alpha)}\Gamma_{ent}\Gamma^{(\alpha)}}{\left(E - E_r^{(\alpha)}\right)^2 + \Gamma^2/4} \qquad (10)$$

where $\omega^{(\alpha)}$ is a spin statistics factor, Γ_{ent} and $\Gamma^{(\alpha)}$ are partial widths for the entrance and exit (α) channels, respectively, and Γ is the total width.

II.C. Incomplete Thermalization with a Shifted Maxwell–Boltzmann Distribution

As a lowest–order solution to the Boltzmann transport equation, the local M–B distribution for deuterons in clusters can be written as[15]

$$f(\vec{r}, \vec{v}, t) = f(\vec{v}) = \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-m(\vec{v}-\vec{v}_d)^2/2kT} \qquad (11)$$

where m is the deuteron rest mass and $\vec{v}_d$ is the average deuteron transport velocity. Both $\vec{v}_d$ and T are functions of $\vec{r}$ and t. Before the cluster impacts on the target, $\vec{v}_d(\vec{r}, t)$ has a constant value $\vec{v}_0$ which is related to E_t by $m\, v_0^2/2 = E_t m/(\alpha m + \beta M)n$ with rest mass M for the atom X. $f(\vec{v})$ as given by eq. (11)

has the following properties: $\langle\vec{v}\rangle = \int \vec{v} f(\vec{v}) d^3v = \vec{v}_d$, $\langle m(\vec{v}-\vec{v}_d)^2/2\rangle = 3kT/2$, and $f(\vec{v}) \rightarrow \delta(\vec{v}-\vec{v}_0)$ in the limit as $kT \rightarrow 0$, corresponding to a monoenergetic deuteron beam with deuteron kinetic energy $mv_0^2/2$ (no thermalization after impact). We note that the deuteron transport kinetic energy $mv_d^2/2$ during the impact time ($\Delta t \sim 10^{-14}s$) is restricted by $0 \leq mv_d^2/2 \leq mv_0^2/2$. The average kinetic energy $\langle mv^2/2\rangle$ for a deuteron due to impact thermalization is now given by

$$\langle mv^2/2\rangle = (m/2)\int v^2 f(\vec{v}) d^3v = mv_d^2/2 + 3\ kT/2\ . \tag{12}$$

The thermalization energy $3kT/2$ comes from energy transferred from the heavy atoms of mass $M >> m$ by multiple collisions between the deuterons and the heavier atoms. For complete thermalization, $v_d = 0$ in eq. (11) (similarly, $v_X = 0$ in an equation like eq. (11)) so that $3kT/2 = 3kT_{max}/2 = E_t/(\alpha+\beta)n$ (and $kT = kT_{max}$ also for the X atoms) using the equipartition theorem for thermal equilibrium. Total energy conservation for each cluster requires that $mv_d^2/2 + 3kT/2 = 3kT_{max}/2$ and $Mv_X^2/2 + 3kT_X/2 = 3kT_{max}/2$ with the restrictions that $mv_d^2/2 \leq mv_0^2/2$ and $Mv_X^2/2 < Mv_0^2/2$. At thermal equilibrium, $kT_X = kT = kT_{max}$ ($v_d = v_X = 0$), while for the nonequilibrium situation, $kT_X \neq kT$ ($v_d \neq 0$, $v_X \neq 0$). Although the M–B distribution with $\vec{v}_d = 0$ in eq. (11) has been used in previous theoretical studies,[7-10] the $\vec{v}_d \neq 0$ case for cluster–impact fusion was first studied by us.[12].

We assume that the deuteron flux described by $f(\vec{v})$, eq. (11), after impact thermalization, impinges on the target (TiD, etc.). For the local M–B distribution, $f(\vec{v})$, eq. (11), the fusion rate R_{calc} for the reaction $D(D,p)T$ is given by

$$R_{calc} = (\Phi/v_0)\int v f(\vec{v})\ P(v)\ d^3v \tag{13}$$

where $\Phi = n_i A v_0$ (number of incident $D's$ per unit time) is the initial D flux incident on the target area A with an incident deuteron density n_i, and $P(v)$ is the probability for a deuteron to undergo a fusion reaction while slowing down in the target, which can be written as $P(v) = n_D \int_0^{E_i} dE_D\ \sigma(E_{DD})/|dE_D/dx|$ with $E_i = mv^2/2$. E_D and E_{DD} are the deuteron kinetic energies in the laboratory (LAB) and CM frames, respectively ($E_{DD} = E_D/2$), dE_D/dx is the stopping power[15] and $\sigma(E)$ is the $D-D$ fusion cross-section.

For order of magnitude estimates, the $D-D$ fusion reaction rate, R_{calc}, eq. (13), can be approximated as

$$R_{calc} \approx g(\Phi/v_0)\Delta x \Lambda(E_d) = g(0.261\times 10^{-12}s)\Phi\Lambda(E_d) \tag{14}$$

where Δx is an effective interaction thickness ($\sim 10^2 - 10^3$ Å) of the target given by $\Delta x = \int_o^{E_o} |dE_D/dx|^{-1} dE_D \approx 0.81\times 10^{-5}(E_0(\text{in keV}))^{1/2}\ cm$ with $E_0 = mv_0^2/2$, and $\Lambda(E_d)$ is given by

$$\Lambda(E_d) = n_D\langle\sigma v\rangle = n_D\int\sigma(v)vf(\vec{v})d^3v\ , \tag{15}$$

for a deuteron density n_D in the target and $E_d = mv_d^2/2$. n_D is assumed to be the same as the titanium density $n_{Ti} = n_D = 5.7\times 10^{22}\ cm^{-3}$.

Following initial contact with the target, the cluster is no longer a closed system and a small fraction of the incident atoms is lost out of the interaction region mostly in the backward hemisphere. The factor g in eq. (14) is included to account for the fraction of incident D's that are lost due to backscattering. In the calculations, g is set to 0.5, which is appropriate for the case of a completely thermalized cluster. For incomplete thermalization, g should be between 0.5 and 1.0, but, as a conservative estimate, it is kept at 0.5.

With $f(\vec{v})$ given by eq. (11), $\Lambda(E_d)$, eq. (15), becomes

$$\begin{aligned}\Lambda(E_d,kT) &= n_D\frac{2}{v_d}\left(\frac{2}{\pi mkT}\right)^{1/2}\int_0^\infty dv\ e^{-2(E_G/m)^{1/2}/v}S\left(mv^2/4\right)\\ &\times\ e^{-m(v^2+v_d^2)/2kT}\left(e^{mvv_d/kT}-e^{-mvv_d/kT}\right)\ .\end{aligned} \tag{16}$$

For the case of $v_d = 0$ corresponding to a completely thermalized M–B distribution, eq. (15) or eq. (16) reduces to[17]

$$\tilde{\Lambda}(E_T) = \Lambda(0,kT) = n_D\left(\frac{8}{m\pi}\right)^{1/2}\frac{1}{(E_T)^{3/2}}\int_o^\infty\sigma(E/2)e^{-E/E_T}EdE \tag{17}$$

with $E_T = kT$ for E in the LAB frame, and

$$\tilde{\Lambda}(E_T) = \Lambda(0,kT) = n_D\left(\frac{8}{\mu\pi}\right)^{1/2}\frac{1}{(E_T^{cm})^{3/2}}\int_o^\infty\sigma(E_{cm})e^{-E_{cm}/E_T^{cm}}E_{cm}dE_{cm} \tag{18}$$

with $E_{cm}(= E/2)$ in the CM frame, the reduced mass, $\mu = m/2$ and $E_T^{cm} =$ kT/2. In one double backscattering of a D from a target Ti and then from a projectile O, the D increases its energy by a maximum factor of 6.2. For two double backscatterings the maximum energy gain factor is $(6.2)^2 = 38.4$. Thus Rutherford double–backscattering can quickly populate the high–energy tail of the M–B distribution during complete or partial thermalization of the $(D_2O)_n^+$ cluster. Hence, the upper limit of integration in eqs. (16) and (17) is expected to be greater than approximately 500 eV $\times$ 38.4 $\approx$ 19 keV. We therefore set the upper limit to be infinity in our calculations; this is expected to give our results an overestimate of one order of magnitude or less.

Note that for monoenergetic deuterons, $f(\vec{v}) = \delta(\vec{v}-\vec{v}_0)$, and R_{calc} as given by eq. (13) reduces to[18]

$$R_{calc}(mono) = \Phi P(E_0) = \Phi(2.3 \times 10^{-6})\exp(-44.40/\sqrt{E_0(\text{keV})})\,. \tag{19}$$

II.D. Cluster–Size Distribution

As part of the experiments of Beuhler *et al.*[2], the incoming cluster beam before acceleration was mass–analyzed, and found to have a shape that is well–described by a Gaussian or Poisson distribution.[5] The distribution was found to typically have a full-width half-maximum $\Delta n \approx 0.38$; the distribution peak, $\overline{n}$, is the value ascribed to the cluster size (i.e., $(D_2O)^{\pm}_{\overline{n}}$) for a given run of the experiment.

If we represent the cluster size distribution as Gaussian in the experiments of Beuhler *et al.*, and assume complete thermalization ($v_d = 0$ in eq. (11)), we may define the following cluster size (n) dependent M–B–like velocity distribution for use in our calculation:

$$\begin{aligned} f(v,n) &= \tilde{N}\,\exp\left(\frac{-mv^2}{2kT}\right)\exp\left(\frac{-(n-\overline{n})^2}{2\overline{\sigma}^2}\right) \\ &= \tilde{N}\,\exp\left(\frac{-9nE_{cm}}{E_t}\right)\exp\left(\frac{-(n-\overline{n})^2}{2\overline{\sigma}^2}\right)\,, \end{aligned} \tag{20}$$

since $E_{cm} = mv^2/4 = \mu v^2/2$ and $kT = 2E_t/9n$, where

$$\overline{\sigma} = \frac{(\Delta n)\overline{n}}{2\sqrt{ln\ 4}} = \frac{0.19\overline{n}}{\sqrt{ln\ 4}}$$

is the Gaussian width of the $(D_2O)^{\pm}_{\overline{n}}$ mass distribution. We solve for the normalization factor, $\tilde{N}$, via the requirement that $1 = \int d^3v \int dn\ f(v,n)$, and then solve for the fusion rate

$$\Lambda(\overline{n}) = n_D\langle\sigma v\rangle = n_D \int d^3v \int dn\ \sigma v f(v,n)\,. \tag{21}$$

Using eq. (8) for σ, we then find

$$\tilde{N} = \frac{\mu^{3/2}}{4\pi\sqrt{2}}\left[\int_0^{E_c} \sqrt{E}I(E)dE\right]^{-1}\,, \tag{22}$$

and

$$\Lambda(\overline{n}) = \sqrt{\frac{2}{\mu}}\left[\int_0^{E_c} \sqrt{E}I(E)dE\right]^{-1} \int_0^{E_c} S(E)e^{-(E_G/E)^{1/2}}I(E)dE\,, \tag{23}$$

where

$$
\begin{aligned}
I(E) &= \int_{\hat{n}}^{\infty} e^{-9n\ E/E_t} e^{-(n-\overline{n})^2/2\overline{\sigma}^2} dn \\
&= \frac{1}{2}\sqrt{2\pi}\overline{\sigma}\exp\left(\frac{E}{E_T^{cm}} - \frac{(\Delta n)^2}{16\ ln\ 2}\left(\frac{E}{E_T^{cm}}\right)^2\right) \qquad (24) \\
&\times \mathrm{erfc}\left(\frac{\Delta n}{4\sqrt{ln\ 2}}\frac{E}{E_T^{cm}} + \frac{(\hat{n}-\overline{n})}{\sqrt{2}\ \overline{\sigma}}\right) .
\end{aligned}
$$

Here E_c, $\hat{n}$, and erfc(x) are the cutoff energy for the velocity portion of the distribution, the cutoff cluster size for the mass portion of the distribution, and the complimentary error function, respectively. In Eqs. (22) - (24), $E = E_{cm} = mv^2/2$. Note that one can have $\hat{n} \geq 1$; it is claimed by Beuhler et al.[2] that $\hat{n} = \overline{n}/2$.

III. COMPARISON WITH PREVIOUS THEORETICAL WORK

In this section, we discuss some of the previous theoretical work by others in order to clarify differences between their models and ours, to describe the relevance of the previous work to our work, and to indicate some obvious errors and inconsistencies in the previous work.

III.A. Critique of EMR's Work

In a recent theoretical paper,[8] Echenique *et al.* (EMR) claim to provide an explanation for the recent cluster–impact fusion experiments.[1] However, both papers[1,8] contain several errors.

First, both Refs. 1 and 8 address resolving a discrepancy of only 10^{10} between measured and expected reaction rates (assuming a monoenergetic deuterium velocity distribution). However, more correctly, a difference of 10^{25} must be explained.[3,4] Our calculation[3,4] shows a discrepancy of 10^{25} rather than the one of 10^{10} suggested by BFF[1] and addressed by EMR.[8] The difference between 10^{25} and 10^{10} is the difference between properly doing the calculation in the CM frame, and doing it improperly in the LAB frame. Their error[1,8] is due to the incorrect use of $E(LAB)$ (instead of using the correct $E(CM) = E(LAB)/2$) in $\sigma(E)$ (eq. (8)) in their paper,[1,8] as first pointed out by one of us.[3] References 14 and 17 also provide clarification on this point.

Second, eq. (3) of Ref. 8 (compare with our eq. (18)) would be correct for CM energies if $\sqrt{2}$ is eliminated and their $E_0 = kT/2$ assuming a M–B deuterium velocity distribution. However, a crucial topic is the determination of E_0 given N particles obeying a M–B velocity distribution with total LAB cluster kinetic energy E_t. A simple calculation shows that $E_t = N(3\ kT/2) = 3NE_0$, or $E_0 = E_t/3N$. For their example given below eq. (3) in Ref. 8 where $E_t = 300$ keV and $N \sim 1000$, E_0 is given as 500 eV instead of the correct value of 100 eV. When the correct value of 100 eV is used to calculate the fusion rate, a value of $R \approx 10^{-8} s^{-1}$ is obtained instead of the quoted 0.08 s^{-1} for the incorrect $E_0 = 500$ eV.

The choice of E_0 cannot be arbitrarily independent of their choice of distribution (equilibrium, non–equilibrium, etc.). The choice of E_0 is constrained by both the conservation of energy and the conservation of the number of particles. Their eq. (3) incorporates a M–B distribution as they state.[8] They did an equilibrium calculation. The words "non–equilibrium" do not occur anywhere in their paper,[8] though they do suggest future calculations that are conceptually of such a nature. We have carried out a non–equilibrium calculation[12] as described earlier in this paper. We find a significantly lower E_0 than EMR's 500 eV rather than a higher E_0 as claimed by EMR. Our paper shows that a shifted local M–B distribution as a solution to the Boltzmann transport equation gives a lower fusion rate than a fully thermalized distribution precisely because there are fewer particles in the high energy tail. We emphasize that non–equilibrium implies a smaller E_0 than the 500 eV used by EMR,[8] and that this choice by EMR violates conservation of energy and number of particles. Furthermore, EMR never explicitly give E_0 in terms of total cluster energy and cluster size in their paper,[8] thereby rendering Fig. 1 of EMR unverifiable.

Third, the theoretical curve in Fig. 1 of Ref. 8 cannot be reproduced without more information on the dependence of the number of particles in the impact region (N) as a function of the number of D_2O molecules in the cluster (n) and total cluster energy (E_t). With a simple model where the cluster thermalizes upon impact before equipartitioning its energy with the target, one obtains $E_0 = E_t/9n$, and for the example mentioned above with $n = 100$, the result of $E_0 = 333$ eV yields $R \approx 0.003\ s^{-1}$, which is about 25 times smaller than the value of 0.08 s^{-1} calculated with the physically unacceptable value of $E_0 = 500$ eV.

Furthermore, Fig. 1 in Ref. 8 (reproduced as our Figure 1) is misleading if not examined carefully. Their calculated[8] and experimental[1,8] values were normalized to unity at $E_t = 300$ keV, which gives rise to the potentially deceptive conclusion that their calculated rates fit the experimental values. However, for our simple model where $E_0 = E_t/9n$ and a comparison calculation where $E_0 = E_t/6n$, the normalized values differ only slightly from the plotted curve in Fig. 1 of Ref. 8. But, when the actual rates are compared, we find that our calculated values differ from the experimental results by some four orders of magnitude for $E_0 = E_t/9n$ and by two orders of magnitude for $E_0 = E_t/6n$, while it is unclear from Ref. 8 what their actual reaction rates are for the case of $n = 150$ (Fig. 1) since they give neither the details of their model nor a calculated value.

Finally, calculations done with a M–B distribution and $E_0 = E_t/9n$ give reaction rates that differ from those in Fig. 3 of BFF[1] (for $E_t = 300$ keV) by 10 orders of magnitude for $n \approx 1000$. This appears to contradict the statement by EMR[8] that their model qualitatively explains the dependence of the fusion rate R on cluster size.

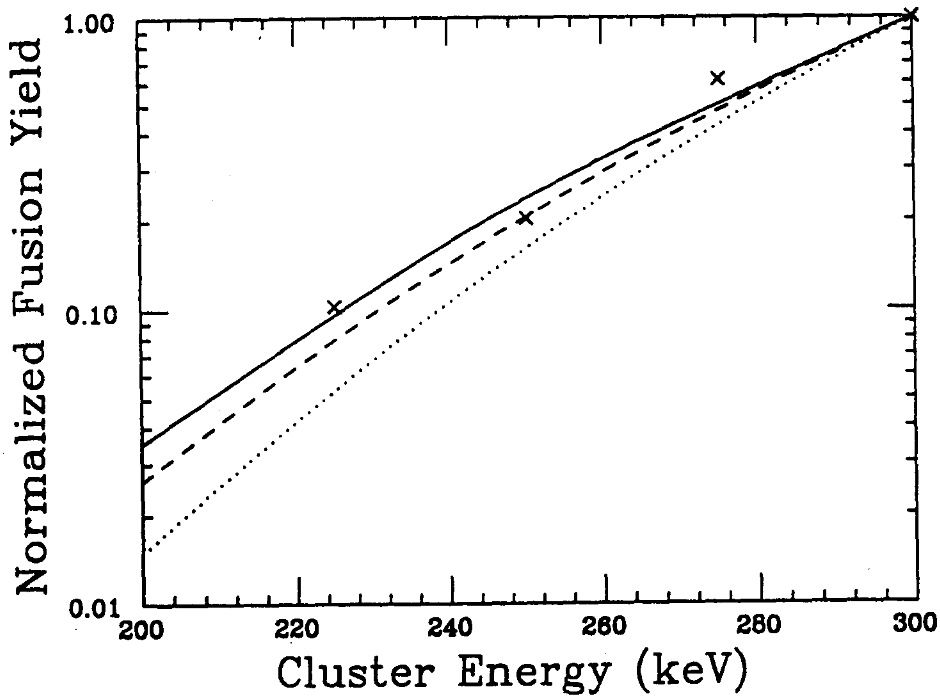

Figure 1: Normalized deuteron-deuteron fusion rate R for $(D_2O)_{150}$ clusters incident on a TiD target as a function of total cluster laboratory energy E_t. The experimental points $(\times)$ and the fit of Echenique et al. (solid line) were extracted from Fig. 1 of Ref. 8. The other two curves are from our fit from eq. (3) of Ref. 8 (i.e., our eq. (18) with E_T^{cm} replaced by E_o) for $E_o = E_t/6n$ (dashed line) and for $E_o = E_t/9n$ (dotted line) for $n = 150$.

III.B. Molecular Dynamics Simulations

Molecular dynamics (MD) simulations carried out by Carraro *et al.*[7] and also by Shapiro and Tombrello[13] show that the density in the interaction region reaches its maximum value of about twice the initial target density during the first $\sim 10^{-14}s$. From the above result of MD simulations, it is tempting to conclude that during this $10^{-14}s$ energy not only is being shared among the atoms of the cluster but among a similar number of target atoms. However, such a conclusion may be premature since it is based on the assumption of the equipartition of energy among both target and incident cluster atoms, which is not applicable to incomplete thermalization.

The increase of the target density during the first $10^{-14}s$ of MD simulations does not necessarily imply equipartition of energy among both target atoms and incident cluster atoms, since they are in a non-equilibrium situation. The incident deuterium atoms will carry most of the available energy due to efficient energy enhancement mechanisms such as the double backscattering mechanism described above, thus contributing to the high velocity components described by the non-equilibrium velocity distribution, $f(\vec{v})$ of eq. (11), while the target deuterium (and Ti and O) atoms in the impact region will share a substantially smaller fraction of the available energy due to the fact that there are no efficient energy transfer mechanisms for them to populate higher velocity components during the first $\sim 10^{-14}s$. Therefore, the effective temperature for the incident projectile deuterium atoms can be substantially higher than that of the target deuterium (and Ti and O) atoms and also higher than if the energy were shared equally among both target and projectile atoms, because not all the target atoms in the impact region can share in the equipartition of energy. For our shifted M–B distribution (when $v_d = v_0$), the effective temperature is 70% of the maximum thermalization temperature. As can be seen for incident D_2O from our Table I, column 6, the fusion rate is decreased very little from the complete thermalization rate, at most by a factor of four for the $n = 75$ case.

A compressional increase in projectile density, n_D^{proj}, and target density, n_D^{targ}, by a factor of two can increase the fusion rate by more than an order of magnitude. The increased density contributes in two ways. The linear dependence of the fusion rate per $D-D$ collision is a minor contributor. The major contribution comes from the greatly increased probability of double backscattering which is proportional to $(n_D^{proj} n_D^{targ})^b$, where b is the number of double backscatterings (see Sect. II.A). For a density increase of two, with two double–backscatterings, the double–backscattering probability is increased by a factor of $(2 \times 2)^2 = 16$. This means a $16 \times 2 = 32$ times increase in the fusion rate from both contributions combined. In presenting a conservative calculation, we have not yet put in the effect of increased density and have only used the uncompressed densities for our results presented here.

Carraro *et al.*[7] carried out MD simulations of the impact of clusters composed of $n = 32$, 54, 80, 128, and 180 heavy–water molecules at $E_t = 100$ keV on a target composed of 1024 heavy–water molecules in a cubic box of 32 Å on a side (~ 10 atomic layers). Their result with a few cluster impacts for the energy spectrum of target deuterons for $n = 128$ at time $t = 4 \times 10^{-14}s$ shows a spectrum approximately proportional to $E^{-1.6}$ with a maximum energy cutoff at ~ 300 eV (~ 4 times the incident deuteron energy of $E_0 = 100$ keV/(10(128)) ≈ 78 eV).

Although their results[7] with an energy cutoff at ~ 300 eV with only a few cluster impacts is consistent with that of a single knock–on process (78 eV $\times$ 3.16 $\approx$ 247 eV), their MD results[7] for the energy spectrum are not applicable to our non-equilibrium velocity distribution $f(\vec{v})$, eq. (11), for the projectile deuterons, since their spectrum is for the target deuterons. Their results for the target deuteron energy spectrum would be relevant to the case of $(H_2O)_{115}$ cluster impact on a $(C_2D_4)_n$ target for which the $D-D$ fusion rate was observed by Beuhler *et al.*[2] to be about 5% of that for $(D_2O)_n$ clusters on the same target. Although Shapiro and Tombrello[13] performed their MD simulations with several thousand cluster impacts, their results are not applicable to the case of D_2O cluster impact, since they simulate the $(Al)_n - Au$ and $(Al)_n - Al$ cases for which double backscattering would be inefficient for energy enhancement and other effective energy–enhancement mechanisms are not available because $(Al)_n$ (like $(D)_n^+$) does not contain heavier atomic partners as in the case of $(D_2O)_n^+$ incident on TiD or $(C_2D_4)_n$. In fact, the results of their MD simulations[13] show that the energy of an individual atom can only increase by a maximum factor of two over the incident energy per atom, with the probability for such events decreasing very rapidly with increasing energy. Their results[13] are relevant to and consistent with our description and results for $(D)_n^+$ (but not for $((D_2O)_n^+)$ cluster impact on TiD or $(C_2D_4)_n$ targets in the context of the cluster–transport impact–fusion mechanism.

There is an error in Carraro et al.[7] Their eq. (10) is incorrect. The text on page 1382 reads, "In the case where a deuteron of energy U backscatters from a titanium atom and then again from the oxygen, the final energy $\tilde{U}$ of the deuteron is $\tilde{U}/U = [((M_0 - M_D)/(M_0 + M_D))(2M_{T_i}/(M_{T_i} + M_D))]^2 \approx 2.23$."[7] This equation with $m = M_D$ should be $\tilde{U}/U = [1 + ((M_0 - m)/(M_0 + m))((M_{T_i} - m)/(M_{T_i} + m))]^2 \approx 2.94$ if we take U to be the maximum knock–on energy a target deuteron can get from a projectile oxygen. That is, $U = mv_d^2/2$, with $v_d = (2M_0/(M_0 + m))V_0$, where V_0 is the velocity of an incident oxygen and v_d is the velocity of a (knocked–on) target deuteron. U is arbitrary in Ref. 7. In general, this ratio is $[(2M_0/M_0 + m)(V_0/v_d) + ((M_0 - m)/(M_0 + m))((M_{T_i} - m)/(M_{T_i} + m))]^2$. Since V_0/v_d can be arbitrarily large, one can have $\tilde{U}/U >> 2.94$. This error propagates into their[7] eq. (11), etc..

The ratio of the final energy of a projectile deuteron, E_{pf}, to its initial energy can also be much larger. As discussed previously, if a projectile deuteron of initial energy E_{pi} backscatters elastically from a titanium and then again from an incoming oxygen, then by conservation of momentum and kinetic energy, $E_{pf}/E_{pi} = [((M_{T_i} - m)/(M_{T_i} + m))((M_0 - m)/(M_0 + m)) + 2M_0/(M_0 + m)]^2 = 6.2$. The total energy gain, E_{tf}, from this process for a target deuteron initially at rest that is knocked–on by a projectile oxygen (triple scattering) is even larger. Since its initial energy is ~zero, let us compare its energy gain relative to the initial energy of a projectile deuteron, $E_{tf}/E_{pi} = (2M_0/(M_0 + m))^2[1 + ((M_0 - m)/(M_0 + m))((M_{T_i} - m)/(M_{T_i} + m))]^2 = (2M_0/(M_0 + m))^2(\tilde{U}/U) = 9.32$. So we see that a much larger energy enhancement is possible than 2.23. There is an oversight in their final conclusion (page 1389) "We found that no deuterium atom ever moves more rapidly than about twice the velocity of the incident cluster. . .."[7] As shown here, significantly larger velocities are possible.

IV. RESULTS

IV.A. General

Using eqs. (4) and (6), the total fusion rates R_{calc} are calculated for both the $(D_2O)_n^+$ and the $(D)_n^+$ cases using $kT_{max} = E_t/3n$ and $kT_{max} = E_t/n$, respectively. For each case, both complete thermalization ($v_d = 0$ in eq. (11)) and partial thermalization ($v_d \neq 0$ in eq. (11)) are considered. The calculated proton counts,

Table I: Comparison of our calculated $D - D$ fusion counts, $\tilde{R}_{calc} = \delta t \epsilon R_{calc}$, with the experimental data of Beuhler *et al.* (BFF)[1] as deduced by Fallavier *et al.*[11] for the case of $(D_2O)_n^+$. The total kinetic energy E_t for the various $(D_2O)_n^+$ clusters is 300 keV. R_{calc} is calculated using eqs. (14) and (16), and the detector efficiency ϵ is assumed to be 10%. The target used in Ref. 1 is TiD. The target deuteron and titanium densities are assumed to be $n_D = n_{Ti} = 5.7 \times 10^{22}$ cm^{-3}.

n	Energy $/D$ (eV)	Incident $D's(10^{15})$	$\tilde{R}_{calc}$ $(v_d = 0)$	$\tilde{R}_{calc}$ $(v_d = v_0/\sqrt{2})$	$\tilde{R}_{calc}$ $(v_d = v_0)$	$\tilde{R}_{exp}$ (Ref. 1)
40	750	6.15	153	137	102	30
60	500	3.3	5.9	5.1	3.4	16
75	400	2.2	0.8	0.7	0.2	8

$\tilde{R}_{calc} = \delta t \epsilon R_{calc}$ (where δt is the acquisition time and ϵ is the detector efficiency) are compared with the experimental results in Tables I and II for the $(D_2O)_n^+$ and $(D)_n^+$ cases, respectively.

As can be seen from Table I, our calculated proton counts agree with the results of BFF[1] to about an order of magnitude. Because there is expected to be less thermalization as the cluster size n decreases, our calculated counts probably overestimate the actual counts for smaller values of n. Furthermore, since Beuhler *et al.*[2] used $(D_2O)_n^+$ beams that contained not just a single cluster size n, but a distribution in cluster size about n, we show below that our calculated counts become increasingly enhanced as the "mean" cluster size n increases due to the contribution of small clusters in the tail of the size distribution when we include the size distribution.

The proton counts for the experiment of Fallavier *et al.*[11] were also calculated with this model, and are seen to be very small (Table II). The $(D)_n^+$ beams are not expected to have such a high degree of thermalization as the $(D_2O)_n^+$ beams (see above), so calculations for the cases where half of the kinetic energy becomes thermal ($v_d = v_0/\sqrt{2}$) and none of the kinetic energy becomes thermal (δ–function velocity distribution) are included. Clearly these calculations show that the proton count (reaction rate) falls precipitously as the degree of thermalization decreases.

Because the parametrization of the cross section[14] used here is appropriate only for the scattering of bare deuterons, the effects of electron screening[3,18,19] in the target have not been taken into consideration in our calculations. However, at the energies relevant in these experiments,[1,2,11] electron screening is expected to increase the reaction rates only one order of magnitude or less.[3,10,20]

When we apply eqs. (4) and (6) to the case of large clusters (e.g., $(D_2O)_{1000}^+$), we find that even when complete thermalization ($v_d = 0$) is assumed, the proton count will be $\tilde{R}_{calc} = \delta t \epsilon R_{calc} = 4.04 \times 10^{-14}$ per 10^{16} D's using the same value

Table II: for the case of $(D)_n^+$. The total kinetic energy per cluster is n times the energy per deuteron. The detector efficiency ϵ is assumed to be 10%. The target deuteron and titanium densities are assumed to be $n_D = n_{Ti} = 5.7 \times 10^{22}$ cm^{-3}. $R_{calc}(v_d = 0)$ and $R_{calc}(v_d = v_0/\sqrt{2})$ are calculated using eqs. (14) and (16). $\tilde{R}_{calc}(mono)$ is calculated with a delta function (monoenergetic) distribution using eq. (19). The experimental values of $\tilde{R}_{exp}$ are all zero.[11]

n	Energy /D (eV)	Incident $D's(10^{15})$	Target	$\tilde{R}_{calc}$ ($v_d = 0$)	$\tilde{R}_{calc}$ ($v_d = v_0/\sqrt{2}$)	$\tilde{R}_{calc}$(mono) (δ–function)
200	750	6.15	$(CD_2)_n$	1.71×10^{-2}	1.64×10^{-3}	1.00×10^{-13}
200	500	3.68	$(CD_2)_n$	1.78×10^{-4}	9.40×10^{-6}	4.32×10^{-19}
200	500	2.96	$TiD_{1.7}$	1.43×10^{-4}	7.56×10^{-6}	5.02×10^{-19}
250	400	2.27	$TiD_{1.7}$	9.05×10^{-6}	3.30×10^{-7}	2.50×10^{-22}
300	400	2.15	$TiD_{1.7}$	8.57×10^{-6}	3.13×10^{-7}	1.68×10^{-22}

of $\epsilon = 0.1$ as above. The equivalent proton count per 10^{16} D's from BFF[1] is $\tilde{R}_{exp} \approx 2.4$, which is some 14 orders of magnitude larger than $\tilde{R}_{calc}$ (see Fig. 2). Therefore, impact thermalization by itself is inadequate to explain the large cluster (low–energy deuteron) results of Beuhler *et al.*,[1,2] and thus some other mechanism—e.g., contaminants, low energy $D-D$ fusion resonances,[4] cluster size distribution ("mass dispersion"),[2,7] and/or electron screening[3,9,19]—must also contribute to explain these results. However, when compared to the traditionally calculated mono–energetic rate (i.e., when $f(\vec{v}) = \delta(\vec{v}-\vec{v}_0)$), $\tilde{R}_{mono} = 1.08 \times 10^{-102}$ per $10^{16} D's$, the use of a velocity distribution such as eq. (11) in $\tilde{R}_{calc}$ does account for most of the discrepancy between $\tilde{R}_{mono}$ and $\tilde{R}_{exp}$, as can be seen from Fig. 2.

In Fig. 3, we include the effects of the mass distribution. The dashed line is the case with no mass distribution (eq. (14)), the solid line is the case with $\hat{n} = \overline{n}/2$ for the cutoff of the distribution integral (eq. (24)), and the dotted line is the case with $\hat{n} = 1$ for the cutoff of the distribution integral (i.e., no cutoff). Note that for $\overline{n} = 1000$ (corresponding closely to the cold fusion case, with $E_{cm} \approx 10$ eV), the inclusion of a mass distribution with $\hat{n} = \overline{n}/2$ (the situation claimed by Beuhler *et al.*[2]) increases $\tilde{R}_{calc}$ from 5.04×10^{-14} to 2.22×10^{-11} per 1.25×10^{16}—a factor of ~ 400, but still some eleven orders of magnitude below $\tilde{R}_{exp}$. However, for the case of a mass distribution with no cutoff, $\hat{n} = 1$, $\tilde{R}_{calc}$ is now 8.59, about ~ 4 times larger than $\tilde{R}_{exp}$. This indicates that if there is some cluster breakup between the mass spectrometer and the entrance to the accelerator column in the experiments of Beuhler *et al.* that "replaces" a portion of the "missing" part of $f(n, v)$ below $\hat{n} = \overline{n}/2$, then $\tilde{R}_{calc}$ will be enhanced at least by several orders of magnitude. However, since at $n \approx 100$, $\tilde{R}_{calc}(\hat{n} = 1)$ is still more than an order of

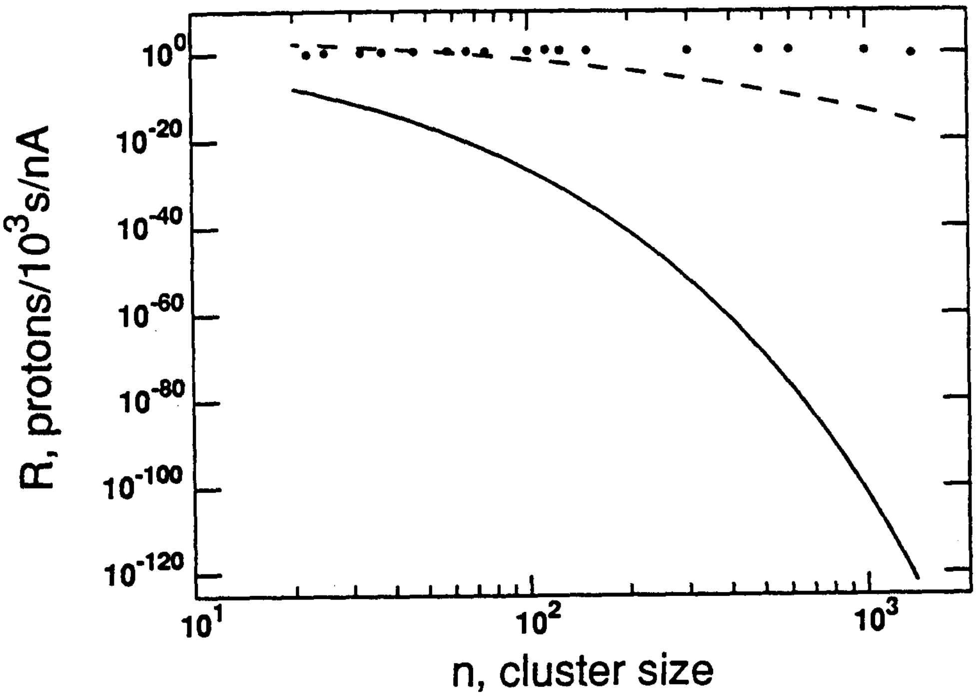

Figure 2: Proton counting rate, $\tilde{R} = \delta t\, \epsilon\, R$, as a function of cluster size, n. The units of $\tilde{R}$, $10^{-3}s^{-1}(nA)^{-1}$, is equivalent to $1.25 \times 10^{12}n$ clusters when $\epsilon = .1$ and $\delta t = 10^3 s$. The data (dots) are from Fig. 3 of Ref. 1. For comparison, we show the results for a conventional nuclear theory calculation assuming monoenergetic deuterons (solid line, eq. (19)), and for a Maxwell-Boltzmann (M-B) distribution of completely thermalized deuterons (dashed line, eq. (14) with eq. (18) for $v_d = 0$).

magnitude below $\tilde{R}_{exp}$, there are still contributing processes not yet considered to be included in our theory, which may also be important to cold fusion.

IV.B. Low–Energy Resonances

One possible candidate for the missing contribution is the existence of low-energy $D-D$ fusion cross–section resonances.[4] An example of the effect of such a resonance is shown in Fig. 4, where we have added a Breit–Wigner resonance, eq. (10), to eq. (8), and included a mass–velocity distribution, eq. (24), with $\hat{n} = \overline{n}/2$ (note that for simplicity, we do not consider interference terms here). The parameters of this Breit–Wigner resonance are as follows: the peak energy of the resonance, $E_r^{(pT)}$; the total width of the resonance, Γ; and the partial width of the $D-D$ entrance channel, Γ_{ent}, are all taken to be 400 eV; the partial width of the $p-T$ exit channel, $\Gamma^{(pT)}$, is set to 2.03×10^{-8} eV. To insure that the cross–section converges to zero as $E \rightarrow 0$, we have multiplied eq. (10) by a factor