Tunneling of atoms, nuclei and molecules

Carlos Bertulani (Texas A&M University-Commerce, USA)

Collaborators

A.B. Balantekin(Wisconsin)V. Flambaum (Sydney)M. Hussein (Sao Paulo)D. de Paula (Rio)V. Zelevinsky (Michigan)



Int. Workshop on Critical Stability, Santos, October 13, 2014



Well-known. Used in device technology. E.g. Resonant Diode Tunneling device.



Resonant tunneling (with single barrier)

(composite particle + single-step barrier)



Poorly known. Occurs in atomic, molecular and nuclear systems. E.g. fusion of loosely-bound nuclei.

Feshbach Resonances



internuclear separation



Schroedinger equation

$$H = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) + V(x_1) + V(x_2) + U(|x_1 - x_2|)$$

Step barrier

Square-well

$$V(x) = \begin{cases} V_0, & -a/2 \le x \le a/2 \\ 0, & \text{otherwise} \end{cases}$$

 $U(x) = \begin{cases} 0, & -d/2 \le x \le d/2 \\ \infty, & \text{otherwise} \end{cases}$

change of variables

 $\mathbf{x} = \left(\frac{\mathbf{x}_1 + \mathbf{x}_2}{2}\right), \qquad \mathbf{y} = \mathbf{x}_1 - \mathbf{x}_2 + \frac{\mathbf{d}}{2}$ c.m. relative $\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{x}^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial \mathbf{y}^2} + \mathbf{U}(\mathbf{y} - \frac{\mathbf{d}}{2}) + \mathbf{W}(\mathbf{x}, \mathbf{y})\right]\Psi(\mathbf{x}, \mathbf{y}) = \mathbf{E}\Psi(\mathbf{x}, \mathbf{y})$





(b) d/2 < a



Tunneling of Molecules



$$\mathcal{H} = \frac{\mathbf{P}^2}{4m} + \frac{\mathbf{p}^2}{m} + U\left(Z - \frac{z}{2}\right) + U\left(Z + \frac{z}{2}\right) + V(r)$$

basis expansion
$$\left[\frac{\mathbf{p}^2}{m} + V(r)\right]\phi_n(\mathbf{r}) = \varepsilon_n\phi_n(\mathbf{r}) \quad \Psi(Z,\mathbf{r}) = \sum_{n=0}^{\infty} \psi(Z)\phi_n(\mathbf{r})$$

effective potential

$$U_{nm}(Z) = \frac{4m}{\hbar^2} \int \left[U\left(Z + \frac{z}{2}\right) + U\left(Z - \frac{z}{2}\right) \right] \phi_n^*(\mathbf{r}) \phi_m(\mathbf{r}) d\mathbf{r}$$

effective equation for cm motion

$$\left(\frac{d^2}{dZ^2} + k_n^2\right)\psi_n(Z) - \sum_m U_{nm}(Z)\psi_m(Z) = 0 \qquad k_n^2 = \frac{4m}{\hbar^2}(E - \varepsilon_n)$$

$$\psi_{nl}(Z) = e^{ik_{n}Z}\delta_{nl} + \frac{1}{2ik_{n}}\sum_{m=0}^{\infty}\int_{-\infty}^{\infty}e^{ik_{n}(Z-Z')}U_{nm}(Z')\psi_{ml}(Z')dZ'$$

$$R_{nl}(Z) = \frac{1}{2ik_n} \sum_{m=0}^{\infty} \int_{-\infty}^{\infty} e^{ik_n Z'} U_{nm}(Z') \psi_{ml}(Z') dZ'$$

$$T_{nl}(Z) = \delta_{nl} + \frac{1}{2ik_n} \sum_{m=0}^{\infty} \int_{-\infty}^{\infty} e^{-ik_n Z'} U_{nm}(Z') \psi_{ml}(Z') dZ'$$

Reflection and transmission probabilities

$$\mathbf{R}_{1} = \sum_{n=0}^{\infty} \frac{k_{n}}{k_{1}} |\mathbf{R}_{nl}|^{2}, \quad \mathbf{T}_{1} = \sum_{n=0}^{\infty} \frac{k_{n}}{k_{1}} |\mathbf{T}_{nl}|^{2}$$

Transition probability

50

40

30

20

10

0

-10

-20

-30

-1

mi

$$\mathbf{P}_{n \to 1} = \frac{k_n}{k_1} \left(\left| \mathbf{R}_{nl} \right|^2 + \left| \mathbf{T}_{nl} \right|^2 \right)$$

-0.5





 $\widetilde{Z} = Z/a$

Goodvin, Shegelski, PRA 72, 042713 (2005)



Tunneling of a (two-particle) nucleus



delta barrier

$U_0 a \rightarrow \delta(Z)$

For d + d \rightarrow ⁴He

With *a* and U_o simulating Coulomb barrier

For large Z's, A's

 \rightarrow Many resonances possible, if <r2> large (loosely-bound)

Problem: strong interactions are too strong!

Electron screening in fusion reactions



Small effects

- Thermal motion, lattice vibrations, beam energy spread
- Nuclear breakup channels (in weakly-bound nuclei)
- Dynamics of tunneling

Balantekin, CB, Hussein, NPA 627 (1997)324

Corrections	
Vaccuum Polarization	$\sim 1\%$
Relativity	10^{-3}
Bremsstrahlung	10^{-3}
Atomic porarization	10^{-5}
Nuclear polarization	$< 10^{-10}$

all ≤ 1%

Not a solution! (we need ~ 100%)



Vacuum polarization

Wrong extrapolation of stopping power

Bang, PRC 53 (1996) R18 Langanke, PLB 369 (1996) 211





Data has to be corrected for stopping power:

 $E' = E - S_p \Delta x$

Very few data on stopping at ultra-low energies: H + He

Golser, Semrad, PRL 14 (1991) 1831

Mainly charge-exchange

Simplest test

CB, de Paula, PRC 62, 045802 (2000) PLB 585, 35 (2004)



Elliptic coordinates

p + H) P + D

Charge exchange (pickup)

Projectile slows down to carry electron with



e⁻

change of variables

$$\begin{split} \xi &= \frac{r_1 + r_2}{R}; \qquad \eta = \frac{r_1 - r_2}{R}; \quad \varphi \\ \Psi &= F(\xi)G(\eta)e^{im\phi} \end{split}$$

Two-center wfs (molecular orbitals):

$$\frac{\mathrm{d}}{\mathrm{d}\xi} \left[\left(\xi^2 - 1\right) \frac{\mathrm{d}F}{\mathrm{d}\xi} \right] + \left[\frac{\mathrm{R}^2 \xi^2}{2} \mathrm{E} + 2\mathrm{R}\xi - \frac{\mathrm{m}^2}{\xi^2 - 1} \right] \mathrm{F}(\xi) = 0$$
$$\frac{\mathrm{d}}{\mathrm{d}\eta} \left[\left(1 - \eta^2\right) \frac{\mathrm{d}G}{\mathrm{d}\eta} \right] - \left[\frac{\mathrm{R}^2 \xi^2}{2} \mathrm{E} + 2\mathrm{R}\xi + \frac{\mathrm{m}^2}{\eta^2 - 1} \right] \mathrm{G}(\eta) = 0$$

Expansion basis: molecular orbitals for p+H



$$l_z \Phi_s = \pm \lambda \Phi_s$$

Value of λ 0123Code letter σ π δ ϕ, \cdots





Coupled-channels calculation



H⁺ + He collisions (two-active electrons)

 $\phi = Nr^{n-1} e^{-\xi r} Y_{lm}(\theta, \phi)$

Two-center basis for two-electrons Hartree-Fock equations

 $\mathbf{F} \cdot \mathbf{C} = \mathbf{S} \cdot \mathbf{C} \cdot \mathbf{E}$

Slater-type orbitals

$$\Phi_{i} = \sum_{i=1}^{n} \left[c_{ji}^{A} \phi_{i}^{A} + c_{ji}^{B} \phi_{i}^{B} \right]$$

$$F_{\mu\nu} = H_{\mu\nu} + \sum_{\lambda\rho} P_{\lambda\rho} \left[\left(\mu\nu \,|\, \lambda\rho \right) - \frac{1}{2} \left(\mu\rho \,|\, \lambda\nu \right) \right]$$

$$H_{\mu\nu} = \iint \phi_{\mu}^{*}(1) \left[-\frac{1}{2} \nabla_{1}^{2} - \sum_{A} \frac{1}{r_{1A}} \right] \phi_{\nu}^{*}(1) d\tau_{1}, \qquad P_{\lambda\rho} = 2 \sum_{i=1}^{occ} c_{\lambda i} c_{\rho i}$$

$$\left(\mu\nu\,\mathsf{I}\,\lambda\rho\right) = \iint \phi_{\mu}(1)\,\phi_{\nu}(1)\frac{1}{r_{12}}\phi_{\lambda}(2)\,\phi_{\rho}(2)\,\mathrm{d}\tau_{1}\mathrm{d}\tau_{2}\,,\quad S_{\mu\nu} = \int \phi_{\mu}(1)\,\phi_{\nu}(1)\,\mathrm{d}\tau_{1}\,\mathrm{d}\tau_{2}\,$$

+. d. coupled-channels equations

Damping of resonant exchange $H(1s) \Leftrightarrow He(1s2s)$



19

Stopping power at very low energies

p + H

e⁻

D

Threshold effect

$$E_{\rm P} \ge \frac{\mu^2}{4M_{\rm P}m_{\rm e}} \Delta E \ge 8 \quad \text{keV}$$

He: $1s^2 \rightarrow 1s2s$: 19.8 eV



CB, PLB 585, 35 (2004)

Virtual particles enhance tunneling



Baron Muenchhausen escaping from a swamp by pulling himself up by his own hair. G.A. Buerger (1786).



QFT: a "physical" particle consists of a "naked" particle "dressed" in a cloud of short-lived "virtual" particles.

Quantum Muenchhausen

Flambaum , Zelevinsky, PRL 83, 3108 (1999)









Tetraneutron

Loosely-bound nuclei Tetraneutron?

halo

Marques et al, PRC 65, 044006 (2002)

HOW THE GANIL TEAM CREATED AND DETECTED TETRANEUTRONS

Firing beryllium-14 nuclei at a carbon target produces a spray of nuclear fragments that fly into over 100 separate detectors. When this nuclear debris hits a detector, it's energy is transformed into a flash of light



New scare links food to blindness

Row over 'turning rivers around'

NASA's new vision emerges

LATEST NEWS

Tetraneutron as a dineutron-dineutron molecule



CB, Zelevinsky, J. Phys. G 29 (2003) 2431

Antissimetrization (Pauli-principle)

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4) = \mathsf{A}\left\{\psi(\mathbf{R})\phi_{\mathrm{a}}(\mathbf{r}_1,\mathbf{r}_2)\phi_{\mathrm{b}}(\mathbf{r}_3,\mathbf{r}_4)\right\}$$

With realistic NN potentials v_{ij}

$$\mathbf{H} = \mathbf{T}_{R} + \mathbf{T}_{a} + \mathbf{T}_{b} + \sum_{i < j} \mathbf{v}_{ij}(\mathbf{r}_{ij})$$

Effective wave equation

$$\left[\frac{\mathbf{P}^2}{2m_{\rm N}} + U_1(\mathbf{R}) + U_2(\mathbf{R})\right]\psi(\mathbf{R}) = E\psi(\mathbf{R})$$

- Effective potential repulsive
- No margin for pocket or state
- no tetraneutron in singlet, or triplet state!
- Confirmed by Pieper, PRL 90 252501 (2003)

Fusion of halo nuclei

Model Hamiltonian



¹¹Lj

CB, Balantekin,

PLB 314, 275 (1993)

$$\mathbf{H} = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + \mathbf{V}_{A}(\mathbf{r}_{1A}) + \mathbf{V}_{B}(\mathbf{r}_{1B}) + \mathbf{V}_{A}(\mathbf{r}_{2A}) + \mathbf{V}_{B}(\mathbf{r}_{2B})$$

Landau approximation $\Psi_{\pm} \cong N \left[\Psi_{A}(r_{1A}) \pm c_{\pm} \Psi_{B}(r_{1B}) \right]$

 \mathbf{r}_{2A}

Loosely bound nuclei are like Rydberg states in atoms

²⁰⁸Pb

1

 r_{1A}

Covalent bond

r

R



$$\mathbf{I} = \left\langle \Psi_{A} \right\| V_{B}(\mathbf{r}_{1B}) \| \Psi_{A} \right\rangle$$

$$\mathsf{L} = \left\langle \Psi_{\mathrm{A}} \right\| \mathsf{V}_{\mathrm{B}}(\mathsf{r}_{\mathrm{1B}}) \| \Psi_{\mathrm{B}} \right\rangle$$

$$\mathbf{O} = \left\langle \Psi_{A} \mid \Psi_{B} \right\rangle$$







Effective covalent potential $V(R) = E(R) - S_{2n}$

Fusion cross section

$$\sigma(E_{cm}) = \frac{\pi}{k^2} \sum_{l} (2l+1) T_l(E_{cm})$$

More on fusion with weakly-bound nuclei :

Canto, Gomes, Donangelo, Hussein, Phys. Rep. 424, 1 (2005)



Time-dependent analysis

Power emitted:		
dP	1	$dE(\omega)$
dE_{γ} =	E_{γ}	dE_{γ}

CB, de Paula, Zelevinsky, PRC 60, 031602(R) (1999)

Momentum

Solving for t.d. w.f. \rightarrow power emitted:

$$dE(\omega) = \frac{8\pi\omega^2}{3m^2c^3} Z^2 e^2 \left| \int \Psi(\mathbf{r},t) \left[-i\hbar\nabla\Psi(\mathbf{r},t) \right] d^3r \right|^2$$





t [fm/c]



Finite size always enhance tunneling probability

Tunneling of Cooper pairs

Zelevinsky, Flambaum, JPG 34, 355 (2005)



Both particles see barrier:

Normal modes:

 $\omega_+^2 = \frac{2k+q}{m}, \quad \omega_-^2 = \frac{q}{m}$

$$H = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2}k(x - y)^2 + \frac{1}{2}q(x^2 + y^2)$$

Energy transfer from internal to c.m. motion

Does not depend on $k \rightarrow$ no finite size effect

$$E = E(\infty) + \frac{\hbar\sqrt{2k/m}}{2} - \frac{\hbar\sqrt{(2k+q)/m}}{2}$$

Adiabatic approx. not valid for tunneling through a Josephson junction (more complicated)

Composite particle fusion enhancement

CB, Flambaum, Zelevinsky, JPG 34, 1 (2007)

Particles see different barriers: $H = -\frac{p_x^2}{2m_x} + \frac{p_y^2}{2m_y} + V(x - y) + U(x) + U(y)$ $x \quad y \quad -a/2 \quad a/2$ $R \quad change of variables \quad Adiabatic approximation$ $x, y \rightarrow r, R \quad \Psi(r, R) = \psi(R)\phi(r, R)$

$$\psi(\mathbf{R}) = u(\mathbf{R}) \exp\left[-\int^{\mathbf{R}} \alpha(\mathbf{R}') d\mathbf{R}'\right] \qquad \phi \text{ normal}$$

alized
$$\alpha(R) = \left\langle \phi \right| \frac{\partial \phi}{\partial R}$$

$$\mathbf{u}''(\mathbf{R}) + \frac{2\mathbf{M}}{\hbar^2} \left[\mathbf{E} - \tilde{\mathbf{U}}(\mathbf{R}) \right] \mathbf{u}(\mathbf{R}) = 0$$

$$\tilde{U}(R) = \varepsilon(R) - E_0 + \frac{\hbar^2}{2M} \left[\alpha^2(R) + \alpha'(R) + \beta(R) \right] \qquad \beta(R) = \left\langle \phi \right\rangle$$



CB, Flambaum, Zelevinsky, JPG 34, 1 (2007)

Features probably seen in experiments.

But not disentangled from uncertainties in potentials, polarization effects, etc.

Deuteron tunneling through barrier step.

$$E_0 = -2.225 \text{ MeV}$$

 $r_0 = 2 \text{ fm}$



Optical Lattices



Feshbach Resonances



Diffusion of Strongly Bound Molecules



Probability (arbitrary units)

Probability distribution of strongly bound ($E_b=10$ kHz) rubidium molecules in optical lattice with size D = 2 μ m.

From top to bottom the time is t = 0, t = 10 ms, t = 25 ms and t = 100 ms.

T. Bailey, CB, E. Timmermans, PR A 85, 033627 (2012)

Diffusion of Strongly Bound Molecules



Escape probability of strongly bound rubidium molecules in optical lattice with D=2 μ m, for increasing potential barrier heights.

Barrier heights increase by 1.5 from the solid to dashed-dotted, from dashed-dotted to long-dashed, and from long-dashed to dotted curve.

Diffusion of Loosely Bound Molecules



Integrity probability of loosely bound rubidium molecules in an optical lattice $D = 2 \mu m$, and potential barrier height $V_0=5 \text{ kHz}$.

The binding energies were parametrized in terms of the barrier height, with $E_4 = V_0/20$, $E_3 = V_0/5$, $E_2 = V_0/2$, and $E_1 = V_0/1.2$.

Diffusion of Loosely Bound Molecules



Blue histograms are the relative probability of finding a molecule in its ground state at a given position along the lattice.

Red histograms give the relative probability of finding individual atoms after the dissociation.

Diffusion of Loosely Bound Molecules



Spreading position width of bound molecules, $\sigma_M(t)$, shown by solid line and of dissociated atoms, $\sigma_A(t)$, shown by dotted line. The dashed curve is a fit to the asymptotic time dependence $\sigma_M(t) \sim t^{1/2}$.

No clear asymptotic dependence is found for the dissociated atoms.

$$= 0.156 \frac{\hbar^2}{\text{mb}\sigma_0^2} \quad \text{Compared to Einstein} \\ \text{diffusion coefficient} \quad D = \frac{kT}{b} \quad \longrightarrow \quad T \sim \frac{\hbar^2}{\text{m}\sigma_0^2}$$

Conclusions:

"Although a [large] number of theoretical works have studied tunneling phenomena in various situations, quantum tunneling of a *composite particle, in which the particle itself has an* internal structure, has yet to be clarified."

Saito and Kayanuma, J. Phys.: Condens. Matter 6 (1994) 3759

• 20 years after: still remains open to imagination and creativity.