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Highly Relativistic Deep Electrons and the Dirac equation

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Most models for CF recognize the need to overcome the Coulomb barrier between hydrogen nuclei

The electron deep orbits (EDOs) satisfy that basic need and much more. They explain:

- DD fusion to 4He without significant fragmentation.
- An accelerated version of HH => D, via the p-e-p reaction.
- Formation of femto-atoms and molecules, which are strong transmutants.
- Transmutations to stable nuclides as a source of local energy; but,
  - without hard radiation as from neutron activation, and
  - with a preference for any unstable nuclides in the lattice

This presentation updates our on-going work on the theoretical basis for EDOs in the relativistic QM equations

Here we list the properties of EDOs that make them a good model for Cold Fusion. These statements are demonstrated in previous works.

Main arguments for EDO model

- Fusion between a femto-atom and lattice nucleus N is a *3-body interaction* N+p+e. Thus, unlike *neutron activation*, which generally has only a single pathway (N+n), the femto-atom can go *three ways* (N+p, N+ e, & N+n) to get to the *lowest energy state*.

- The intimate presence of the deep-orbit electron to/in the fused nucleus provides a ready means of *dissipating fusion energy locally*, rather than by gamma decay (elimination of the D+D => 4He gamma-decay path is a proven example).

- The *lowest energy-state* "daughter" will generally be *stable*. Neutron activation often cannot even access this path and almost all transmutation paths lead to excited states that can decay only by gammas or energetic-particle decay (unless an EDO is occupied).

- Unstable nuclides are more influenced by the *extremely strong fields of a deep-orbit electron*. Their response to the potentials of a femto-atom, giving a greater *attractive force* (F = -dV/dr) between them, is the basis of "*selective transmutation*".

Now, we give some simple arguments to support them.
It is important to note that a femto-atom can induce a three-body interaction with a lattice nucleus, unlike neutron activation, and the consequences for transmutations.

I. *Initial results with Dirac equation*

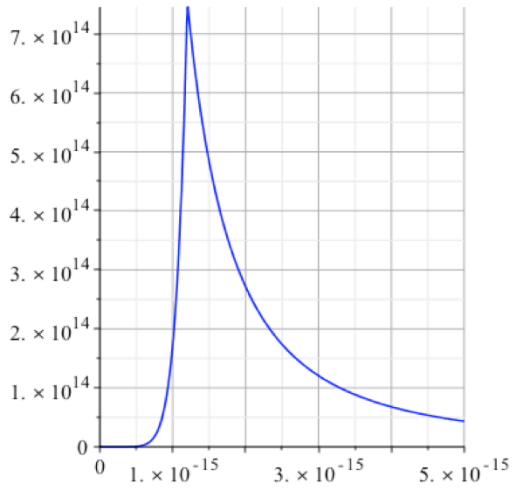
Computations of the Dirac "anomalous" wavefunctions, with finite potential inside nucleus ($r < R$), R close to the nucleus

Improvement and extension of work of Maly & Va'vra [Fus. Sc. Tech. V.24#3, V.27#1]

Example: R = 1.2 F, radial quantum n' =1

Plot of Probability Density

Energy $E \sim 1.8$ kev, mean radius $\langle r \rangle \sim 6.6$ F



To find out *how to populate deep levels*, we need to know more information, and to correct some imperfections:

- *Pb 1*. Ansatz *not allowing* to have *continuous derivatives* at *R*
- *Pb 2*. Energie *E* used to compute a solution for a *finite nucleus* is the energy *E* of solution for *point-like nucleus*
- *Pb 3*. Difficulty to evaluate the *relativistic coeff*. γ, *kinetic energy*, and other energy parameters

From Maly & Va'vra works on "anomalous" solutions of Dirac equation, we computed EDO wavefunctions with an improved ansatz, to connect the solutions inside and outside the nucleus. But it did not allow us to have derivatives continuous at the junction radius, and the energy used to compute the wavefuntion was the energy of solution for *point-like* nucleus case. Moreover, we could not evaluate the relativistic coefficient γ and energy parameters, as the kinetic energy, required for a better understanding of EDOs and possible interaction with nuclear fields.

These Imperfections are listed in the form of three problems.

II. A valuable help: *Semi-classical simulations*

• *Principle*: Radial potential = *sum of inverse power terms*, with *magnetic* interactions and *radiative corrections*.

Necessity to respect the Heisenberg Uncertainty Relation (HUR)

• Our decisive choice: **to take HUR as *Starting Point*** =>

-(i) Electrons confined in deep orbits (EDO) are *highly relativistic*,

$p \sim \hbar/r$ => $\gamma \sim (1- v^2/c^2)^{1/2} \sim [1 + (\lambda\!\!\!^{-}_c/r)^2]^{1/2}$, $\lambda\!\!\!^{-}_c$: *reduc. Compton wavelength*

if $r << \lambda\!\!\!^{-}_c$ = 386 Fermis => $\gamma \sim \lambda\!\!\!^{-}_c/r$ (Case of EDOs)

- (ii*)* Importance of a strong *relativistic* correction of Cb Potentiel *V*:
effective potential energy V_{eff} [Adamenko, Vysotskii. FoPL,17,3 & FoP,34,11]

$V_{eff} = \gamma V + V/2mc^2 \sim (\lambda\!\!\!^{-}_c e^2/r^2) (1- \alpha /2) \sim \gamma V$ in nuclear zone =>

V_{eff} can confine an EDO near the nucleus

• *Relativity, implied by HUR, is the solution for EDO confinement*

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That is why, then, we studied the possible existence of EDO's in a semi-classical way, to better know their energy parameters. First, we directly address the Heisenberg Relation as a starting point, for an electron confined in a sphere of radius *r.* From the momentum *p*, we can compute the relativistic coefficient γ, by an expression involving the *reduced* Compton wavelength. At ICCF21, we gave examples showing the expression of γ gives realistic values.

• We can see electrons confined in deep orbits are *highly relativistic.*

• But a strong relativistic correction to the Coulomb potential *can confine such energetic electrons*

Semi-classical simulations (cont'd)

Looking for a *Local Minimum of Energy* (*LME*) near the nucleus

Considering *Total Energy* TE = E_H + *PE*, *where* $E_H = \sqrt{\frac{\hbar^2 c^2}{r^2} + m^2 c^4}$

Importance of Radiative corrections near the nucleus:

(i) Lamb shift (LS) is very strong in *high electric field*, and has

(ii) *Repulsive* dominant effect (electron self-energy > vacuum polarization)

In recent work : LS expressed as a repulsive quasi-potential in $1/r^3$

Example (computations for ICCF21 paper, JCMNS)

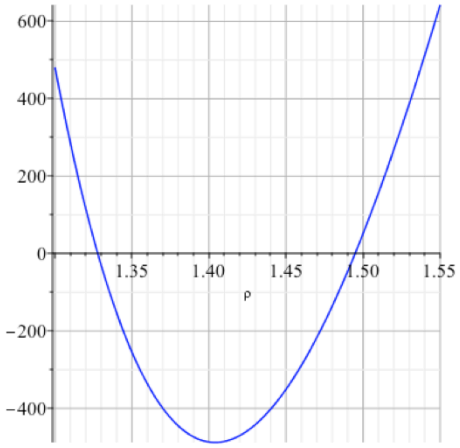
Plot of Binding Energy: BE = TE – mc^2

LME at ~ 1.4 F, $\gamma \sim 275$

Binding Energy (BE) ~ - 509 kev

Pot. Energy (PE) ~ -140.5 Mev

Kinetic Energy (KE) ~ 140 Mev



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5

In order to find EDOs, we look for a Local Minimum of Energy (LME) of electron in a central potential, obtained by a balanced combination of EM potentials near the nucleus.
Recently, we took radiative corrections into account, especially the Lamb shift, whose effects become very strong near the nucleus, because of the strength of the electric field. We expressed LS as a repulsive quasi-potential, by means of extrapolations from data tables on QED effects on orbital parameters.

From semi-classical simulations to Dirac EDO's

1. Electrons confined near the nucleus are ultra-relativistic:

At distance r, $\gamma \sim \lambda_c/r = 386/r$ where r is in Fermis

Example: for $r \sim 2$ F, we have $\gamma \sim 193$

2. For LME obtained by *combinations V* of potentials in various *inverse powers* and with diverse factors, the *virial theorem* is respected (on 4-5 decimals) at the LME radius, in the following form:

$KE / |PE| \sim \gamma/(\gamma+1)$ KE: Kinetic Energy PE: Potential Energy

3. From this, with correspondence *LME radius* --> *mean radius* $\langle r \rangle$ for Dirac EDO solutions with finite nucleus,
we can evaluate γ, TE, KE, BE at $\langle r \rangle$ TE: Total Energy

Example: $TE \sim m_e c^2/\gamma \sim m_e c^2 \langle r \rangle / \lambda_c$ [$m_e c^2 \sim 511$ kev]

=> This allows us to correctly adjust the energy levels of Dirac EDO's solutions (*Pb 2*) and to know all energy parameters (*Pb 3*)

Semi-classical studies provided a lot of useful information for correcting the imperfections of the initial Dirac EDO's for finite nucleus case (at least for two of the "three problems").

- Not only we can evaluate the gamma coefficient, but also all the energy parameters. Moreover we found that the relativistic *virial theorem was respected by ultra-relativist EDOs*, in a very simple form and for various combinations of potentials.

- This allows us to deduce all the energy parameters of the DIrac EDOs, computed at the mean radius of the probability density distribution, and to check their coherence

III. *Back to Dirac equation.*
First: what means solving a quantum equation ?

Quantum (*time-independent*) equation for a *wavefunction*: $H\,\psi = E\,\psi$,
It can be multi-dimensional (example: Dirac equation)

Summarily

-1. *H* is a Hamiltonian operator, including *differential* operators.

(for example: the momentum ***p*** is expressed by $-i\hbar\frac{\partial}{\partial x}$)

H represents the *total energy* of the considered system

---> **we have to solve *a differential equation***

-2. We have to look for ψ, unknown *wavefunction,* and for *E*, unknown eigenvalues which are *energy values* associated with quantum numbers: *energy levels* (*Pb 2*)

---> **we have to solve *a spectral problem*** (spectral theory for QM)

Now we show how to apply this new information to Dirac EDOs.

But first, we give a brief theoretical recall about resolution of a quantum differential equation.

In fact, this problem includes two concomitant mathematical issues:

- To solve a differential equation, and
- To solve a spectral problem: for finding eigenvalues associated with solutions of the differential equation

Quantum Equation for H atom with finite nucleus

We consider H atom with not point-like nucleus of radius $\sim R$

(i). *Outside* the nucleus, the potential is $V_O = -e^2/r$ [Cb potential]

(ii) *Inside* the nucleus, the potential is $V_I = -(e^2/2R)(3-r^2/R^2)$ [full sphere]

- So the whole potential is described by a *piecewise* expression:

  $Pot(r) =$ if $0 \le r \le R \rightarrow V_I$, if $r > R \rightarrow V_O$

- Thus, equations $Eq(r)$ using $Pot(r)$ will have a *piecewise* form:

  $Eq =$ if $0 \le r \le R \rightarrow Eq_I(V_I)$, if $r > R \rightarrow Eq_O(V_O)$

- Consider analytic solutions for Schrödinger eq. (or Dirac eq. system) in *piecewise* formulation:

  $Sol(r) =$ if $0 \le r \le R \rightarrow Sol_I(r)$, if $r > R \rightarrow Sol_O(r)$

- Sol_I and Sol_O *are two complex expressions including very different special functions*

- *It's practically impossible to unify them, But*

- We verify the solutions on *limited* domain and on *whole* set of reals *are identical*

=> For the domain *r > R (outside the nuleus), we can apply the general solution.*

ICCF-22 8

We have to solve radial differential equations, where the radius *r* belongs to two separate domains of the real numbers, associated with inside and outside of the nucleus respectively. And the central potentials are very different in these domains. This implies ***the formal solutions have to be expressed in piecewise form.***

On the other hand, the software Maple can solve a differential equation on a limited domain: here it will be outside the nucleus.

For the Dirac system of radial equations, we observe:

- First, the formal solutions are very different in the two domains, and they are very difficult to unify.

- Secondly, a solution on the considered limited domain is formally the same as on the whole domain of real numbers. Here, this latter corresponds to point-like nucleus case. *So,* ***the general solution for point-like nucleus case, can be used for the domain associated with the nucleus outside.***

Dirac equation for H atom with finite nucleus

- The "outside" solution is given by the general solution

  The couples (*f,g*) of functions solutions of the radial system of equations for H with point-like nucleus have the general form:

$$g = \frac{1}{2} C r^{s-1} e^{-r/a} \left\{ {}_1F_1\left(s+p, 2s+1; 2\frac{r}{a}\right) - \frac{s+p}{k+q} {}_1F_1\left(s+p+1, 2s+1; 2\frac{r}{a}\right) \right\}$$

$$f = -\frac{i}{2\mu} C r^{s-1} e^{-r/a} \left\{ {}_1F_1\left(s+p, 2s+1; 2\frac{r}{a}\right) + \frac{s+p}{k+q} {}_1F_1\left(s+p+1, 2s+1; 2\frac{r}{a}\right) \right\}$$

But some parameters (*a*, *p*, *q*, …) include the unknown eigenvalue *E*

=> when applying the *general solution* to *limited* domain $r > R$, (solutions *outside the nucleus*), the eigenvalue *E' associated with* the *wavefunctions* (f_O ,g_O) *must be different* from the one E_0 of general solutions for point-like nucleus (spectral problem) => *Pb 2*

For doing this, we use a simplified "fixed-point" method

- The "inside" solutions are simply polynomials approximations

Here, we indicate the general solution of system of Dirac radial differential equations, usable outside the nucleus. But some parameters of these functions, are in fact expressions including the energy *E*, eigenvalue of the Dirac Hamiltonian. While applying the general solution to the limited domain *outside a finite nucleus*, we cannot use directly the eigenvalue associated with the *point-like nucleus case.*

But we can solve this issue by an iterative method, looking for a fixed-point to stop the iteration.

Dirac equation for H atom with finite nucleus (cont'd)

Connecting inside and outside solutions

- The couples of inside (f_I, g_I) and outside (f_O, g_O) solutions have to be *connected* at the "surface" of the nucleus:

- We must have the *continuity* at $r = R$,

$$f_I(R) = f_I(R) \text{ and } g_I(R) = g_O(R)$$

- and the *continuity of respectives derivatives*

$$f_I'|_R = f_O'|_R \text{ and } g_I'|_R = g_O'|_R$$

We found out a new ansatz system with 4 free parameters (*Pb 1*)

- While doing this, we have to *preserve the initial coupling* between the two components of the general solution =>

f_O and g_O must share a *same multiplicative factor* (like *C*, slide #7)

- *Notation*. $f_I U f_O$: total function obtained by connecting f_I with f_O at R (and similarly for $g_I U g_O$)

Before the fixed-point process, we consider the question of connecting the couples of inside and outside solutions at the nucleus surface, with continuity of the total functions and their derivatives.

For doing this, we found a mathematical trick allowing us to "simulate" an ansatz with four free parameters, while restoring the initial coupling between the two components of the general solution.

We do not give the different steps that are simple but a bit tedious and time-consuming to develop.

Dirac equation for H atom with finite nucleus (cont'd)

Fixed-Point Method for spectral problem (*Pb 2*)

- Start: E_0 is *eigenvalue* associated with solution in *point-like nucleus case* for given radial quantum nb *n'*.
- Step 0: - [complex computation]----> E_0 determines the wf Ψ_0 with mean orbital radius r_0. Ψ_0 = (F, G) where F = f_I U f_O and G = g_I U g_O

  -[direct relations] --> Total Energy E_1 at r_0
- Step 1: $E_1 \neq E_0$ ---> similarly, E_1 determines a new wf Ψ_1 with mean orbital radius r_1 --> E_2 : energy at r_1

  - if $E_2 \sim E_1$, end --> *The eigenvalue is* E_1 ($\neq E_0$)

  - if $E_2 \neq E_1$, ---> *do Step2 similar to Step 1.*

Results: from a lot of computations, we can stop at Step 1.

Note: The mean radius varies *very slowly* as a function of the energy

=> $r_1 \sim r_0$, rapid stopping of the iteration (*fixed point*)

The iterative process is indicated here, in very simplified form.
For a given value of radial quantum number *n'*, the expression of energy for solution in the point-like nucleus case, gives a value E_0.
- At step 0, we take E_0 to determine the wavefunction and we compute the electron probability density; then we deduce the average orbital radius r_0 and we directly calculate the total energy E_1 of electron at r_0. *Next we go to step one, where a new value r_1 of orbital radius is computed.*
- In fact, we can observe in many computations, that the value of average orbital radius varies very slowly as a function of the total energy at each step. *Finally we can stop the iteration at the step 1, where the fixed point is practically reached.*

EDO from Dirac equation, H atom with finite nucleus

Probability density computed with junction radius R = 1 F

Comparing energies with solutions using "point-like" nucleus (PLN)

For radial quantum nb n'=1 (red) and n'=2 (blue)

- n'=1, <r> ~ 4.5 F, $\gamma \sim 84$

  KE ~ 42.5 Mev

  Tot. Energy E ~ 6 kev

  ~1.8 kev for PLN

  BE ~ - 505 kev

  ~ - 509 kev for PLN

- n'=2, <r> ~ 1.13 F, $\gamma \sim 405$

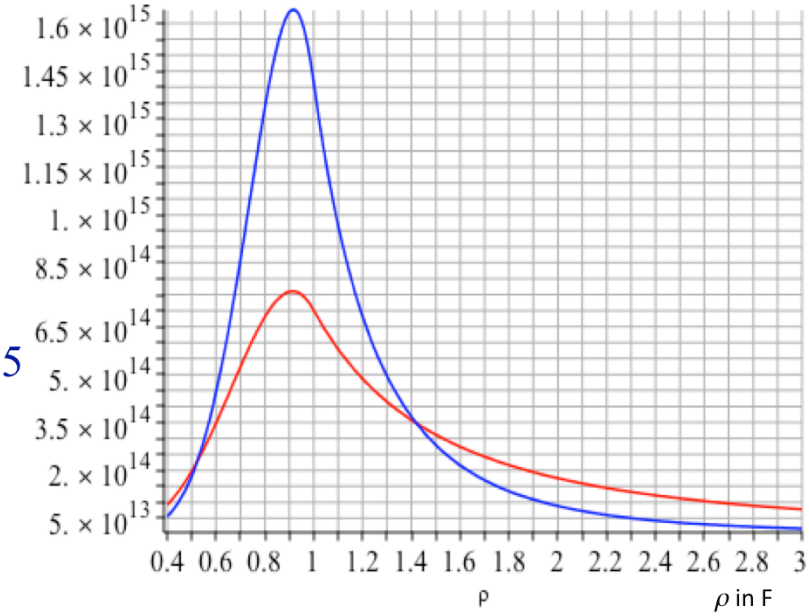
  KE ~ 206 Mev

  Tot. Energy E ~ 1.5 kev

  ~1 kev for PLN

  BE ~ - 509.5 kev

  ~ - 510 kev for PLN



| Remark: <r> ~ $\underline{\lambda_c}\, E / m_e c^2$

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12

Here we plotted the curves of probability density corresponding to values *1* and 2 of radial number.

We indicate the values of γ and Kinetic Energies, not obtained for initial solutions. We give also the new Total and Binding Energies, and compare them with point-like nucleus case (in orange).

Moreover, one can verify the average radius and the total energy satisfy the relationship given in Remark (under the chart). It's also a property deduced from semi-classical studies.

Finally, we observe the shape of curves is similar to orbital 1s of "regular" solutions.

Can EDO states be populated ?

Semi-classical analysis

- KE = $(\gamma - 1)mc^2$: Kinetic Energy

  $V_{eff} = \gamma V + V/2mc^2$: Eff. Pot.

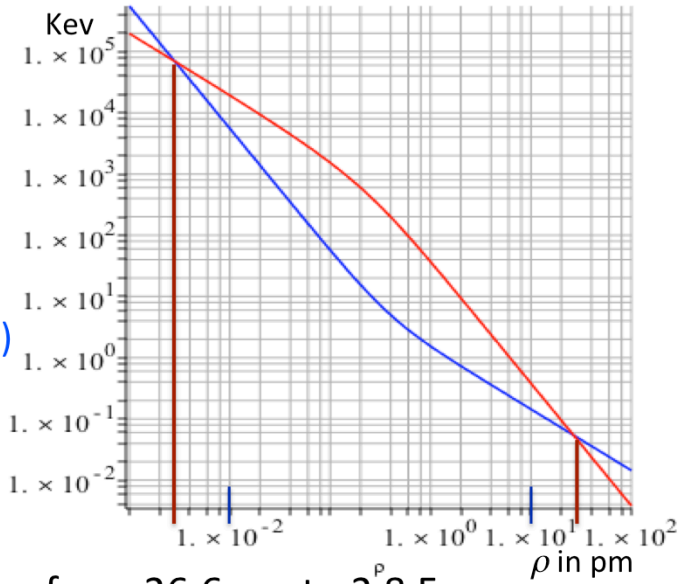
For electron confined at radius ρ

$\gamma \sim [1 + (\lambda_c/\rho)^2]^{1/2}$

- loglog-plot of KE (red), $|V_{eff}|$ (blue)

For 2.8 F < ρ < 27 pm KE > $|V_{eff}|$

EDO zone *Atomic zone*



- "Heisenberg barrier":

For confinement with ρ decreasing from 26.6 pm to 2.8 F, two antagonist interactions, with γ increasing:

(i) Attractive effective relativistic potential V_{eff} increases

(ii) KE increases, *because of the Heisenberg Relation*, and *prevents confinement*. Peak of KE - $|V_{eff}|$: ~ 17 Mev at $\rho \sim$ 5.6 F

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13

Here is a first attempt to evaluate a possible population of EDO states by tunneling from ground state, in the form of superposition of quantum states. We consider two antagonistic interactions, one due to the attractive relativistic effective potential, and the other to the Heisenberg relation, increasing the kinetic energy to prevent the containment of electron: we call it "Heisenberg barrier". This plot for semi-classical analysis was in ICCF21 presentation.

Note these are not static fields, but *dynamic effects* associated with an increasing confinement of the electron.

We could say the "Heisenberg barrier" is a virtual dynamic barrier.

Can EDO states be populated ? (cont'd)

Possible tunneling from atomic zone to EDO zone

- WKB method to compute the *amplitude weakening factor*

$\Delta E = KE - |V_{eff}|$, $K(\rho) = [2m\,\Delta E)]^{1/2}$

K has momentum dimension

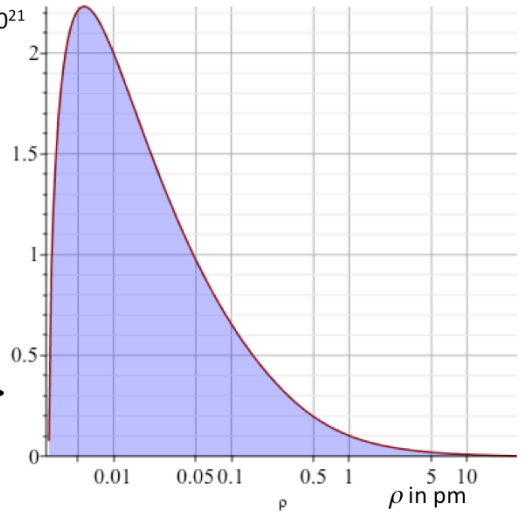
Semilogplot of *K* for 2.8 F < ρ < 27 pm

$Q = \int_{\rho 0}^{\rho 1} K(\rho)\, d\rho$ where ρ_0= 2.8 F, ρ_1= 27 pm

wexp = *Q* / $\hbar$ is a dimensionless number

Weakening factor $w = e^{-wexp} \sim 0.003$ =>

Presence probability: $P = w^2 \sim 9 \times 10^{-6}$



The general wavefunction could be a *linear combination* of EDO state and atomic ground state, with amplitude coefficient $\lambda_{EDO} \sim 0.003$

Note. *WKB : Wenzel-Kramers-Brillouin*

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14

To compute a possible tunneling, we use the WKB approximation in dimension one, similarly to the calculation of Gamow astrophysical factor. The curve of *K* could illustrate the "Heisenberg barrier"; the indicate values on vertical axis are muliplied by 10^{21}. The integral of *K* corresponds to the blue area below the curve. Note *that tunneling effect is extended* here to a *dynamic barrier*, which is unusual.

We obtain a weakened amplitude of wavefunction in EDO zone, and an estimate of probability of EDO state: the general wavefunction of basic state for atom H could be a linear combination of EDO and ground state.

Of course, it would make more sense to use WKB approximation in dim three, but it's much more difficult to do, and for the time,

Conclusion, Prospect

- Semi-classical simulations allowed us to solve questions about EDO as solutions of Dirac equation with finite nucleus

(i) HUR implies strong containment energy and yields the relativistic γ

(ii) So we know *EDO solutions are highly relativistic*, which is an *important result for LENR. Magnitude order of* KE ~ 100 MeV

(iii) We know the relativistic effective V_{eff} can confine EDO's

(iv) Now we can evaluate γ, TE, KE, BE at the mean radius $<r>$

- While going back to Dirac equations, for finite nucleus

(i) We can recalculate the radial wavefunctions of Dirac EDO solutions and determine the correct energy level *E* associated with the radial quantum number *n'*.

(ii) Moreover, we obtain wavefunctions with smooth continuous shapes, having continuous derivatives everywhere.

We emplasize the high energy of the EDOs, very useful for nuclear actions

Conclusion, Prospect (cont'd)

- Nevertheless, we can note the following questions :
  - All semi-classical computations give only one EDO solution.
  - Conversely, Dirac eq. seems to provide a EDO solution for each $n' > 0$
  - Moreover, the semi-classical solutions seem closer to the Dirac solution associated with $n'=2$, than with $n'=1$
- LENR features, such as energy transfer with neither gamma radiations nor energetic particles, requires *enhanced internal conversion*. So, we study possible connections between highly energetic deep electrons and nuclei, hadrons, quarks
- An important problem to solve: how to populate EDO's ?
  A possible lead: look for physical paramaters in condensed matter, allowing *to increase tunneling from atomic to EDO state*

We indicate some question and ideas for future work

Thank You For Your Attention

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17