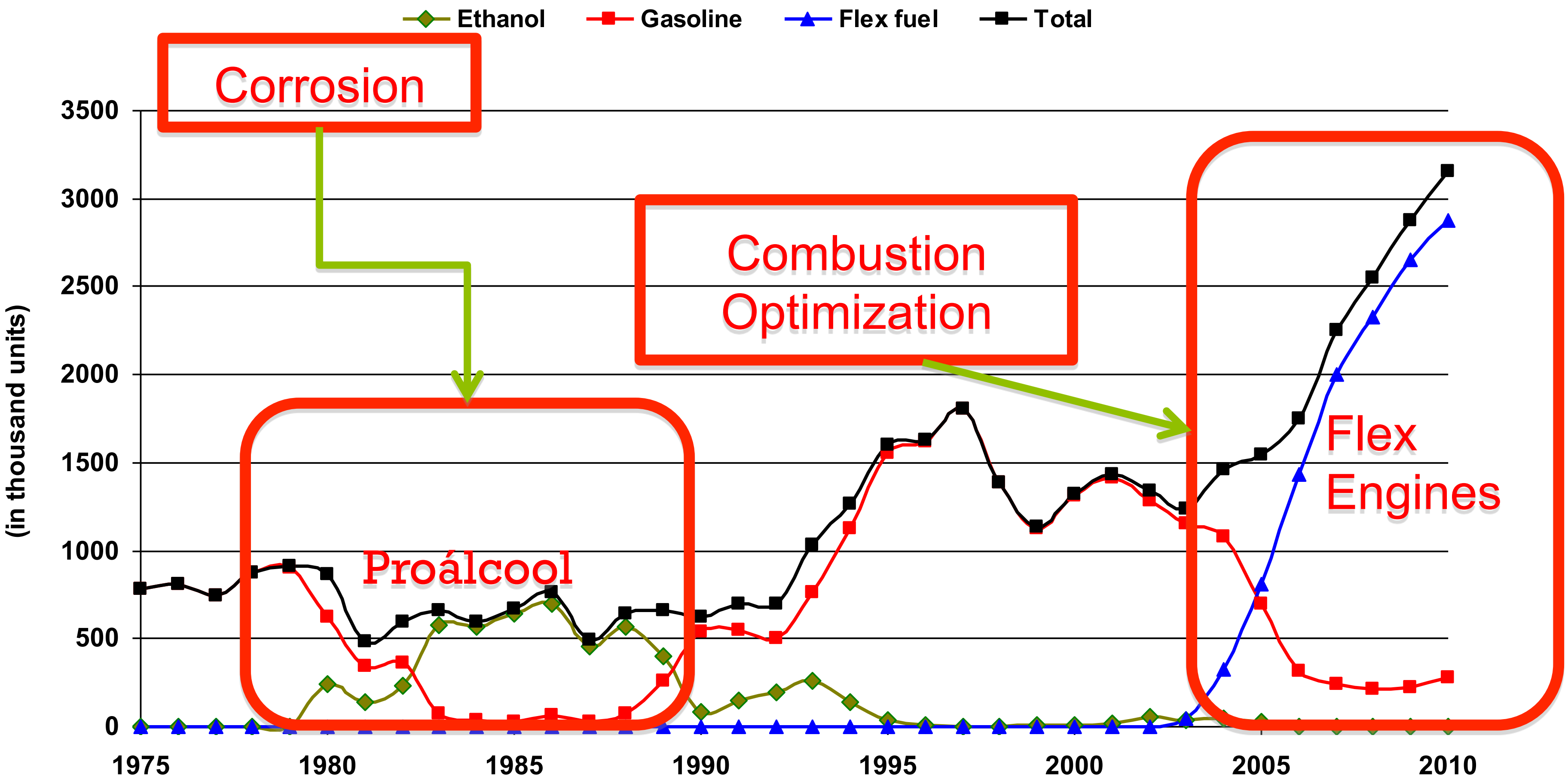
Mecânica quântica, plasmas químicos e produção de etanol: assuntos relacionados de uma agenda científica brasileira.

Marco Aurélio P. Lima
Unicamp

Instituto de Física Gleb Wataghin
UNICAMP

Assuntos aparentemente desconexos

Special motivation I: large scale use of ethanol in engines



Brazilian Sales of light fleet Vehicles (1975-2010)

Ethanol as Fuel: Plasma Ignition for Vehicle Engines

Theoretical support for an application project working on:

- Investigation of processes occurring during the ignition of plasma and its consequences in post-discharge for an internal combustion engine;

- The proper parameters to be applied in cars that operate on "poor mixtures" reducing pollutants released into the atmosphere, especially considering the spark plug discharge.

Special motivation II: large scale production of ethanol

A sugarcane industry of Sugar/Ethanol/Bioeletricity

Special motivation II: large scale production of ethanol

Biomass: a source of energy and carbon

Special motivation II: large scale production of ethanol

Biomass: a source of energy and carbon

Special motivation II: large scale production of ethanol

First generation ethanol: crushing the cane for the juice

Special motivation II: large scale production of ethanol

Bagasse piles
at the mill.

2nd generation
ethanol?
Other high value
bioproducts?

Can we use plasmas on Biomass?

Ambientes de descarga elétrica

From the 80's up to now these scientific topics and applications stimulated the community

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DISCHARGE ENVIROMENTS

This community was inspired by several basic science problems

Natural Phenomena	Aurora Borealis
Astrophysics	Planetary Atmospheres
Biology	DNA dissociation … Plasma Science towards Future Medicine
Quantum Optics	Molecular Lasers

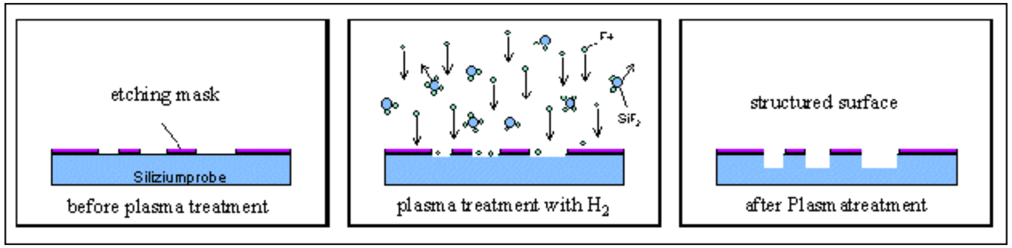
and got further motivated by great applications

- Ozone destruction
- Control of pollution
- Sterilization $$
- Surface treatment $$$$
- Nanofabrication $$$$
- Medical treatment $$$$

Surface treatment with Plasmas

Plasma Processing Gases → Several Industry Applications

Production of reactive species → ETCHING, DIAMANTIZATION, POLIMERIZATION, NITRIDING, CLEANING, and others



IMPROVEMENT NEEDS MODELING AND MODELING NEEDS DATA

Modeling is a big challenge

Electron collision data: cross sections for

Elastic

Inelastic: electronic, rotational and vibrational excitation

Ionization

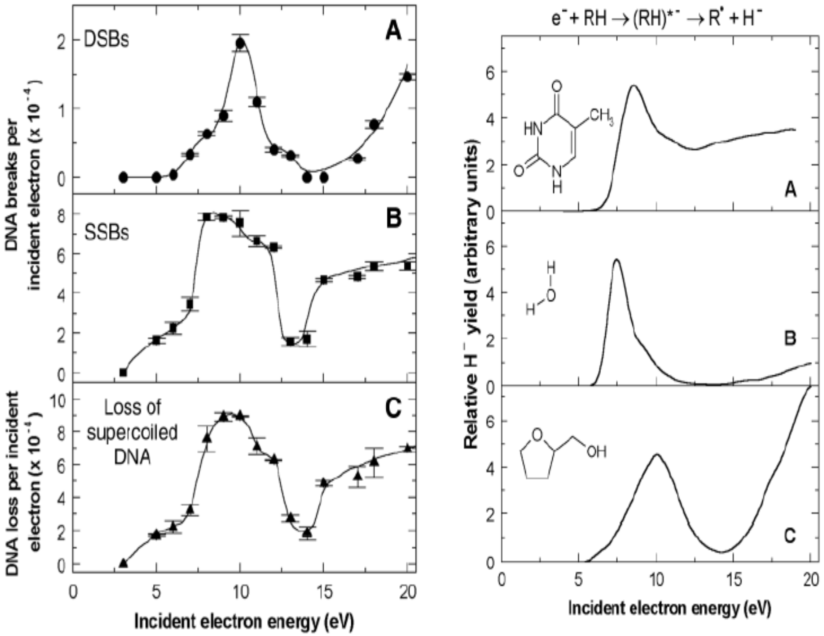
Dissociation

Electron-Induced Damage to Biomolecules

Resonance's inducing dissociation.
How precise the data (position and width) must be?

Resonant Formation of DNA Strand Breaks by Low-Energy (3 to 20 eV) Electrons

Badia Boudaïffa, Pierre Cloutier, Darel Hunting, Michael A. Huels,* Léon Sanche



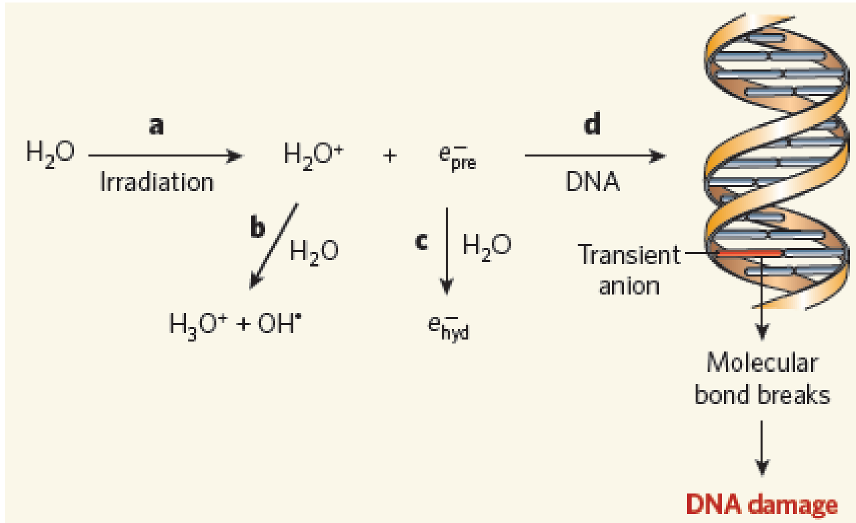
Science, **287** 1658 (2000)

BIOLOGICAL CHEMISTRY

Beyond radical thinking

Léon Sanche

Radiation-induced DNA damage has been attributed to hydroxyl radicals, which form when water absorbs high-energy photons or charged particles. But another product of water's radiolysis might be the real culprit.



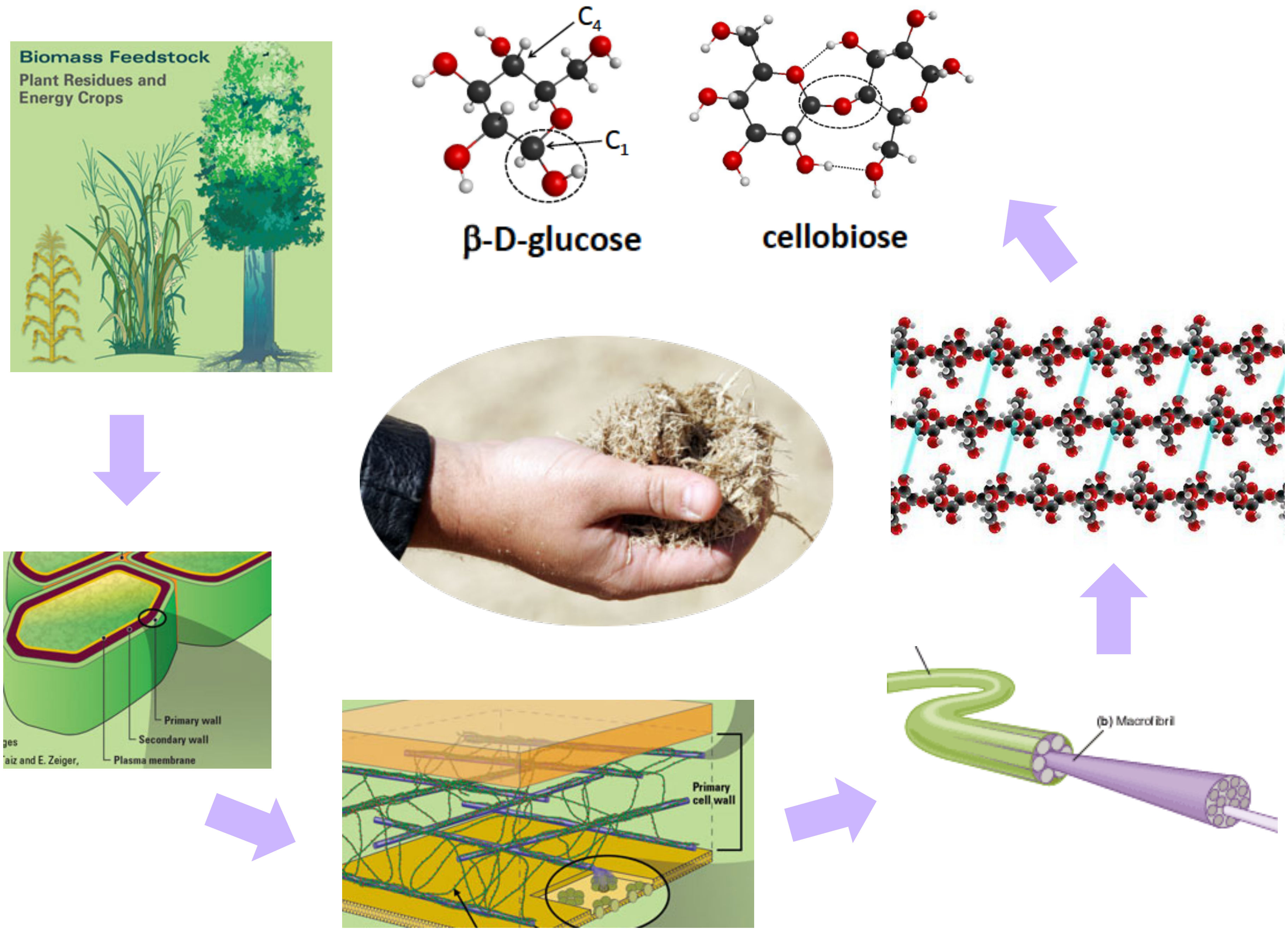
Sanche, Nature **461**, 358 (2009)

J|A|C|S COMMUNICATIONS

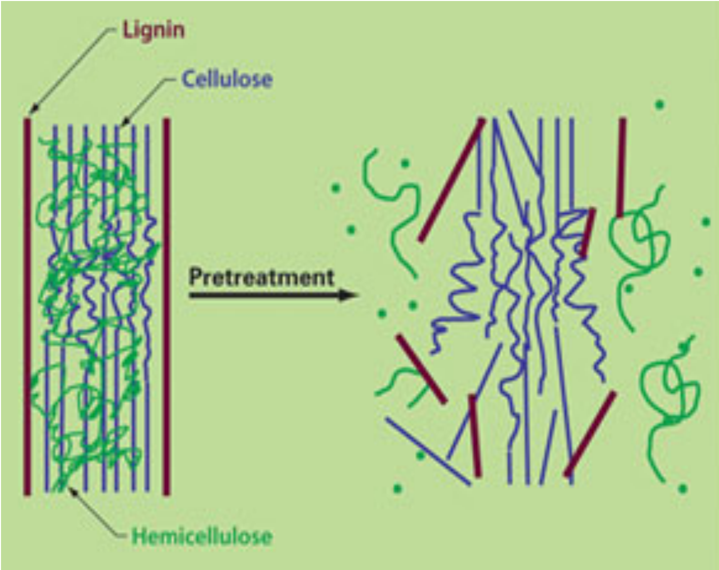
Chun-Rong Wang, Jenny Nguyen, and Qing-Bin Lu*

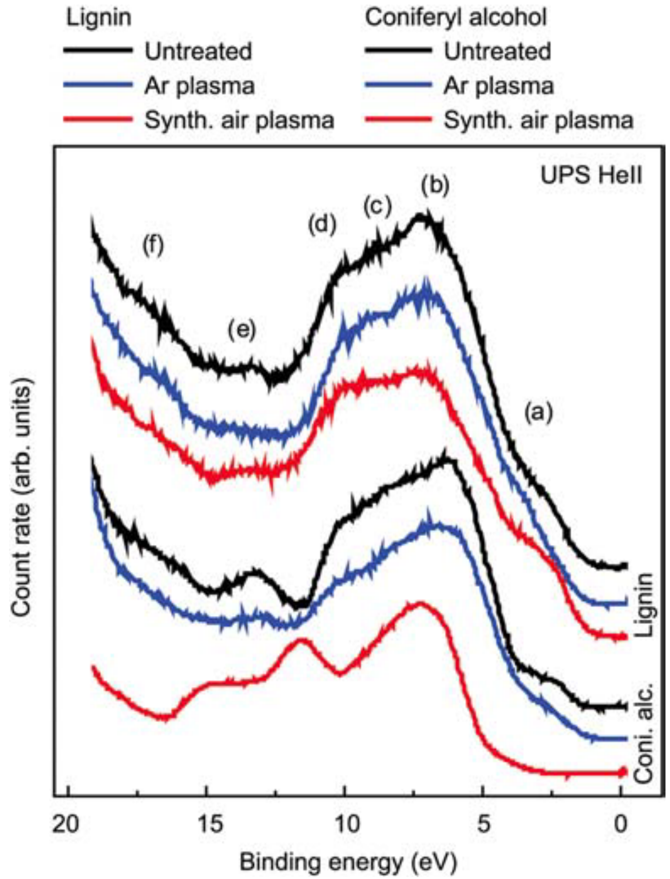
J. AM. CHEM. SOC. 2009, *131*, 11320–11322

Biomass is Made Up with Fermentable Sugars



Lignocellulose is Resistant to Hydrolysis

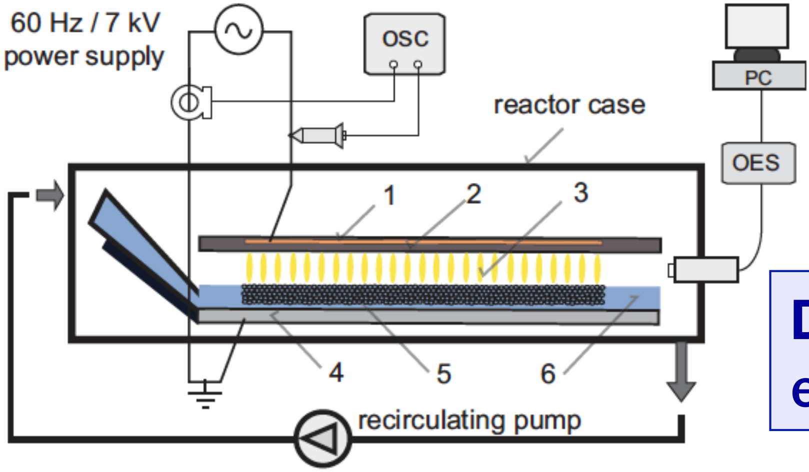




Pretreatment: bio- and physical-chemical processes to expose the cellulose fibers

Lothar Klarhöfer[1], Wolfgang Viöl[2,3,*] and Wolfgang Maus-Friedrichs[1]

Holzforschung, Vol. 64, pp. 331–336, 2010



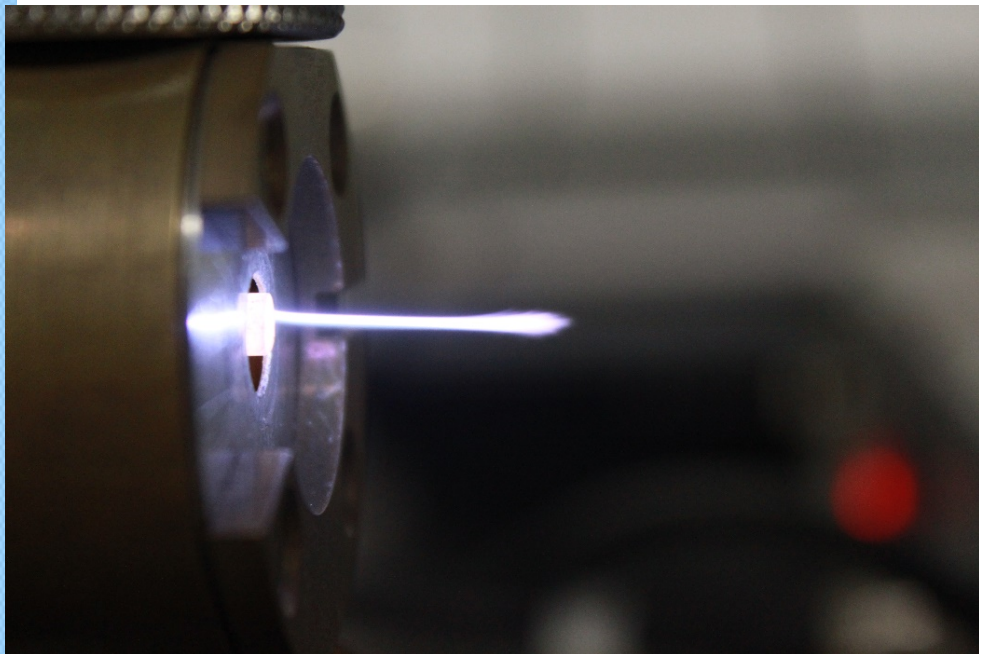
Dielectric Barrier Discharge (DBD): electron flux on substrate ~10^8 cm^{-2} s^{-1}

Experimental Initiative

supported by BIOEN

- Microwave Plasmas in argon at atmospheric pressure

- Exploration of their potential for applications, in particular, to the treatment of biomass (sugar cane bagasse)



By Jayr Amorim, Carlos Oliveira, Jorge A. Souza-Correa, Marco A. Ridenti
Plasma Process. Polym. 2013, DOI: 10.1002/ppap.201200158

FM003
IFGW
UNICAMP

Diffuse Reflectance Fourier Transform Infrared Spectrometry (DRIFT)

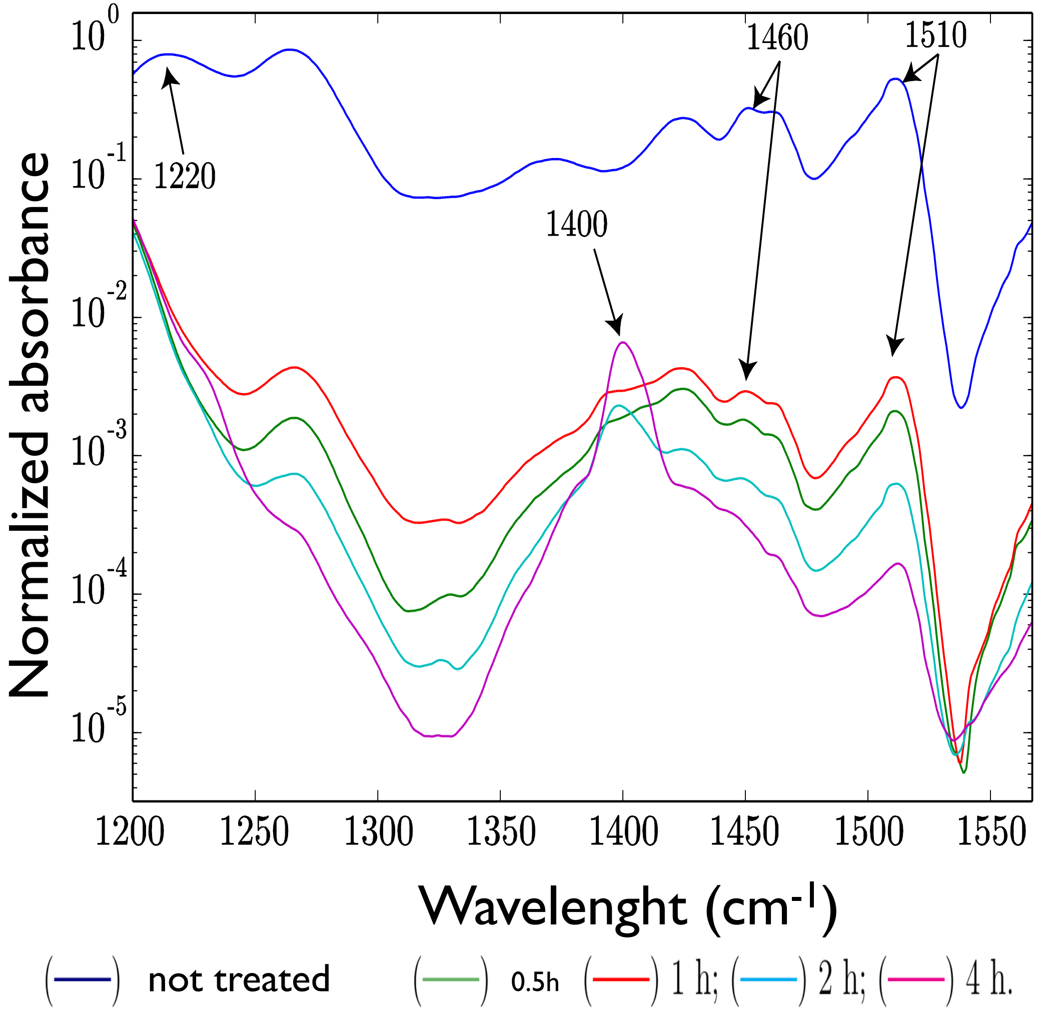
wavelenght:

1220 cm^{-1}

CC plus CO plus CO stretching in Guaiacyl group

1460 cm^{-1}

CH deformations (bend) methoxyl; asymmetric stretching in $–CH_3$ and $–CH_2$

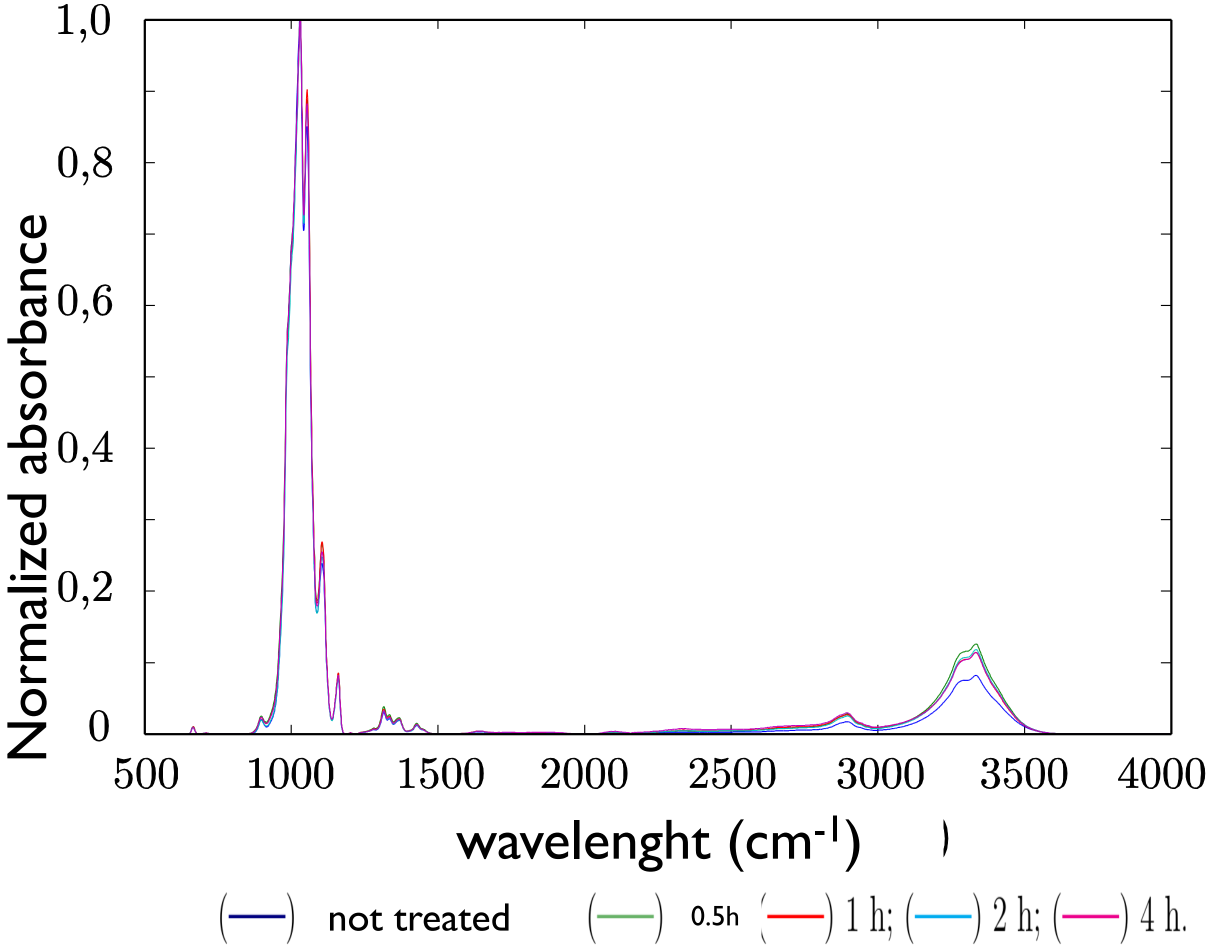


By Jayr Amorim, Carlos Oliveira, Jorge A. Souza-Correa, Marco A. Ridenti
Plasma Process. Polym. 2013, DOI: 10.1002/ppap.201200158

MAPLima

Diffuse Reflectance Fourier Transform Infrared Spectrometry (DRIFT)

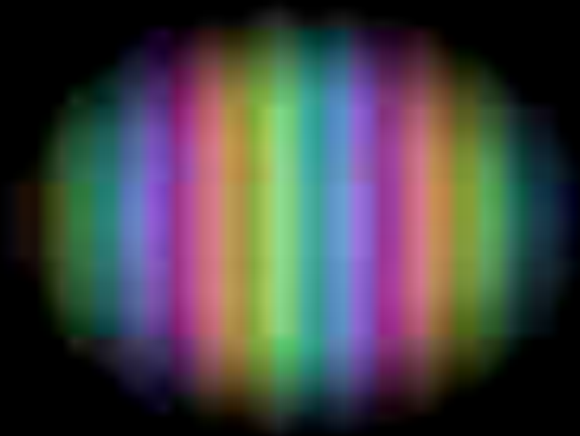
No modification was observed in the spectra after plasma treatment on cellulose



By Jayr Amorim, Carlos Oliveira, Jorge A. Souza-Correa, Marco A. Ridenti

Plasma Process. Polym. 2013, DOI: 10.1002/ppap.201200158

EM COLISÕES QUÂNTICAS,



PARA ONDE VÃO AS PARTÍCULAS?

Trajetória de uma partícula

Lei da inércia permite prever o futuro de uma partícula livre

$$S = S_0 + V_0 t$$

Vocês também sabem o futuro da partícula na presença de uma força constante

$$v = v_0 + at$$

$$S = S_0 + v_0 t + \frac{1}{2} a t^2$$

Ondas

Para se falar em mecânica quântica, é preciso falar sobre ondas. As mais conhecidas são: as ondas do mar, as ondas sonoras, e as ondas eletromagnéticas.

Alguns exemplos e definições:

Tipos de ondas
Amplitude e comprimento de onda
Freqüência
Ondas eletromagnéticas

Comportamento ondulatório das partículas

No começo do século XX, algumas experiências mostraram um comportamento muito estranho das partículas: em situações especiais, elas se comportavam como ondas

http://www.colorado.edu/physics/2000/index.pl
Experiência de duas fendas

No começo do século XIX, de Broglie associou às partículas com momento linear p=mv, uma onda com comprimento de onda λ

$$\lambda = \frac{h}{p}$$

Para achar a partícula é preciso procurar pela onda associada à ela: onde esta onda for diferente de zero temos chance de achá-la

Dualidade partícula/onda da luz

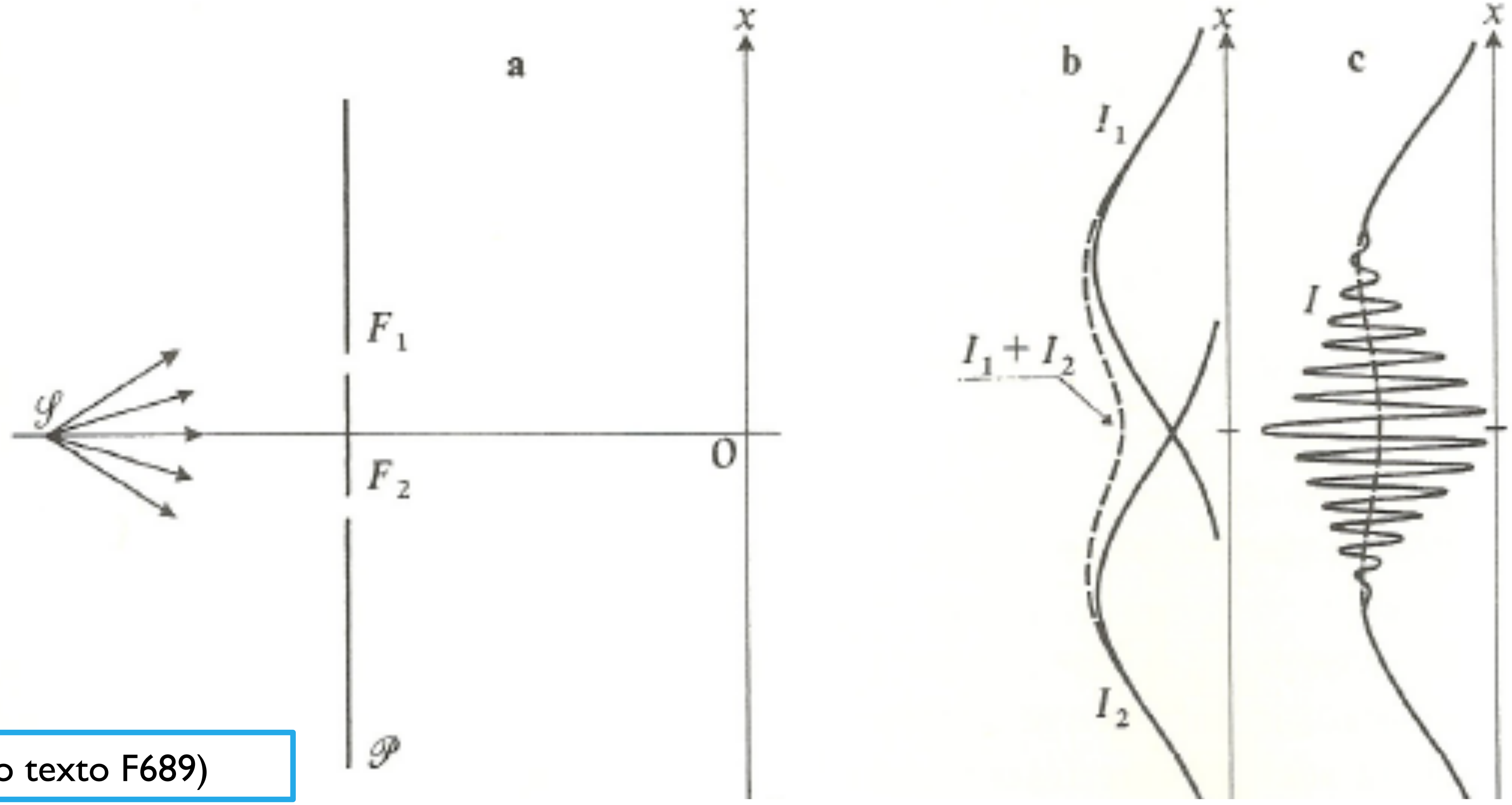


Figura 1 (livro texto F689)

Diagrama do experimento de interferência de dupla fenda de Young (fig. a). Cada uma das fendas F_1 e F_2 produz um padrão de difração na tela ϵ. As intensidades correspondentes são $I_1(x)$ e $I_2(x)$ (linhas sólidas da figura b). Quando as duas fendas são abertas simultaneamente, a intensidade $I(x)$ observada na tela não é a soma $I_1(x) + I_2(x)$ (linha tracejada nas figuras b e c), mas mostram oscilações devido à interferência entre os campos elétricos por F_1 e F_2 (curva figura c).

O que esperar, se: (1) bloquear F_2; (2) bloquear F_1; (3) ambas abertas (partículas); (4) ambas abertas (partícula/onda - caso real)?

Revista Brasileira de Ensino de Física, vol. 38, nº 3, e3309 (2016)
www.scielo.br/rbef
DOI: http://dx.doi.org/10.1590/1806-9126-RBEF-2016-0052

Artigos Gerais

Quantum "Ghosts"

"Fantasmas" na Mecânica Quântica

Gabriela M. Amaral, David Q. Aruquipa, Ludwing F. M. Camacho,
Luiz F. C. Faria, Sofía I. C. Guzmán, Damaris T. Maimone, Melissa Mendes, Marco A. P. Lima*

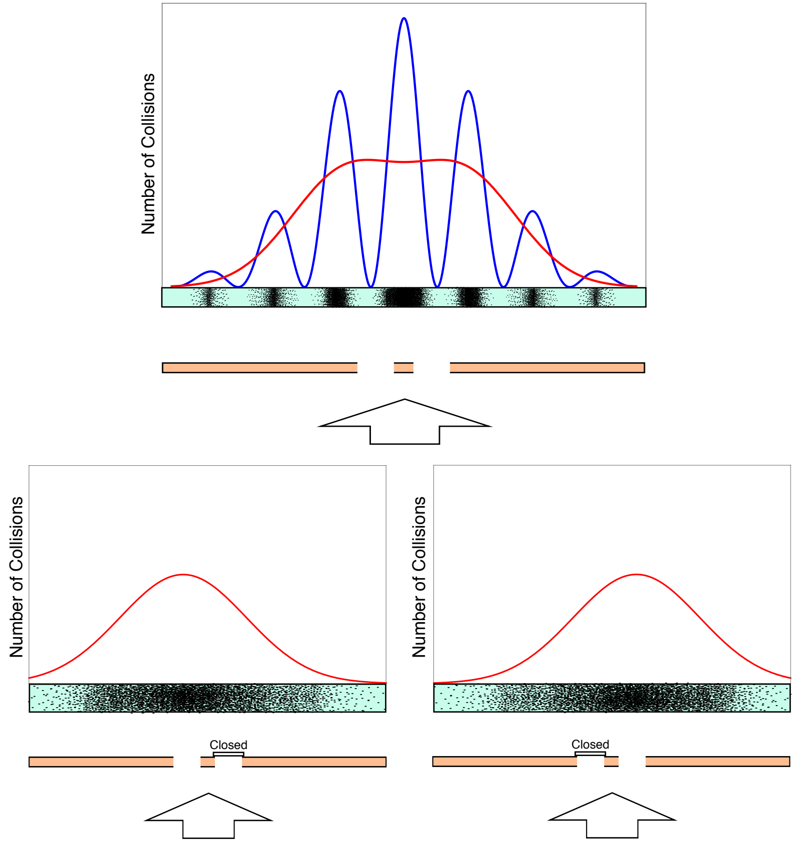
Instituto de Física "Gleb Wataghin", Universidade Estadual de Campinas, 13083-859, Campinas, São Paulo, Brazil

Recebido em 9 de março de 2016. Aceito em 19 de março de 2016

Can you pick a complex subject in quantum mechanics and discuss it with a minimum number of equations, in a simplified form that the general scientific public could understand? This was a question presented to graduate students of the one-year Quantum Mechanics course based on the text book *Modern Quantum Mechanics* by J. J. Sakurai and Jim Napolitano, at the State University of Campinas (UNICAMP), Brazil. The first seven authors of this paper are graduate students (alphabetical order) that accepted to try it. The chosen subject was "delocalized quantum states", and it will be discussed using colloquial terms like quantum *ghosts*, spooky action, splitting beings and invisibility cloak.
Keywords: delocalized state, interference effects, double slit experiment.

Pode-se escolher um tópico complexo em mecânica quântica e discuti-lo com um número mínimo de equações, e de forma simplificada para que um público com apenas conhecimento básico em física possa entender? Essa foi a pergunta apresentada aos alunos de pós-graduação das disciplinas de um ano de Mecânica Quântica I e II da Universidade Estadual de Campinas (UNICAMP), baseadas no livro "Quantum Mechanics" de J. J. Sakurai e Jim Napolitano. Os primeiros sete autores desse artigo são os alunos de pós-graduação (em ordem alfabética) que aceitaram o desafio. O tópico escolhido foi estados quânticos delocalizados, e será discutido utilizando termos coloquiais como fantasmas quânticos, ações fantasmagóricas, entidades divididas e capa de invisibilidade.
Palavras-chave: estados delocalizados, efeitos de interferência, experimento de dupla fenda.

Experimento de duas fendas com elétrons



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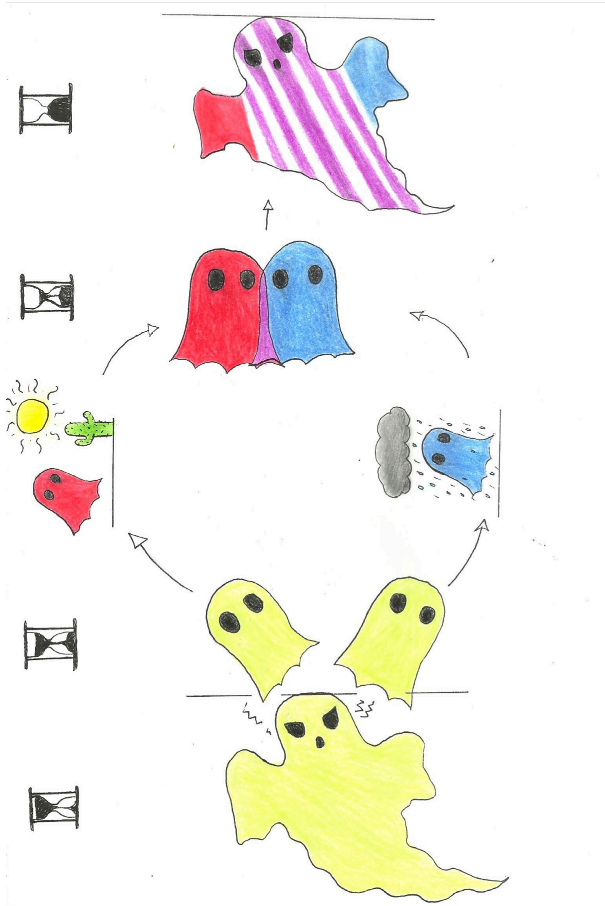

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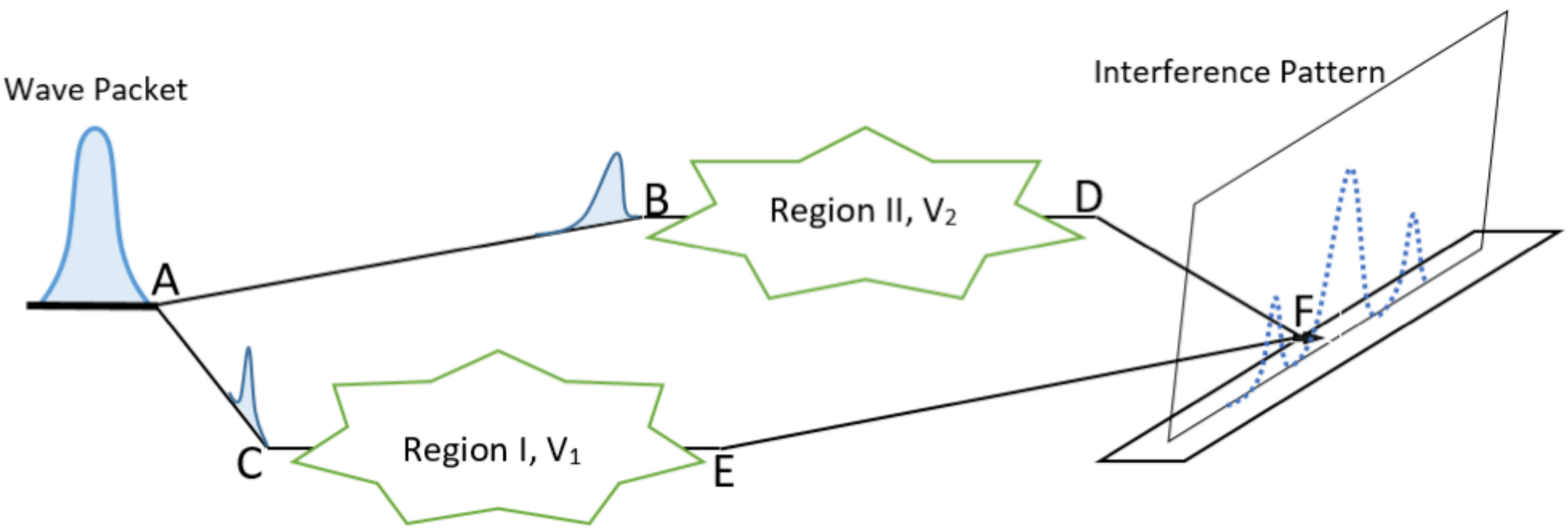
O Ambiente interage com pedaços da função de onda



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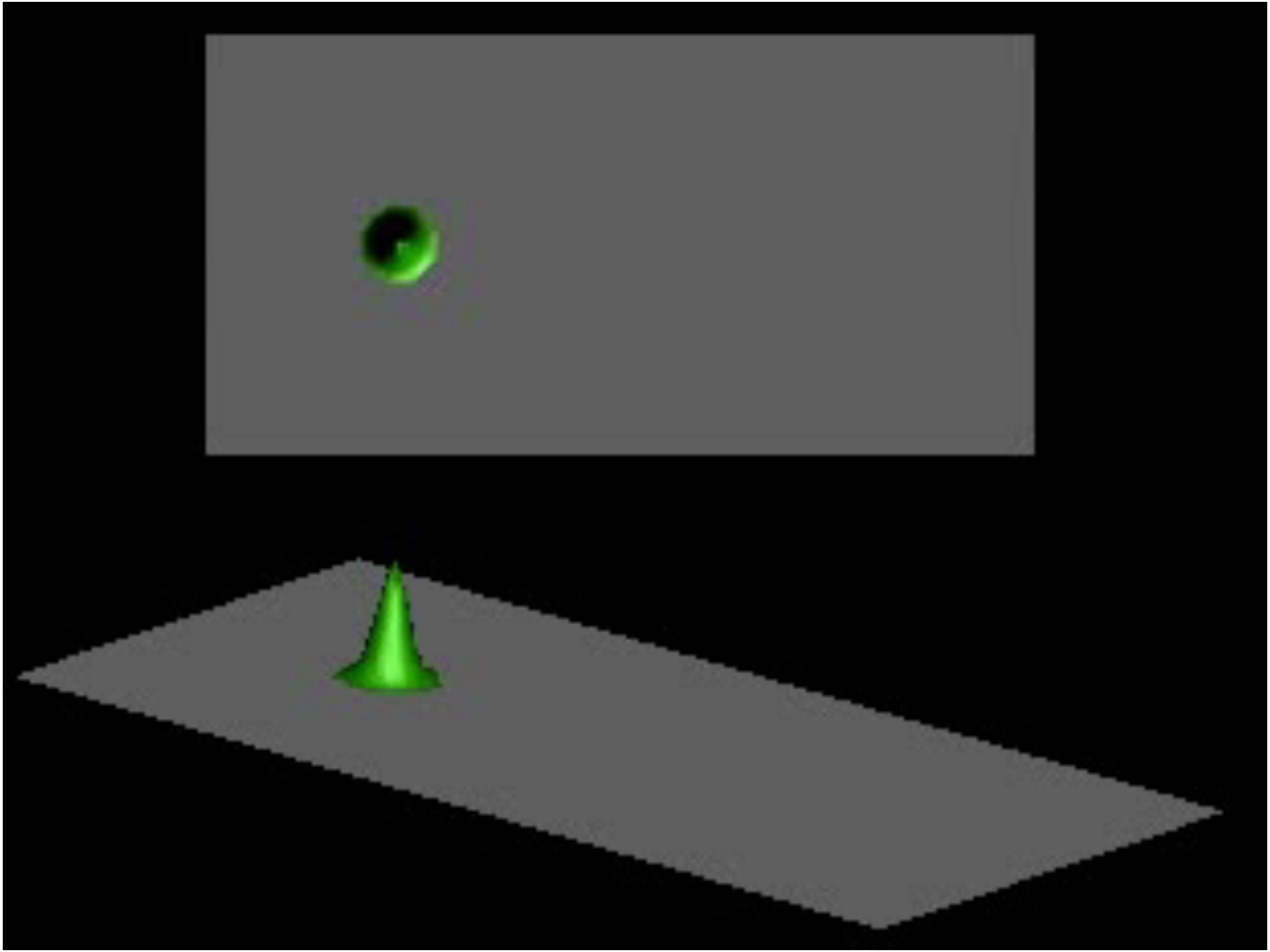
Relação de incerteza de Heisenberg

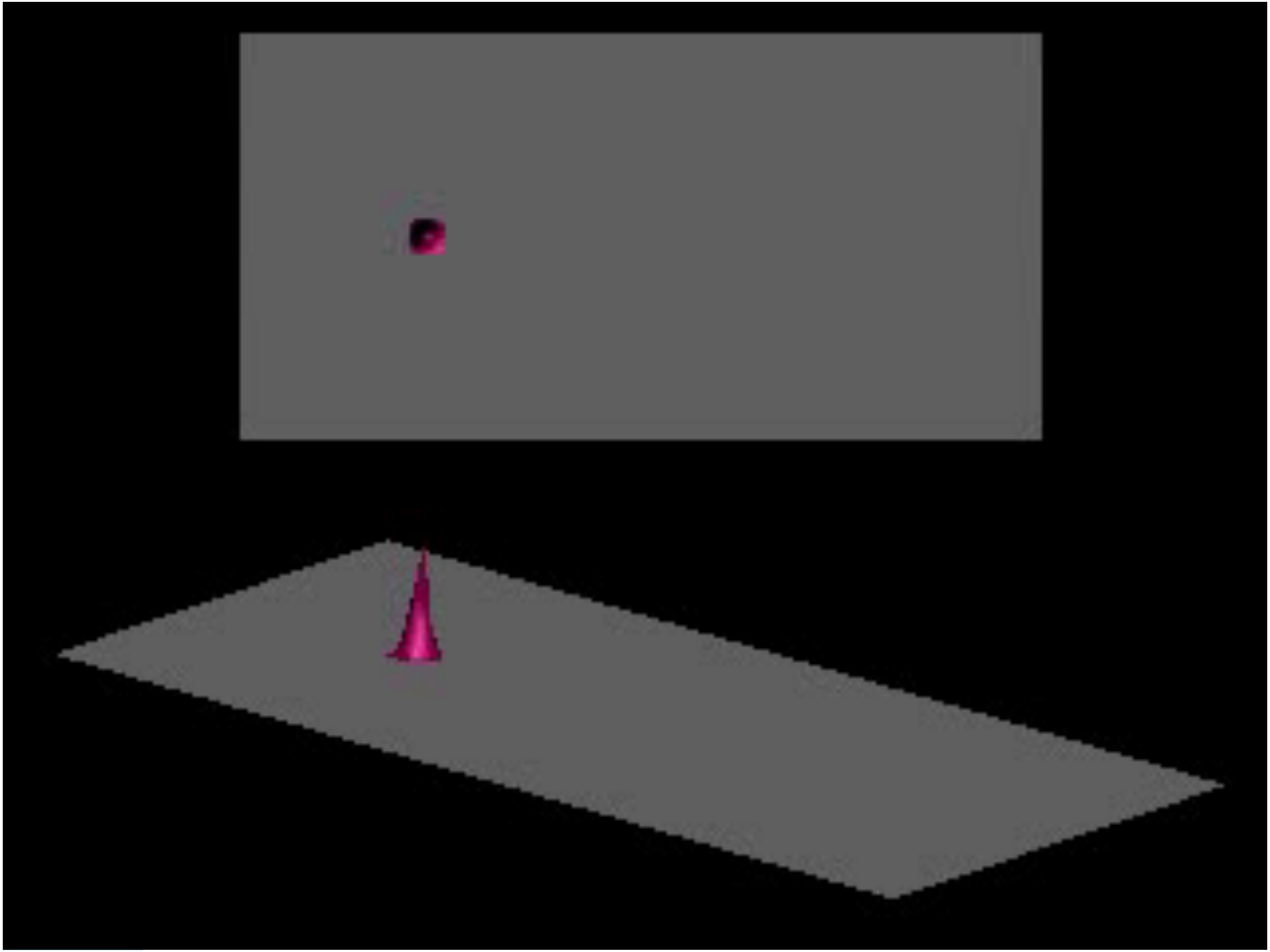
Todas as ondas respeitam esta relação:

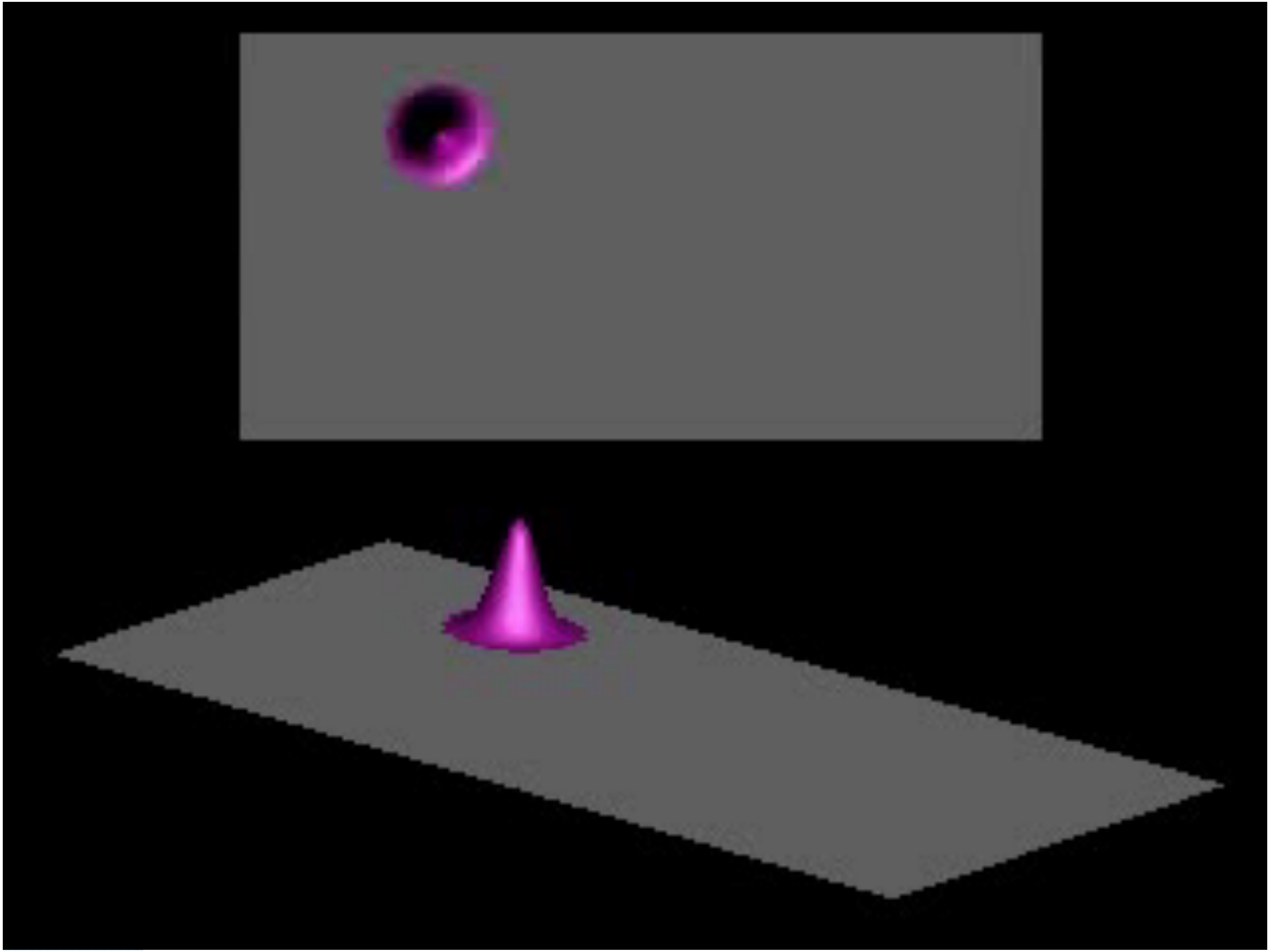
$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

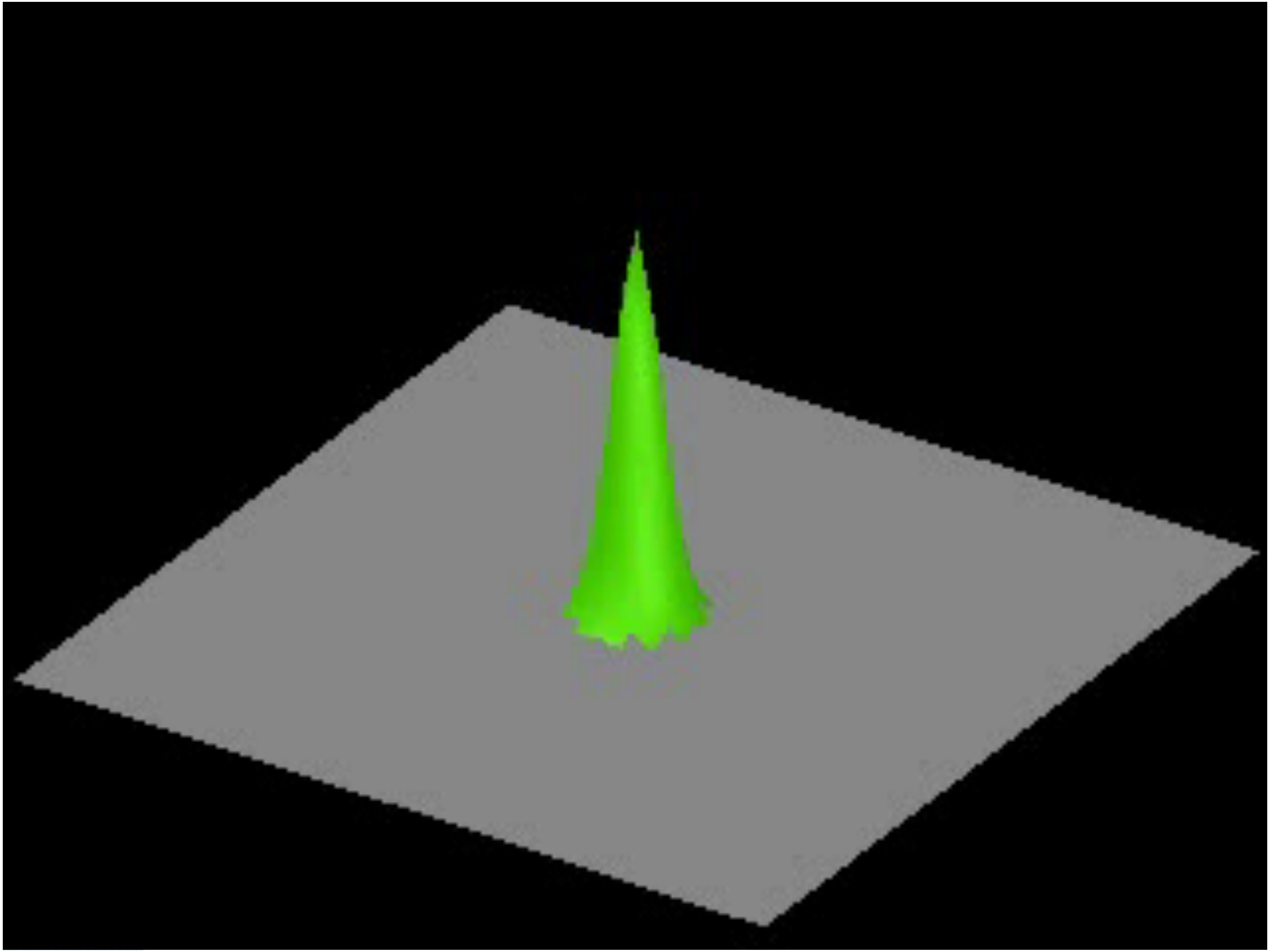
$$x = x_0 \pm \frac{\Delta x}{2} \qquad p = p_0 \pm \frac{\Delta p}{2}$$

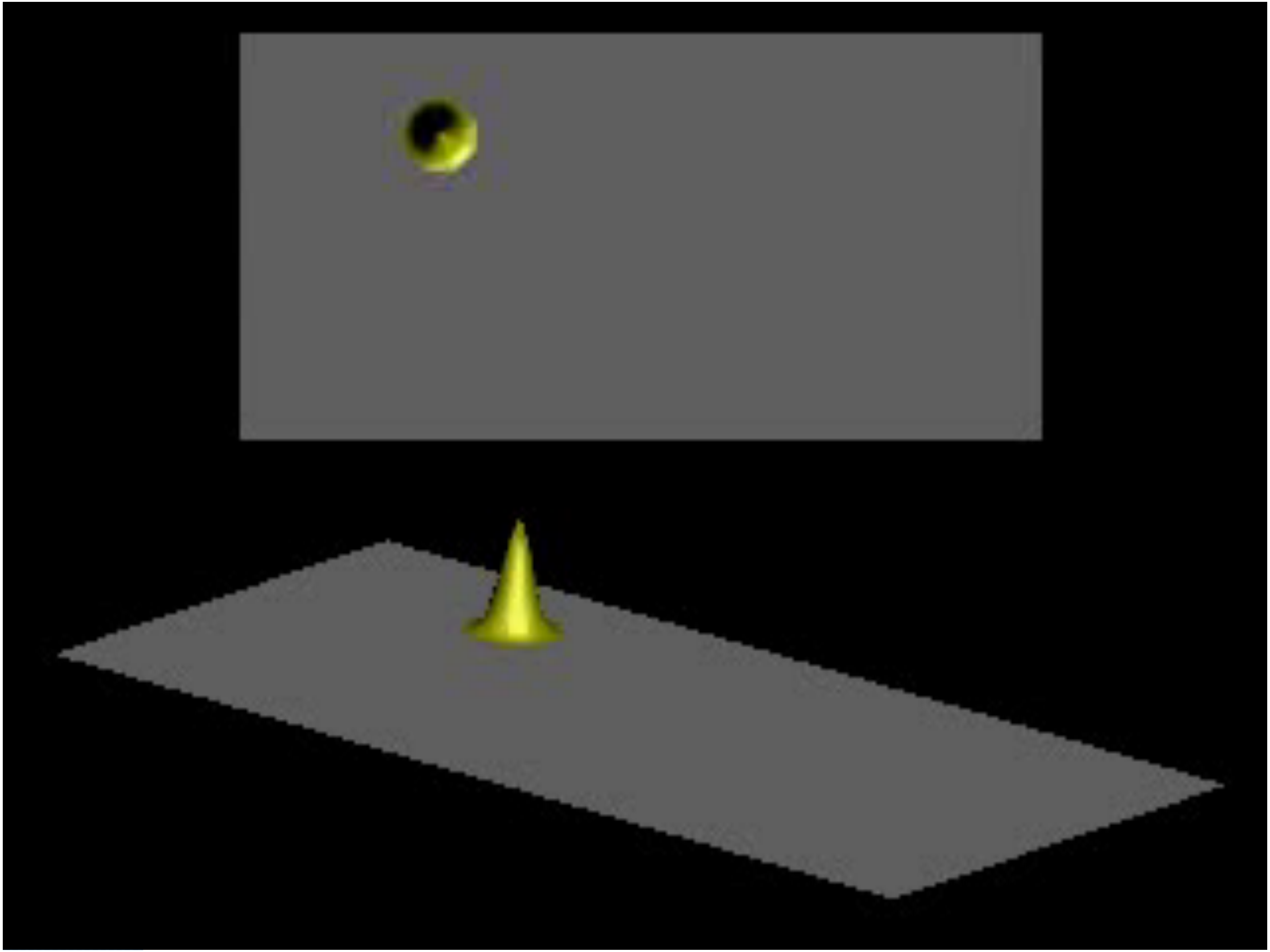
Somando ondas

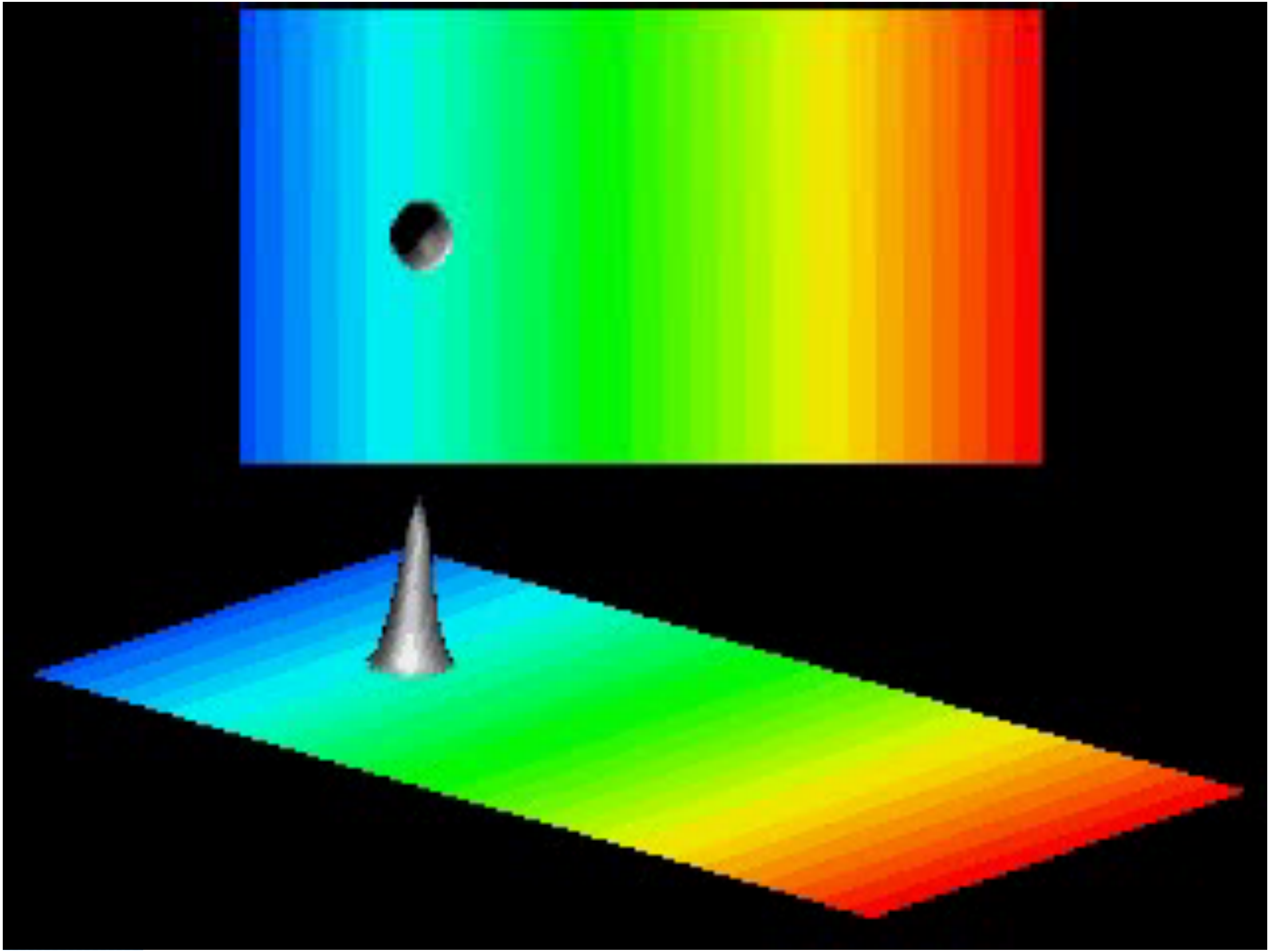


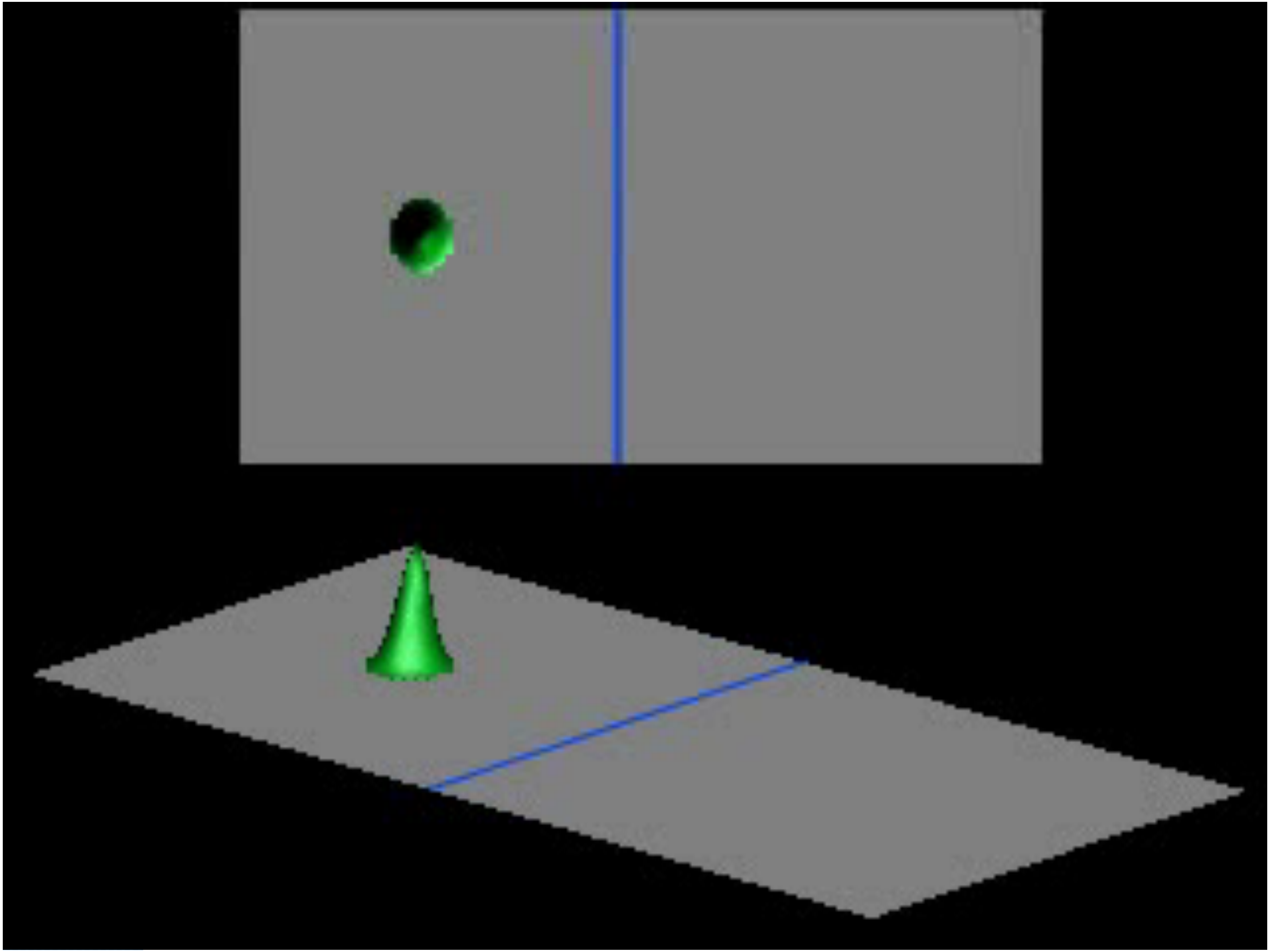


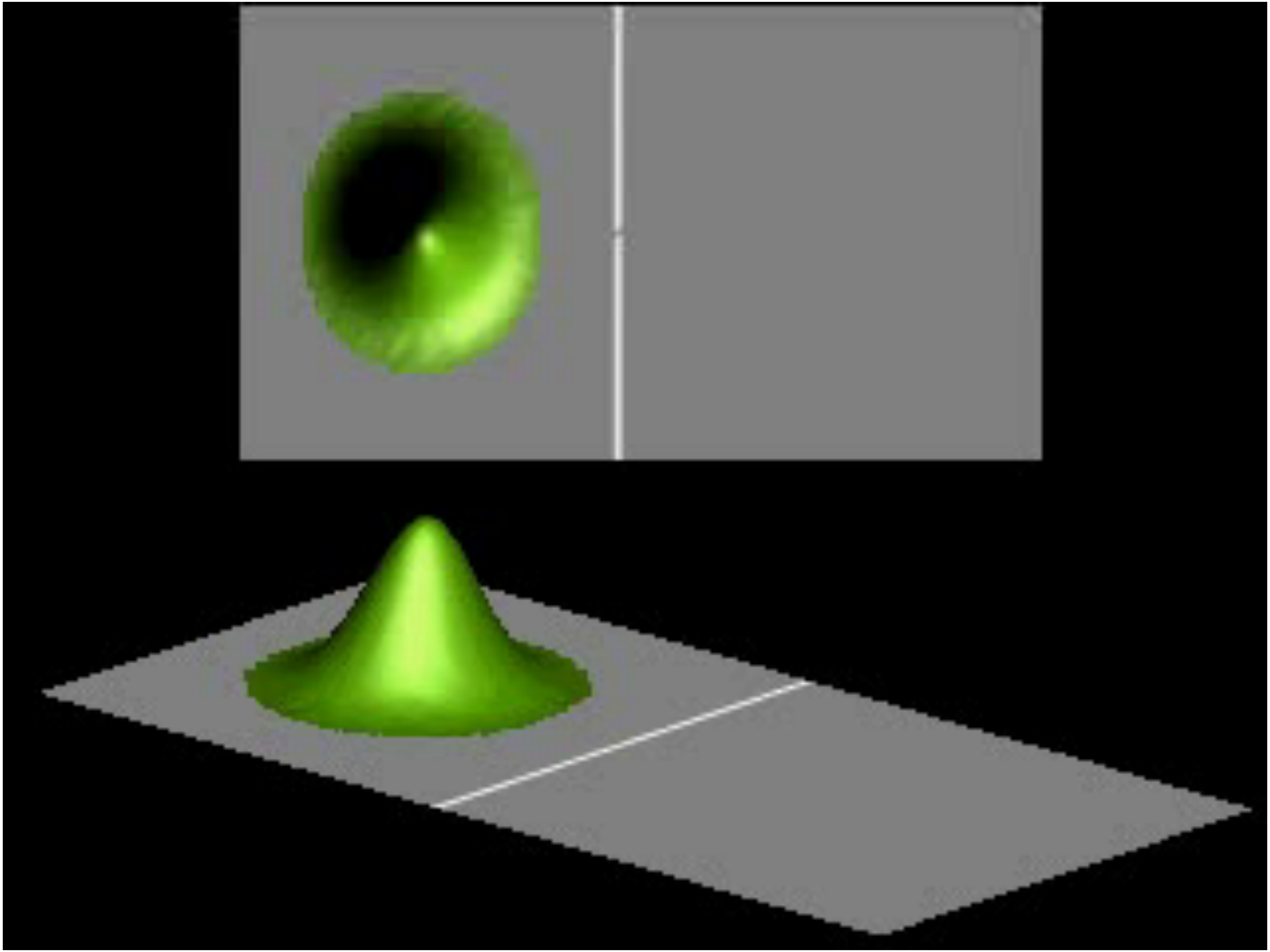


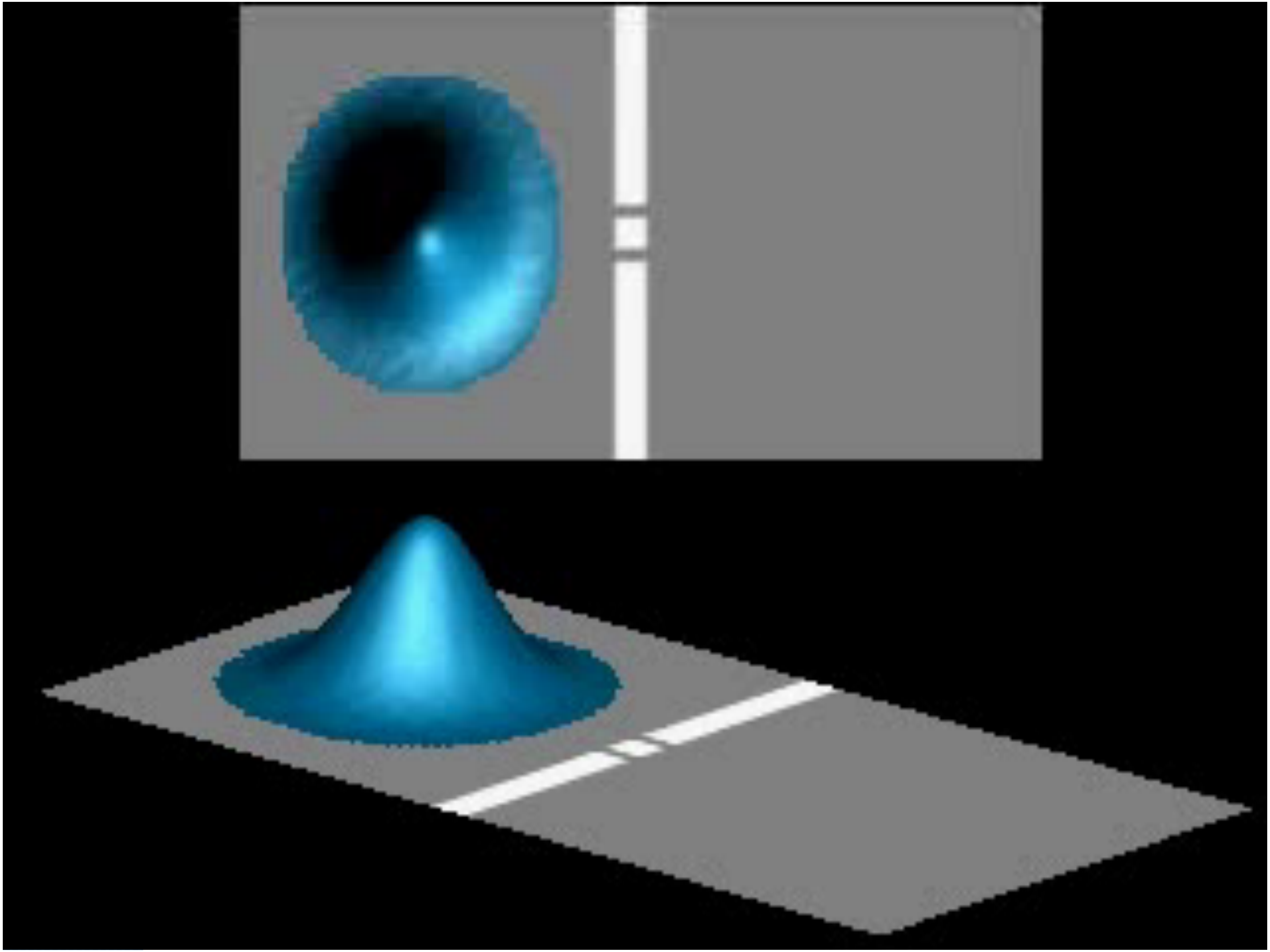




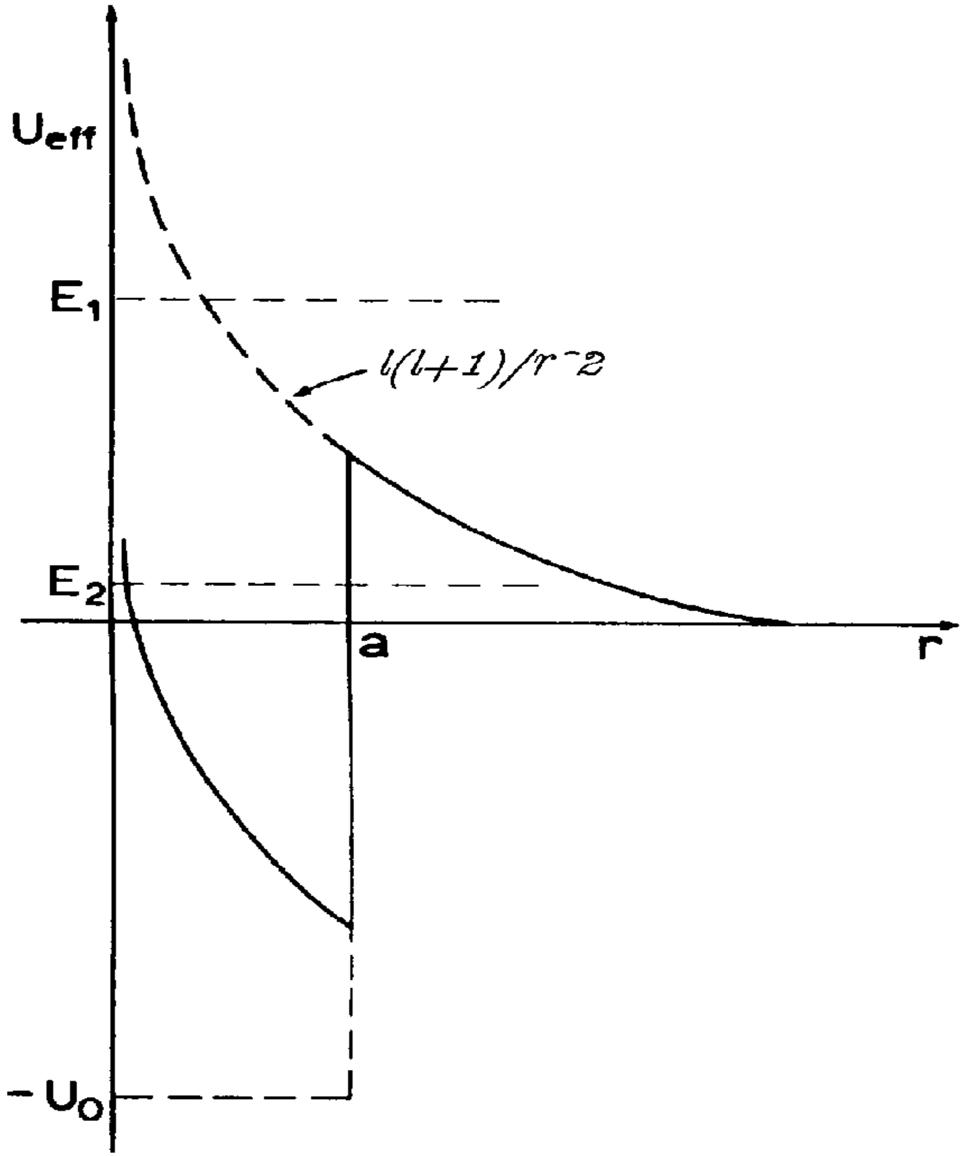






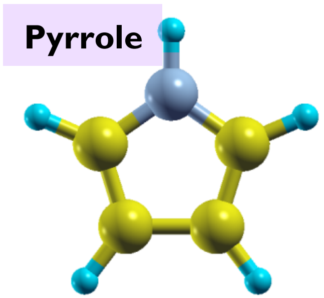


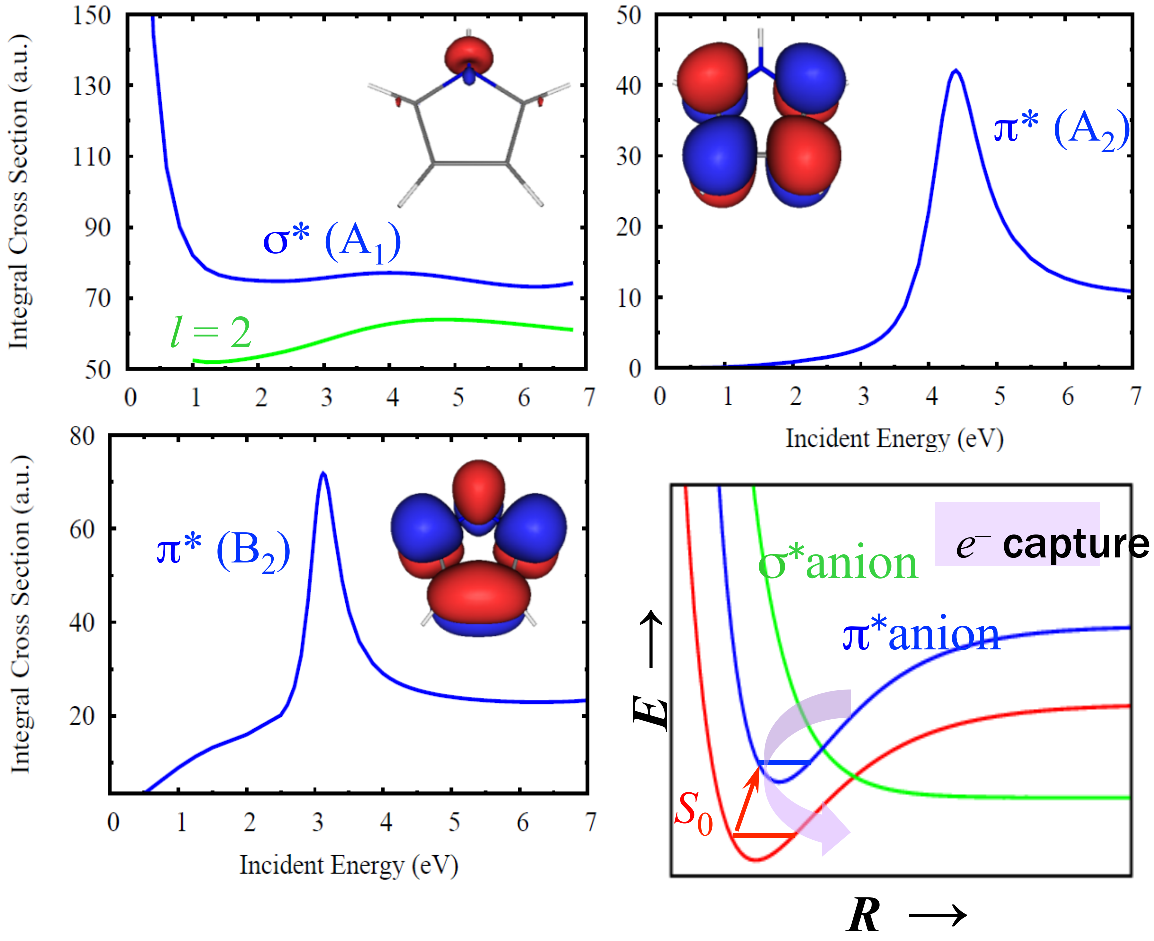
Shape resonances are related to angular momentum traps



Low energy elastic electron scattering from pirrole

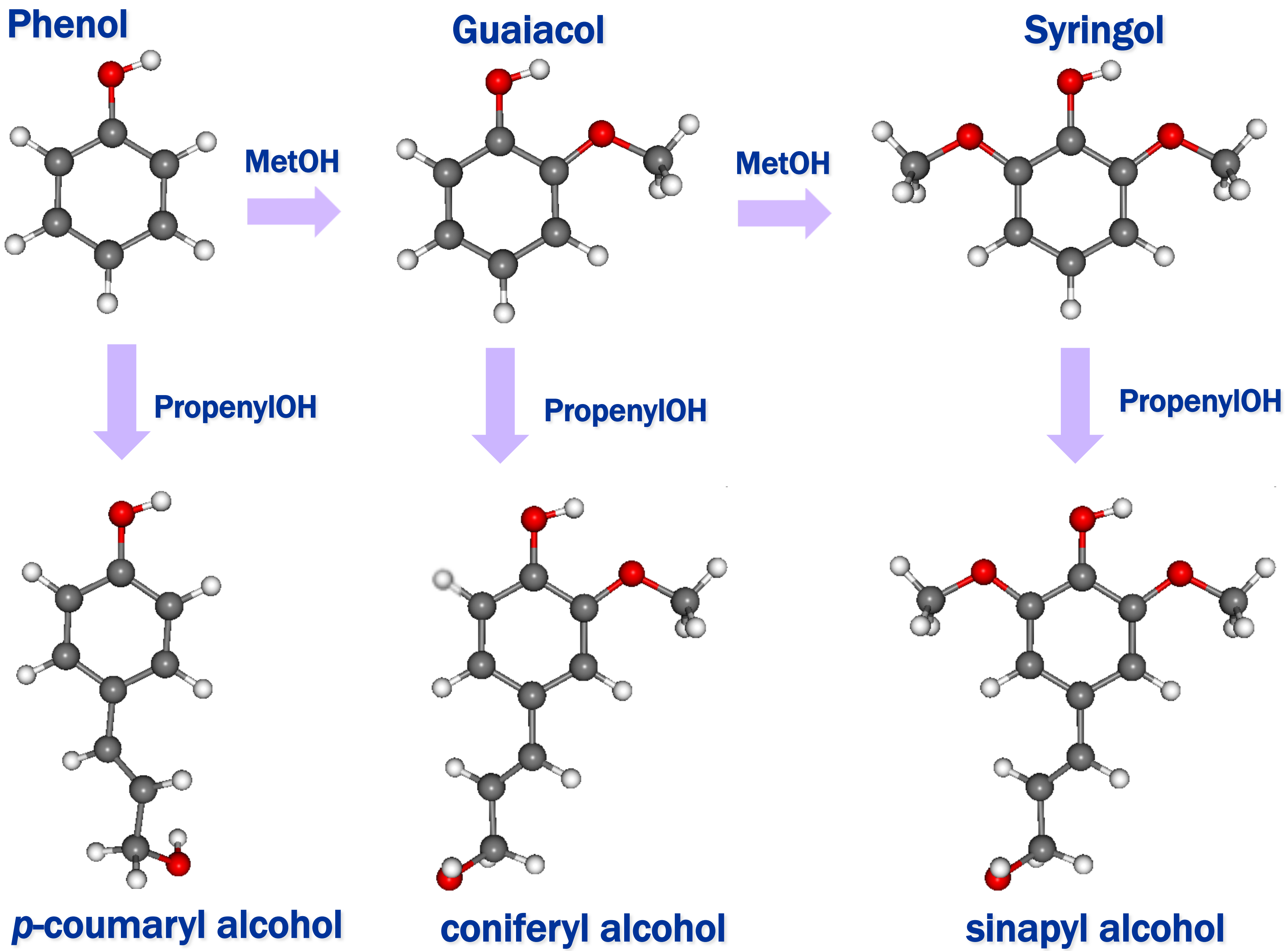
- There are π* (ring) and σ* (N–H) shape resonances in pyrrole. Nice prototype!





de Oliveira EM, Lima MAP, Bettega MHF, Sanchez SD, da Costa RF, and Varella MTD, J. Chem. Phys. **132**, 204301 (2010)

Lignin Subunits

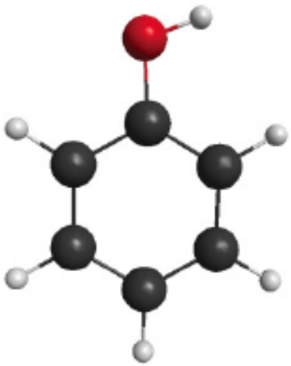


RAPID COMMUNICATIONS

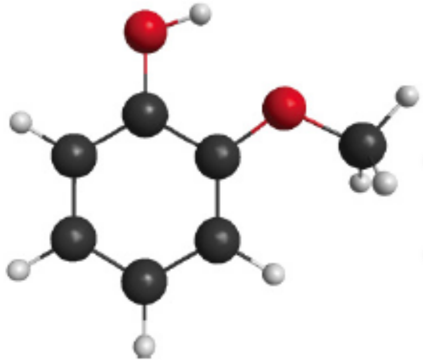
Shape resonance spectra of lignin subunits

PHYSICAL REVIEW A **86**, 020701(R) (2012)

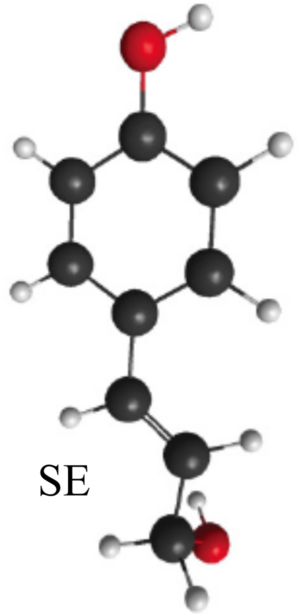
By E. M. de Oliveira, S. d'A. Sanchez, M. H. F. Bettega, A. P. P. Natalense, M A. P. Lima, and M. T. do N. Varella.

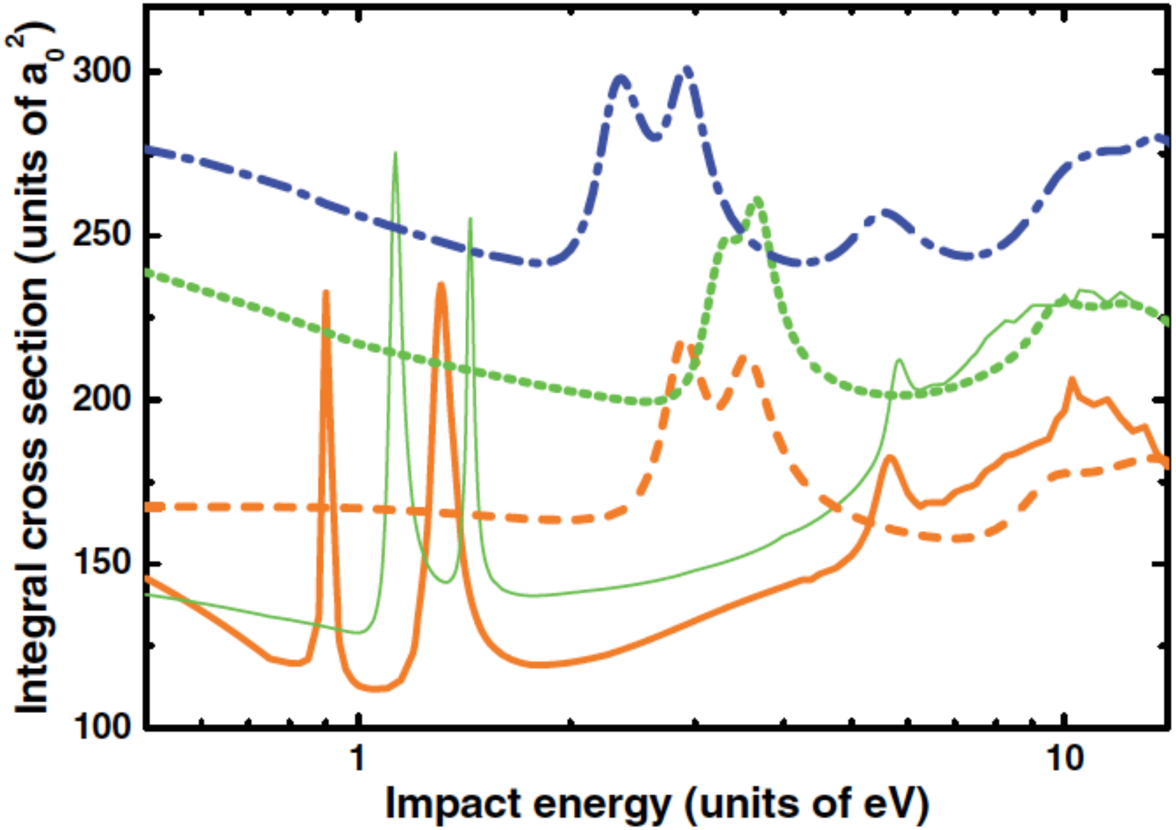


phenol



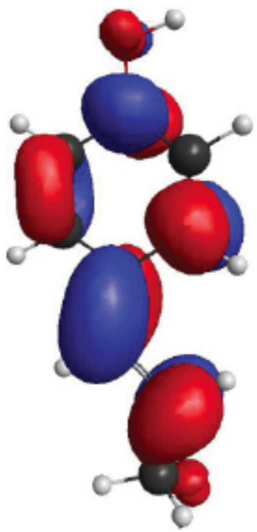
guaiacol



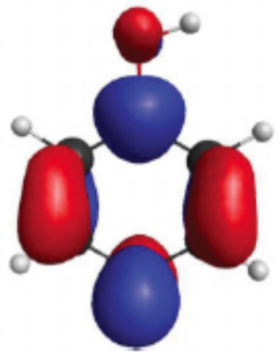


***p*-coumaryl alcohol**

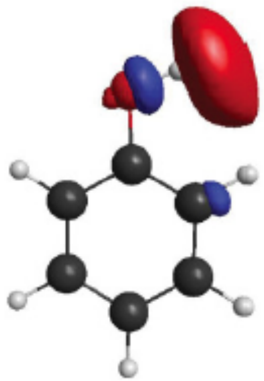
p-Cu (LUMO)



Lots of low-energy resonances!

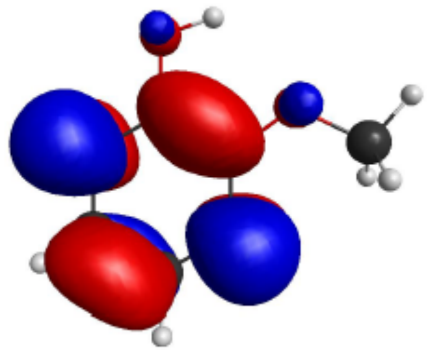


π* (LUMO+1)

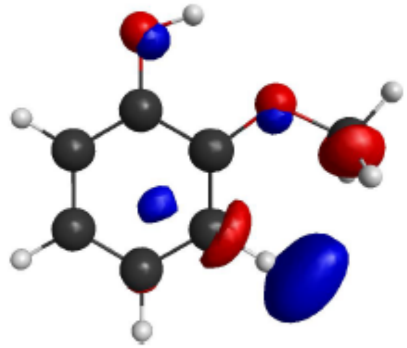


σ* (LUMO+2)

Phenol: Calculations, ET spectra and DEA data indicate H elimination from π*/σ* coupling.

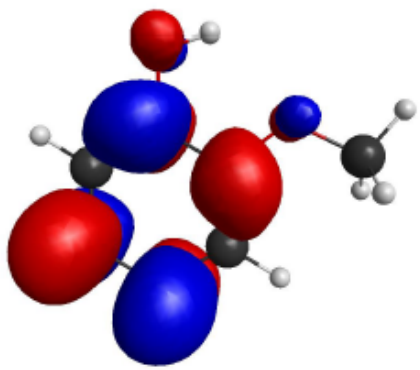


π* (LUMO)

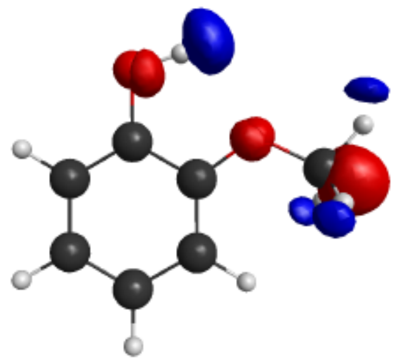


σ* (LUMO+2)

Guaiacol: Methoxilation is expected to give rise to other dissociation channels. H elimination should be also observed.



π* (LUMO+1)

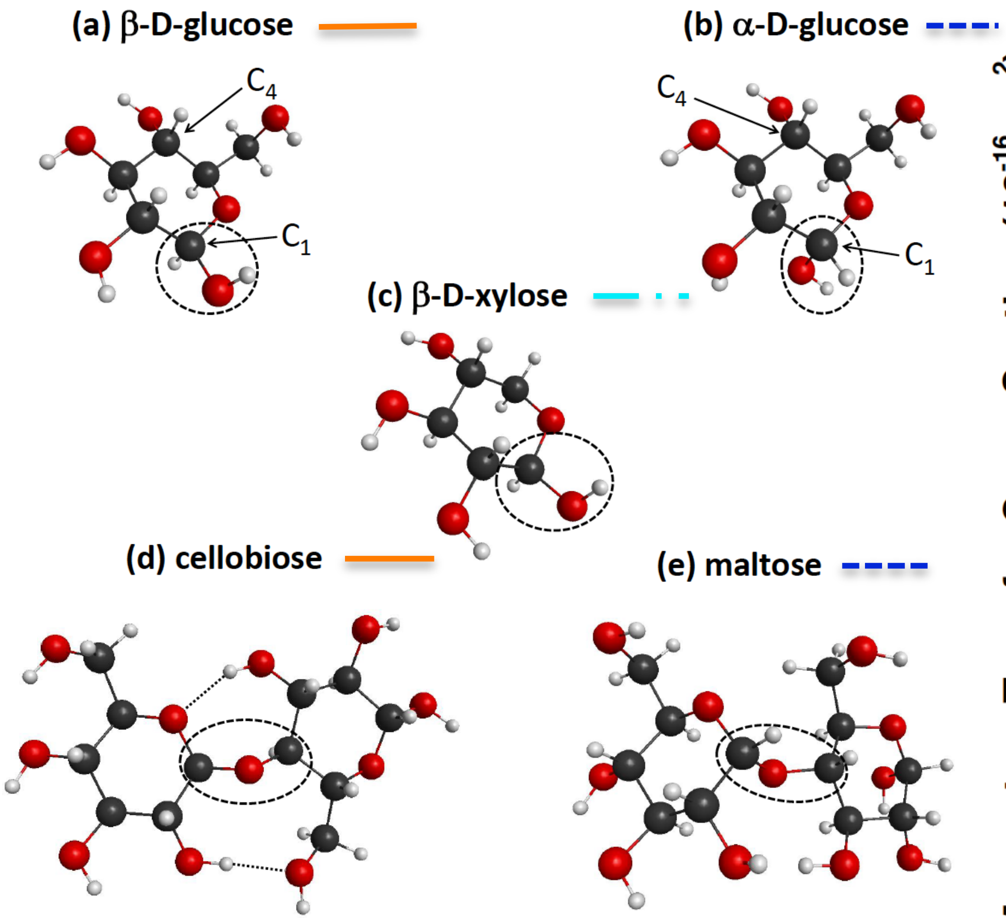


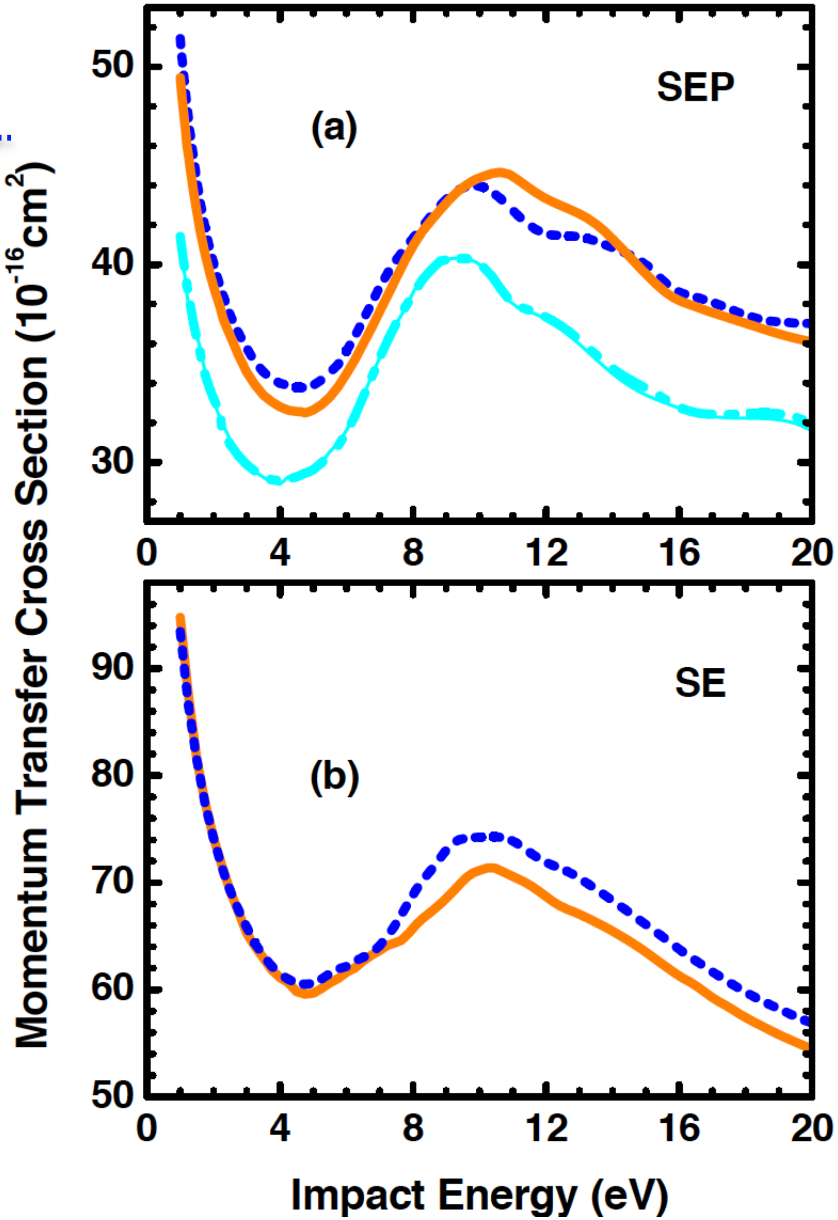
σ* (LUMO+3)

Low-energy electron scattering by cellulose and Hemicellulose components

Phys. Chem. Chem. Phys. **15**, 1682 (2013).

By E. M. de Oliveira, R. F. da Costa, S. d'A. Sanchez, M. H. F. Bettega, A. P. P. Natalense, M. A. P. Lima, and M. T. do N. Varella,





No low-energy resonances! Is this sufficient to explain why the discharge attacks the lignin and not so much the cellulose and hemicellulose?

Obrigado pela atenção, pessoal!

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