The Abdus Salam
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Computational Photonics: Forces and Quantum Fluctuations

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Computational Nanophotonics: Forces and Fluctuations

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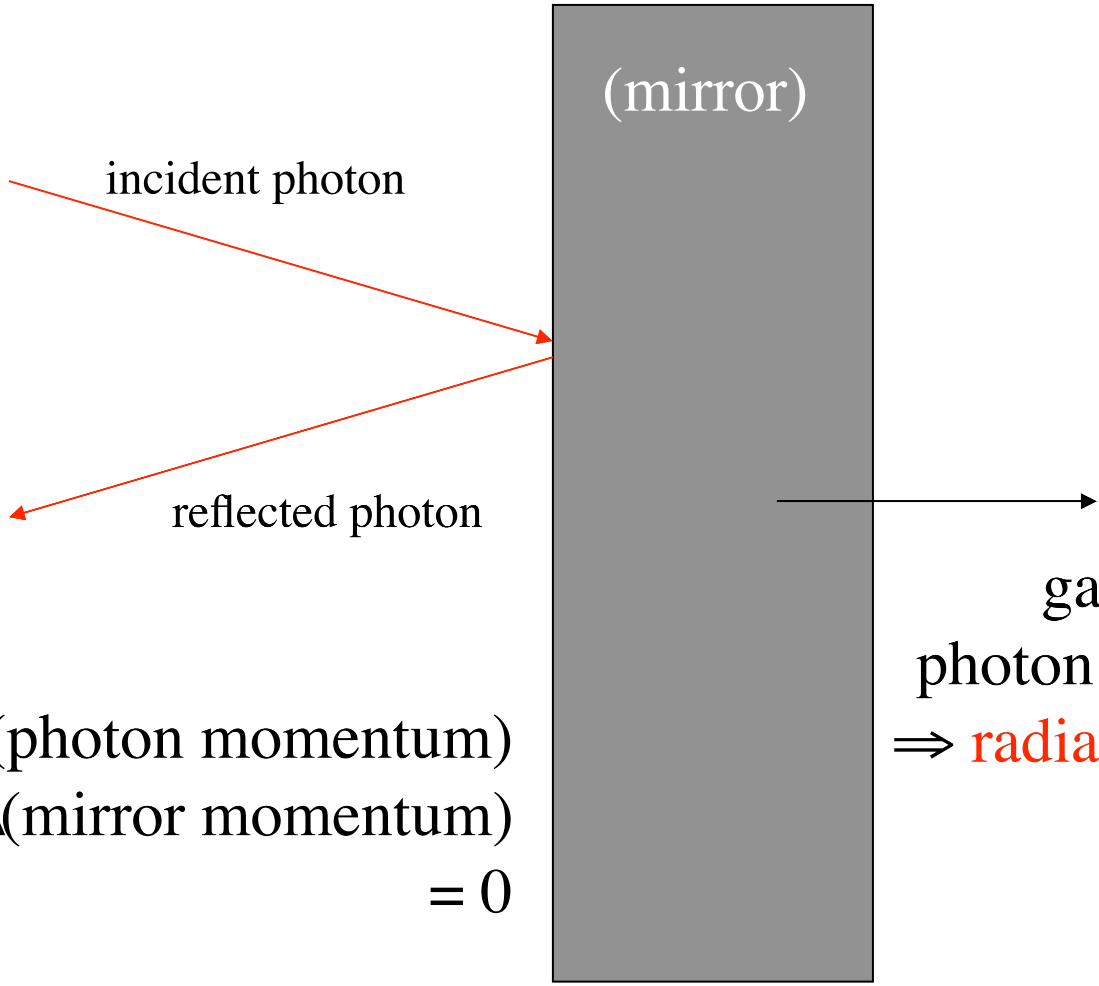
[here,
forces from *oscillating* fields (light),
not electrostatic forces]

Radiation Pressure

[Maxwell, 1871]

photon has momentum $\hbar\omega/c$

(classically, $\mathbf{E}\times\mathbf{H} / c^2$ = momentum density)



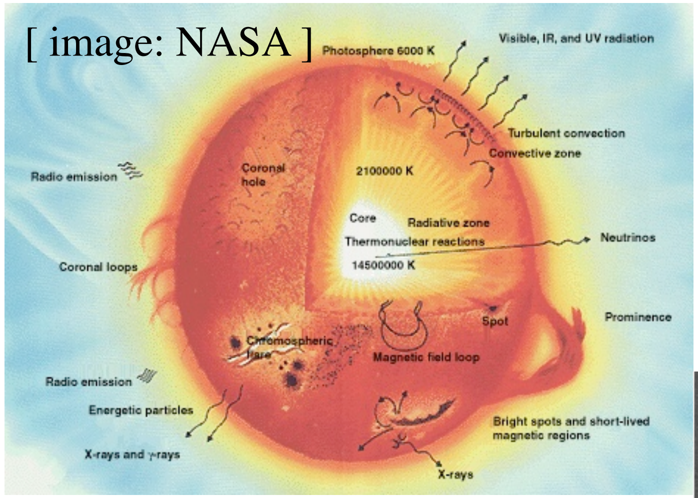
gains 2 ×
photon momentum
⇒ radiation pressure

Δ(photon momentum)
+ Δ(mirror momentum)
= 0

Observations of Radiation Pressure

[observed since 1901]

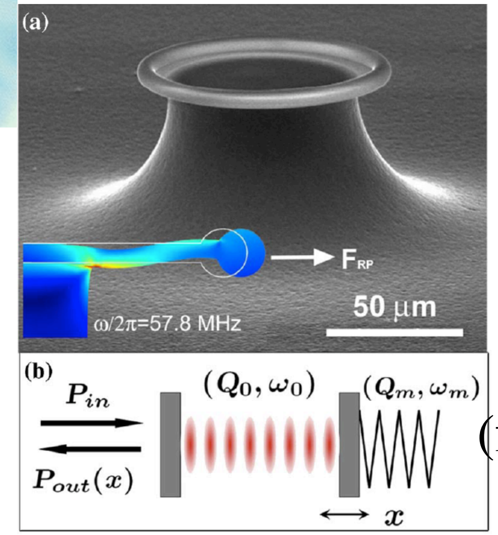
very *large* scales:



important in determining stellar structure

very *small* scales:

laser cooling of atoms



radiation-pressure cooling of microdisk resonators via opto-mechanical coupling

[Schliesser et al., *PRL* **97**, 243905 (2006)]

(for detecting tiny displacements, gravitational waves, etc.)

we also want forces

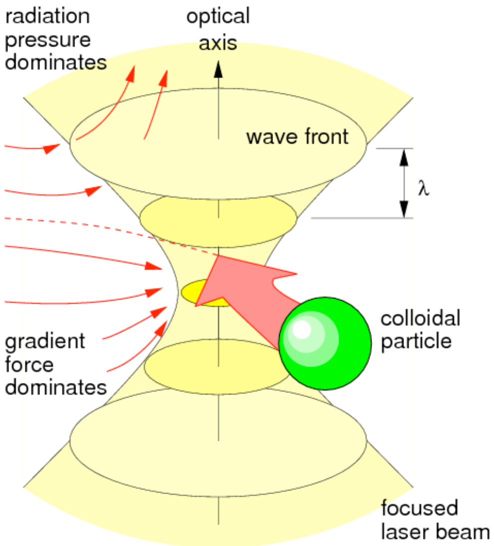
from *confined* light

(not free-space propagation)

to enhance/control interactions

Gradient Forces
and Evanescent Coupling

gradient force
in optical tweezers



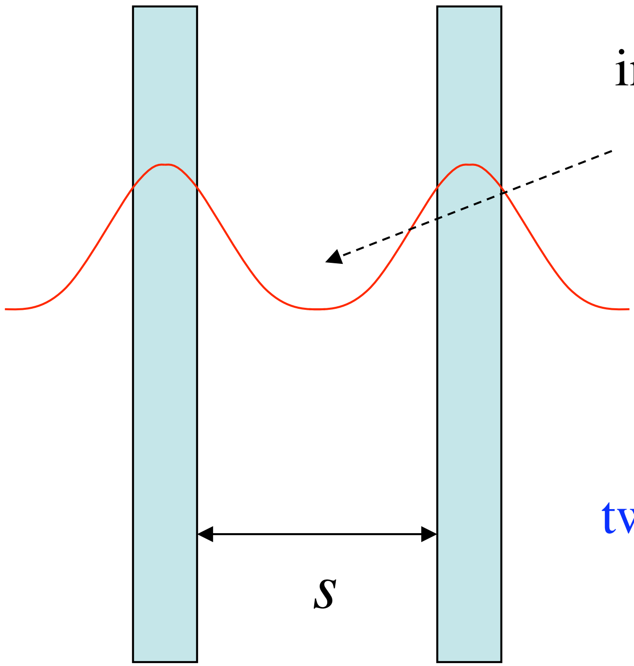
physics.nyu.edu/~dg86

force ~ $-\nabla(-\mathbf{p}\cdot\mathbf{E})$

~ $\alpha\nabla(|\mathbf{E}|^2)/2$

for particle polarizability α

evanescent coupling
between two waveguides

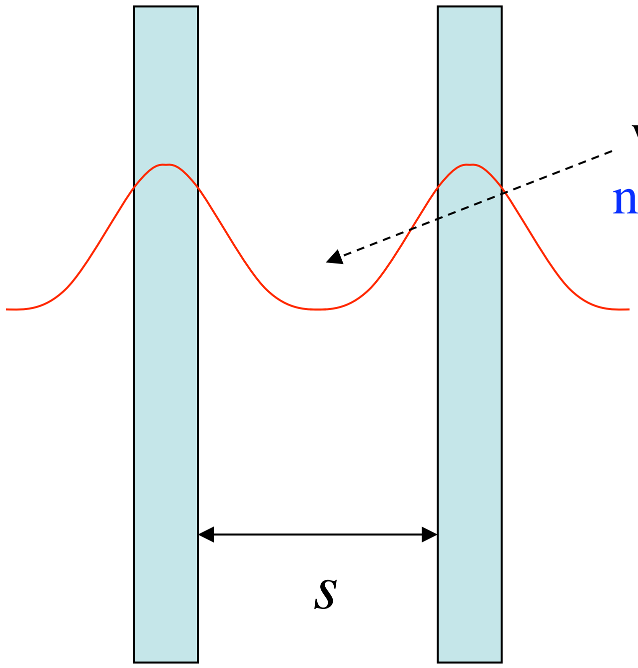


in between waveguides
is a nonzero Maxwell
stress tensor
~ $E^2 + B^2$
~ force/area

interaction between
two waveguides is key…

Evanescent-Coupling Forces

from frequency shifts



in between waveguides is a nonzero Maxwell stress tensor $\sim E^2 + B^2$ ~ force/area

evanescent coupling between two waveguides

equivalently:

finite *s* affects mode frequency ω, Δ*s* = change in photon energy ħω, hence a force

force/length

$= -(\text{\# photons/length})\, d(\hbar\omega)/ds$

$= -(U / \hbar\omega)\, d(\hbar\omega)/ds$

$= -U/\omega\, d\omega/ds$

for a total energy/length *U*

(can also be derived classically)

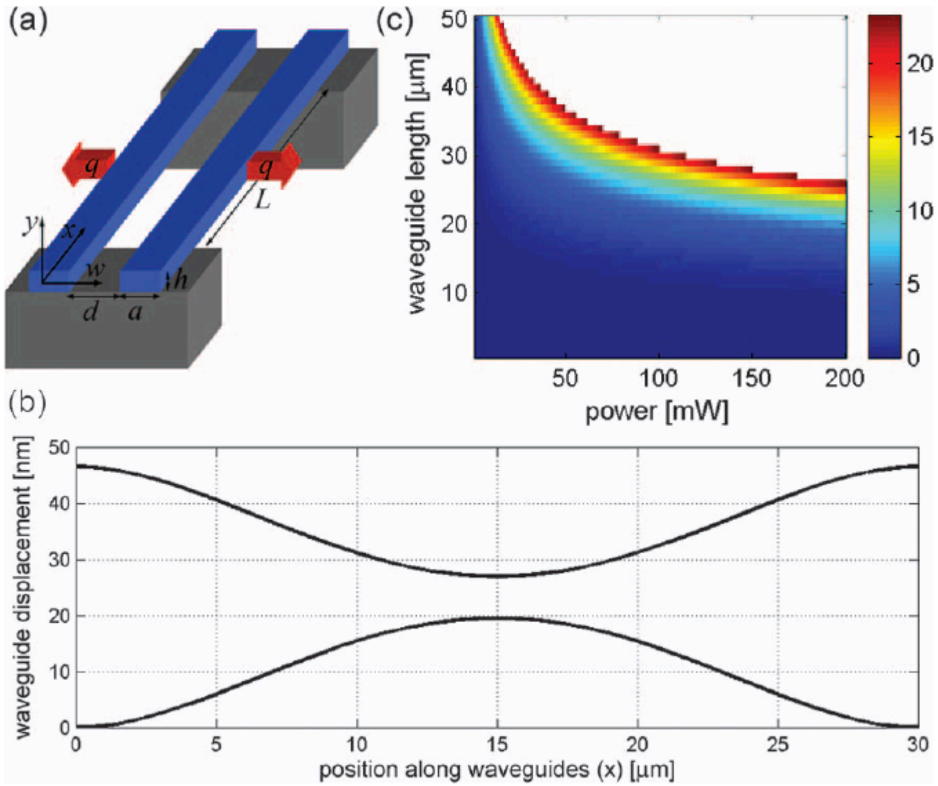
[Povinelli *et al*., *Opt*. *Express* **13**, 8286 (2005)]

Attraction and Repulsion Between Waveguides

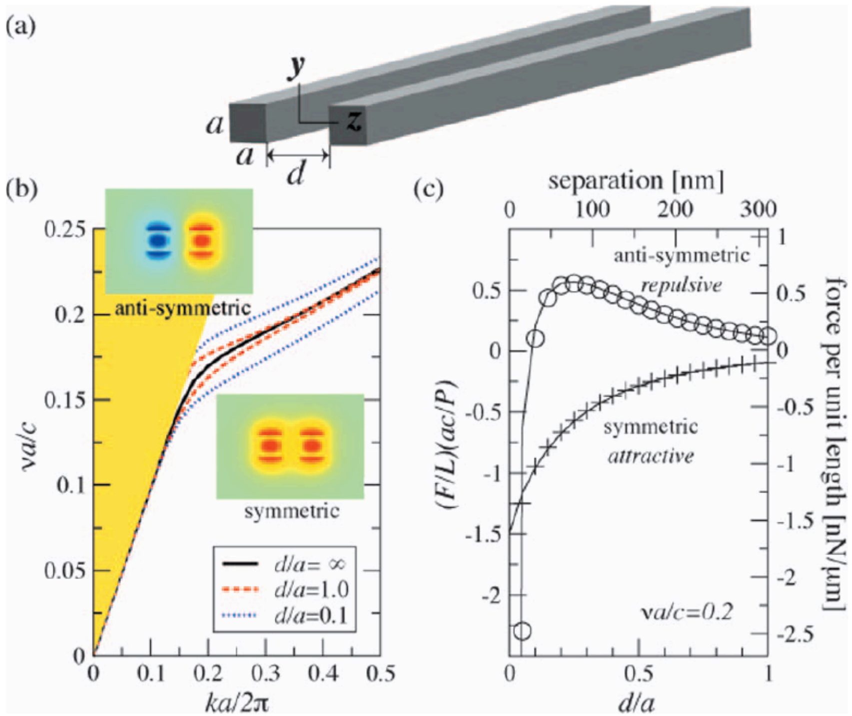
[Povinelli *et al*., *Opt*. *Lett*. **30**, 3042 (2005)]

mechanical displacement calculation (SOI air-bridge waveguides)

optical force calculations



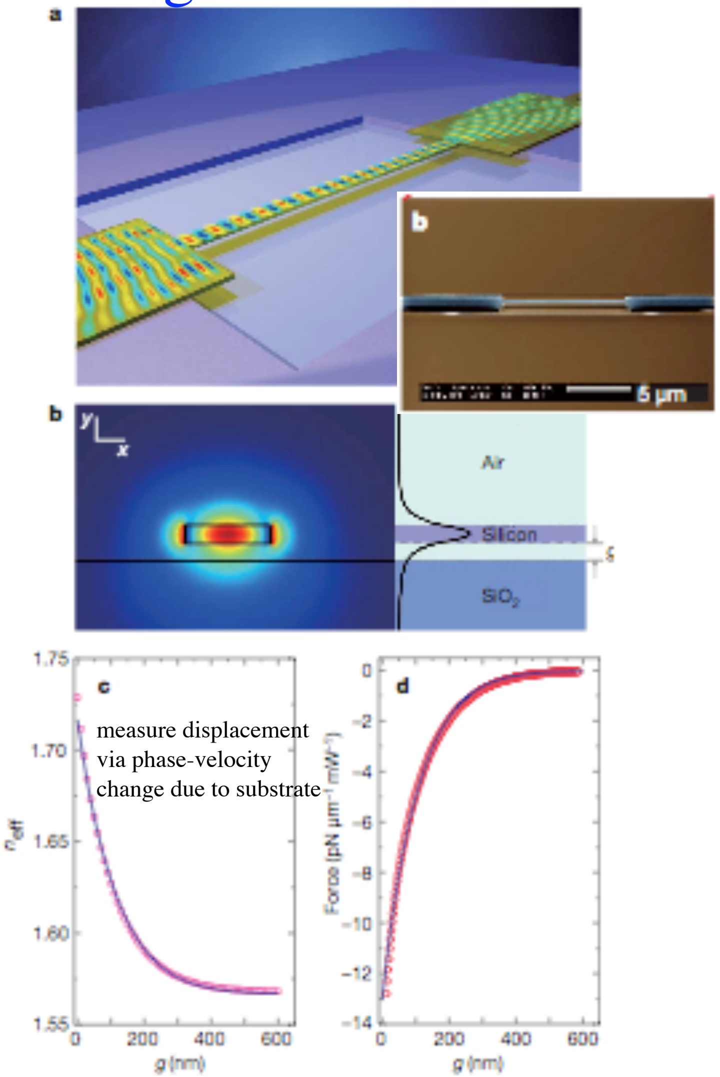
(λ=1.55μm, power = 100mW)



symmetric/antisymmetric modes haveattractive/repulsive force

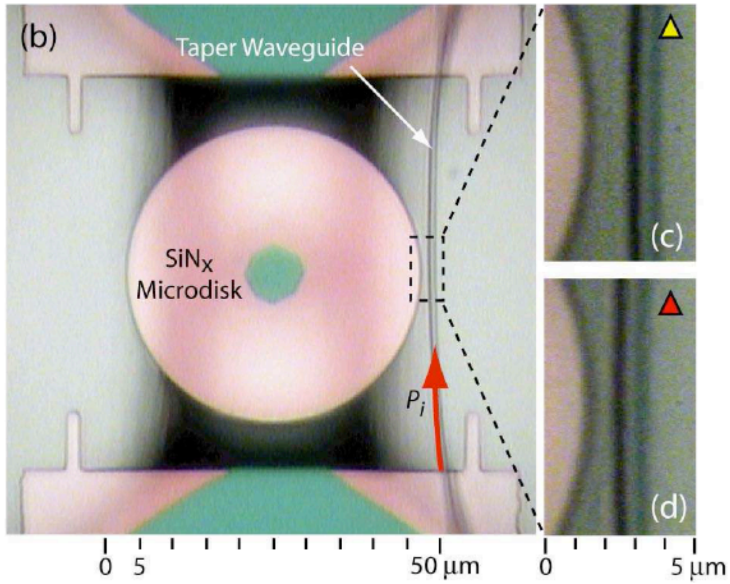
Recent Experimental Realizations

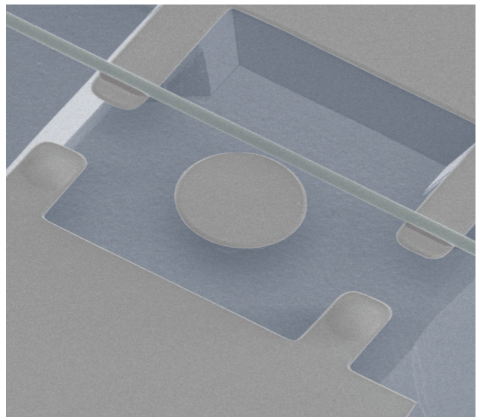
waveguide/substrate force



[Li et al. *Nature* **456**, 480 (2008)]

waveguide/microdisk force

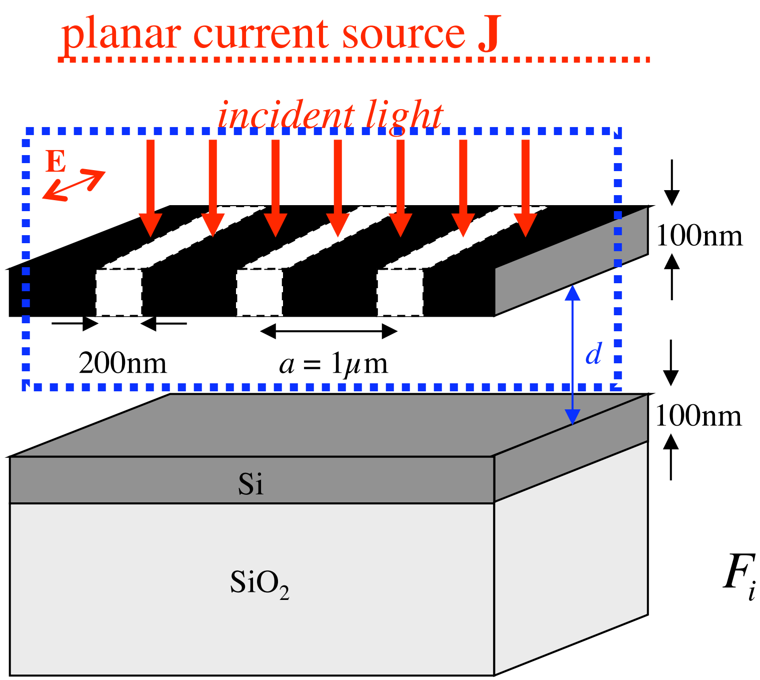




[Eichenfield et al. *Nature Photonics* **1**, 416 (2007)]

Computing forces via stress tensors

example system:



Frequency-domain approach:

1) put in planar current source **J** at ω to generate incident wave.

2) compute resulting **E**, **H**

3) integrate Maxwell stress tensor over bounding box to get force at ω

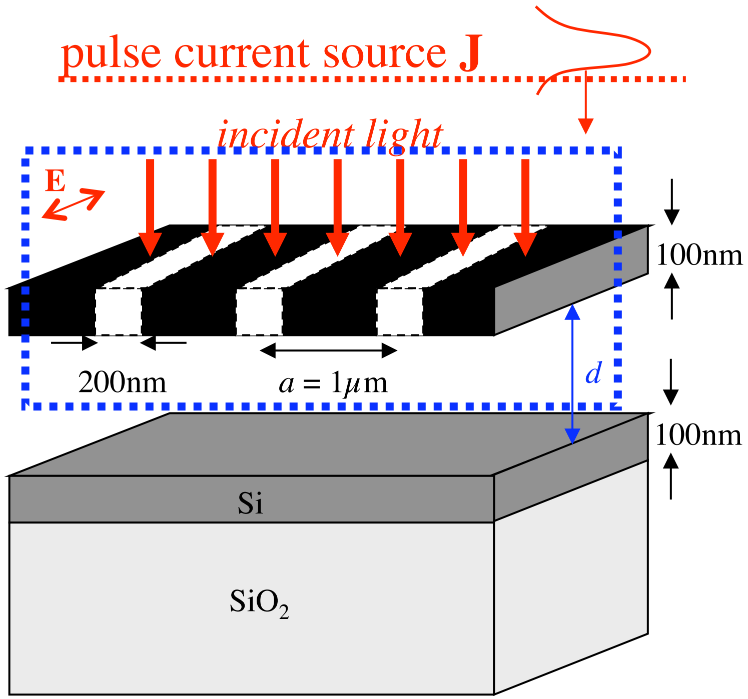
$$F_i = \oint\!\!\oint \sum_j \left[E_i E_j + H_i H_j - \delta_{ij} \frac{|\mathbf{E}|^2 + |\mathbf{H}|^2}{2} \right] dA_j$$

4) repeat for each desired ω

… yuck

Computing whole spectrum at once

example system:

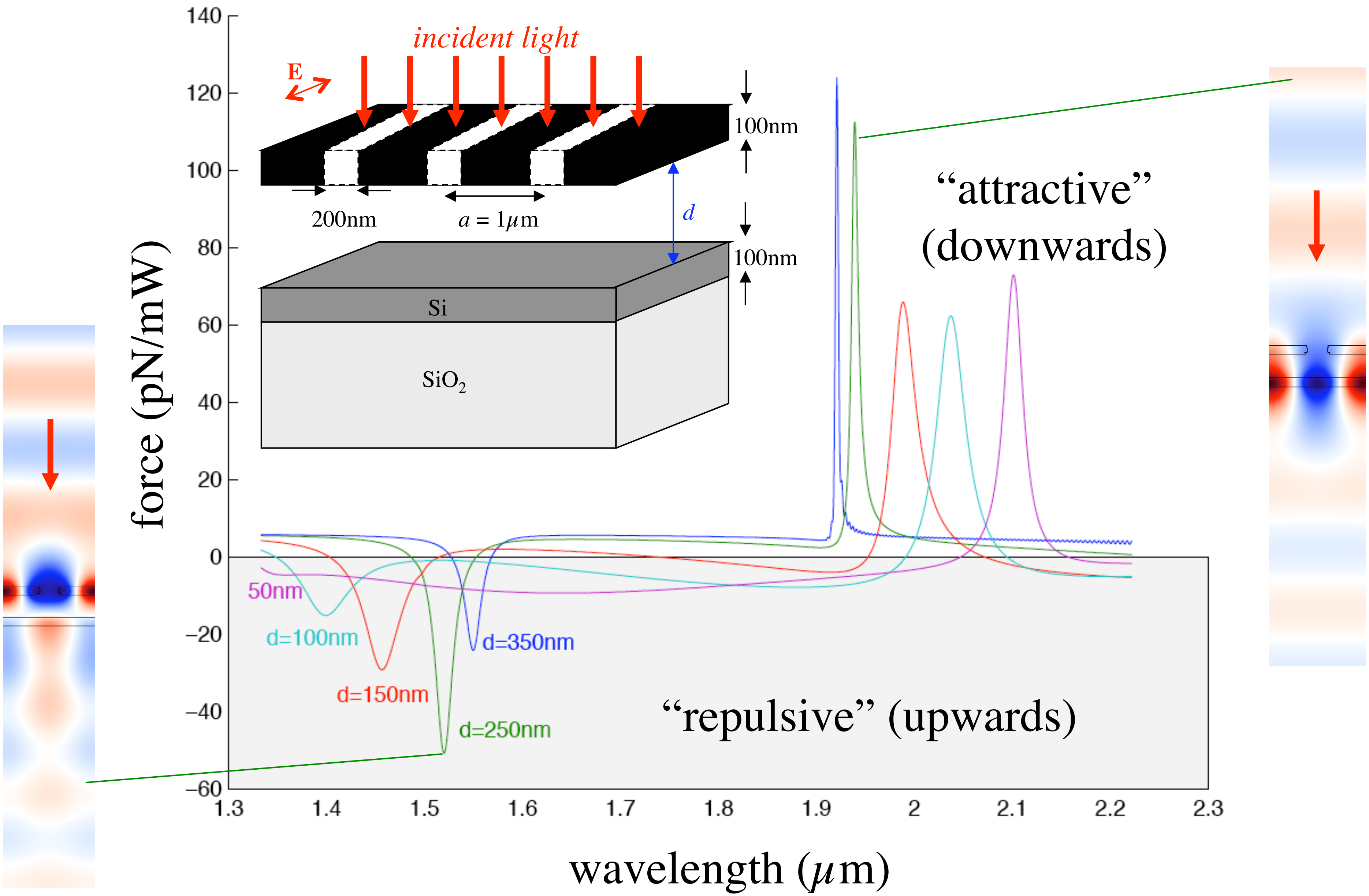


Time-domain approach:

1) put in planar current source **J** as a short pulse to generate incoming pulse.
2) record resulting **E**(t), **H**(t) on bounding box
3) Fourier transform to obtain **E**(ω), **H**(ω) on bounding box
4) integrate Maxwell stress tensor over bounding box to get force at each ω

$$F_i = \oiint \sum_j \left[E_i E_j + H_i H_j - \delta_{ij} \frac{|\mathbf{E}|^2 + |\mathbf{H}|^2}{2} \right] dA_j$$

Classical Optical Force on Membrane



What happens when there is

no input power,

no light,

no net charge

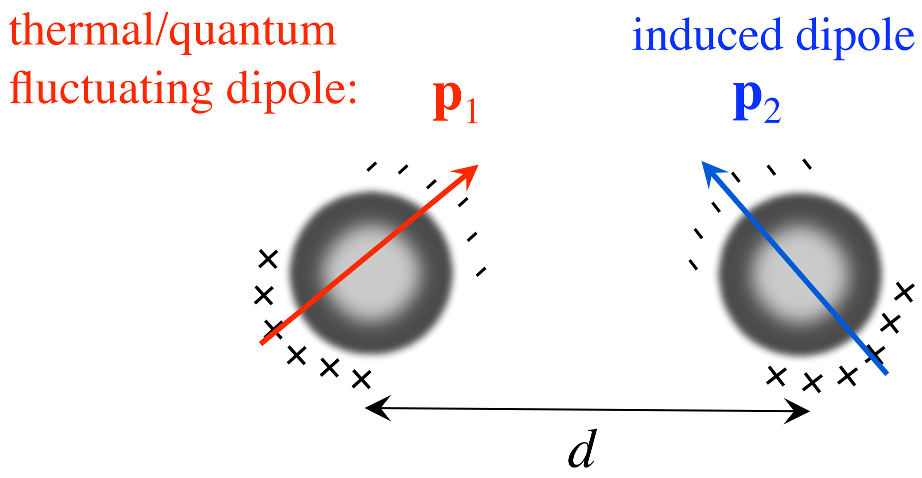
. . .

$\Rightarrow$ no electomagnetic force?

No, there ***is*** an EM force.

Fluctuation-Induced Interactions

Attractive forces between otherwise neutral atoms



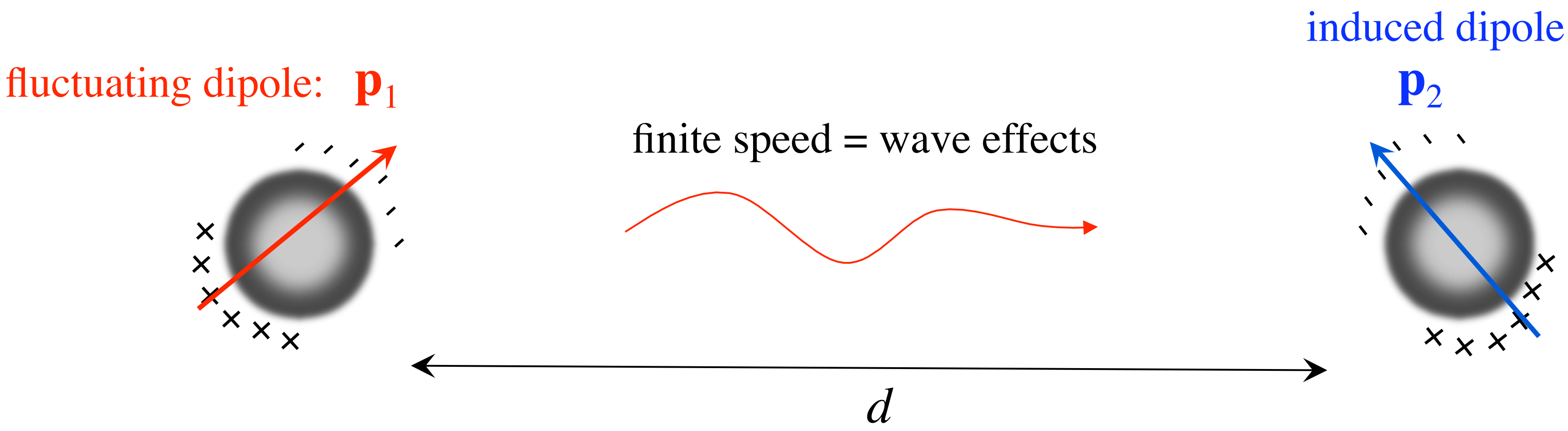
van der Waals force

(close proximity)

$$U \sim -\frac{1}{d^6} \quad \Rightarrow \quad F \sim -\frac{1}{d^7}$$

Fluctuation-Induced Interactions

Attractive forces between otherwise neutral atoms



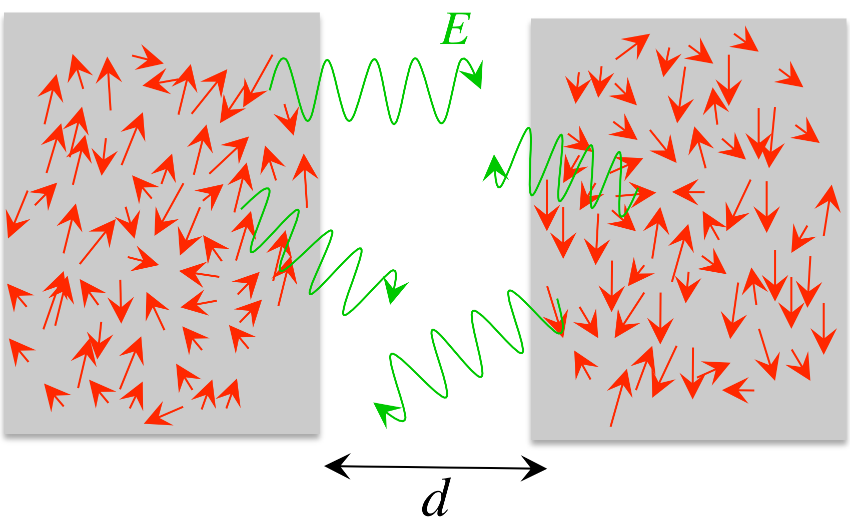
Casimir–Polder force

(separations >> resonant wavelength)

$$U \sim -\frac{1}{d^7} \quad \Rightarrow \quad F \sim -\frac{1}{d^8}$$

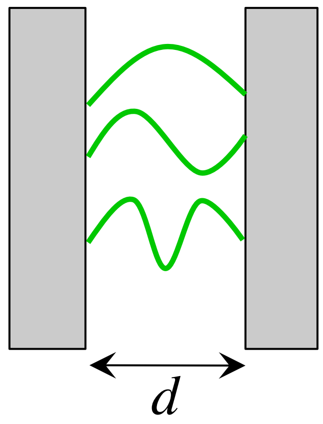
Casimir Effect

macroscopic objects
(many interacting dipoles)



Hendrik Casimir (1948)

perfect metal plates



$$F/A = -\frac{\hbar c \pi^2}{240 d^4}$$

attractive, monotonically decreasing

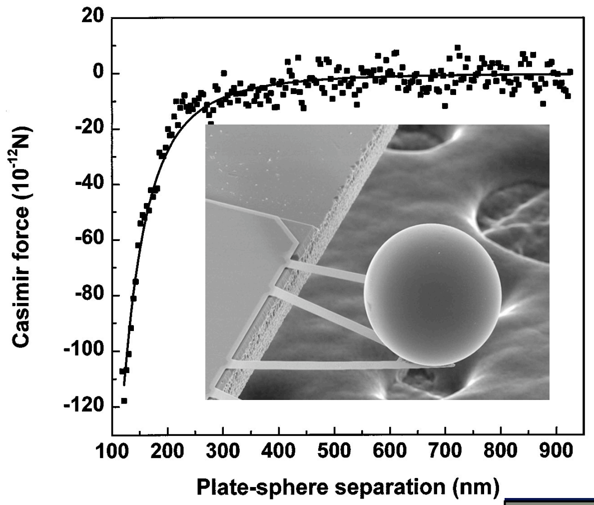
pressure ~ 1 atm at d=50nm

Geometry & materials important:

Electromagnetic field must satisfy boundary conditions at material interfaces.

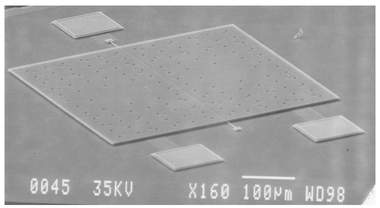
Experiments

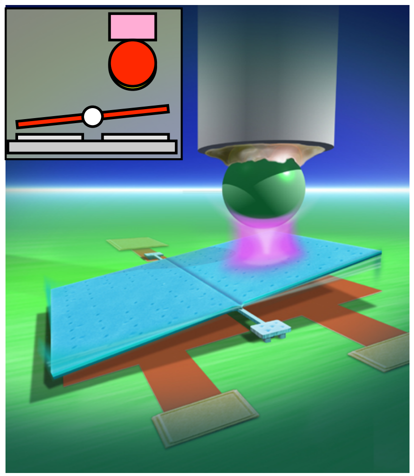
- Van Blockland, Overbeek 1978
  first clear qualitative observation
- Lamoreaux 1997 – first high-precision



[U. Mohideen *et. al.* PRL, 81 (1998)]

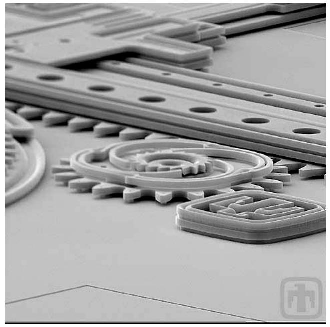
[Chan *et. al.*, *Science* **91**, (2001)]

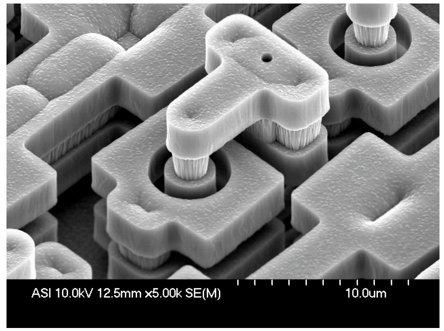


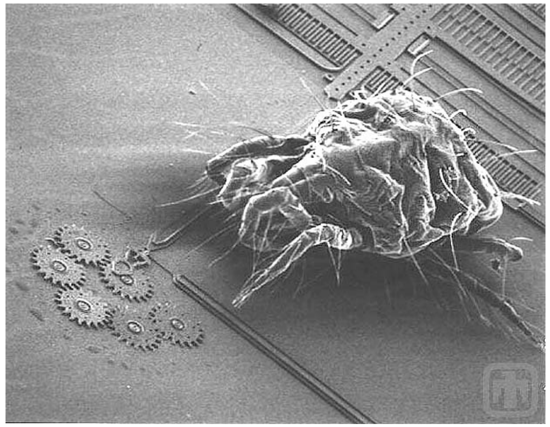


Applications

Microelectromechanical Systems





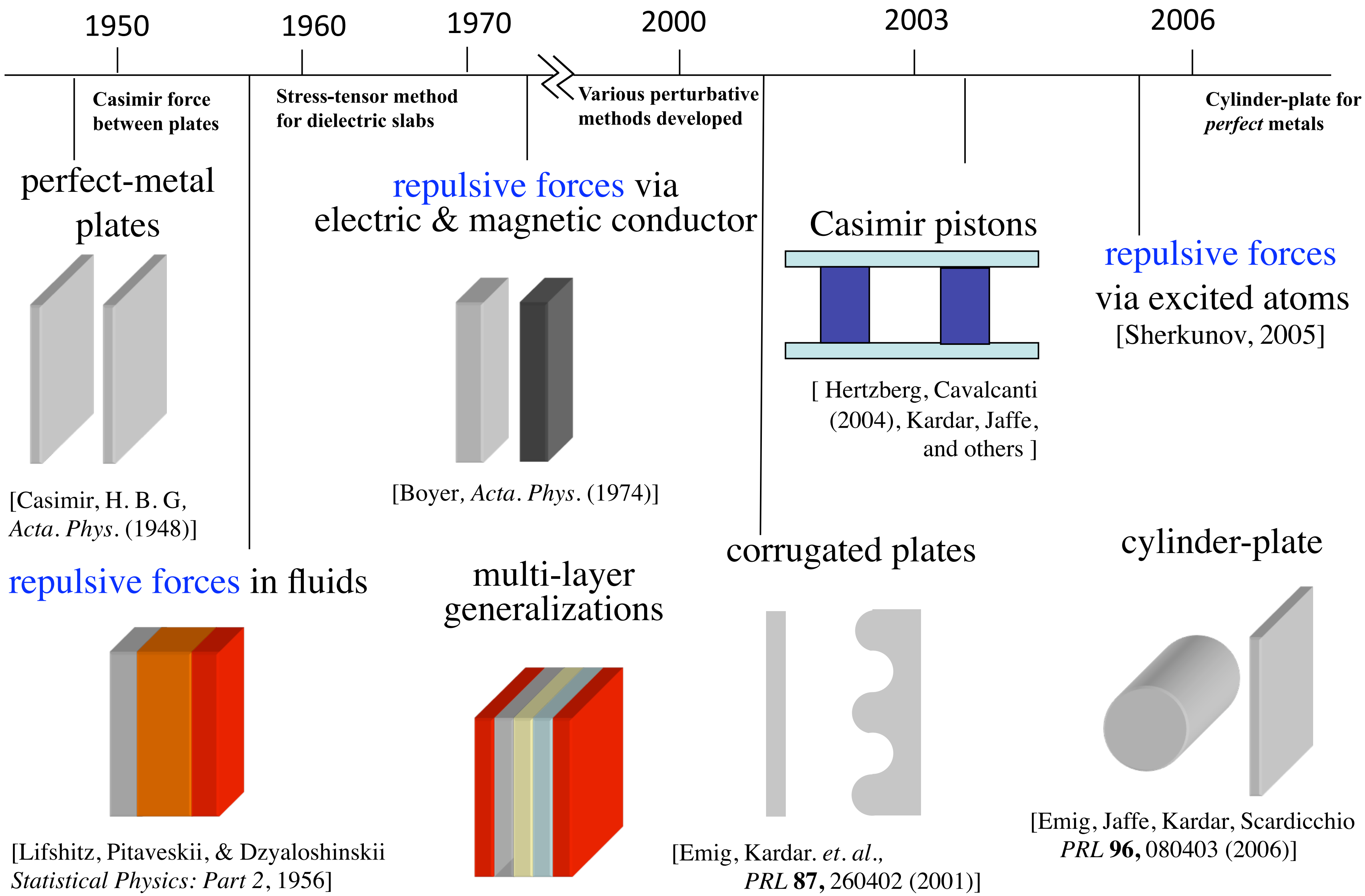


stiction problems!

study complicated geometries:
reduce stiction? new effects?

how?

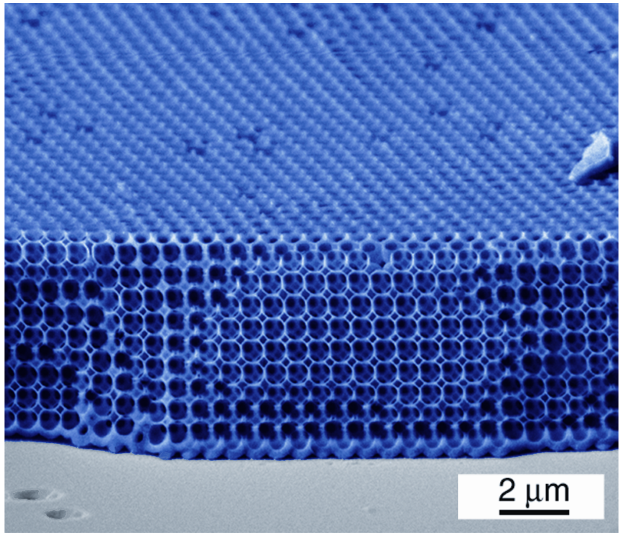
Selected pre-2007 theoretical work



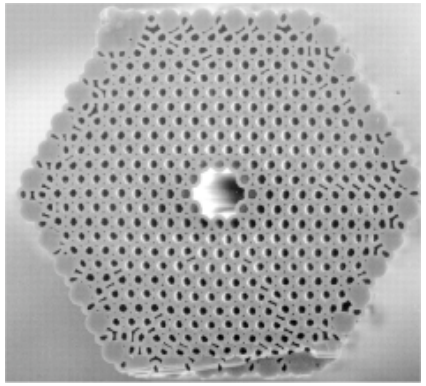
Nanophotonics

classical electromagnetic effects can be altered by λ-scale structures

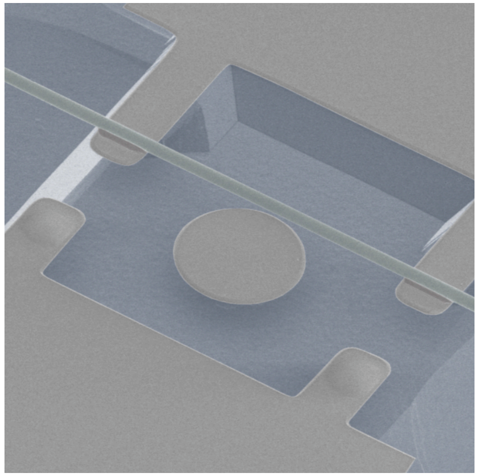
optical insulators



[D. Norris, UMN (2001)]

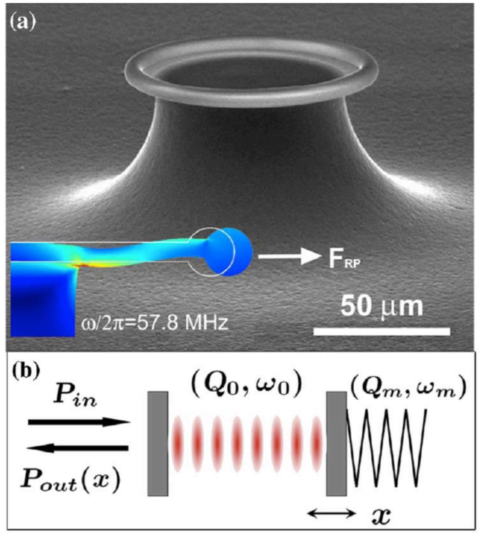


trapping/guiding light in vacuum



coupled to mechanical force/vibration

[Eichenfield et al. *Nature Photonics* **1**, 416 (2007)]



[Schliesser et al., *PRL* **97**, 243905 (2006)]

many recent advances in nanofabrication

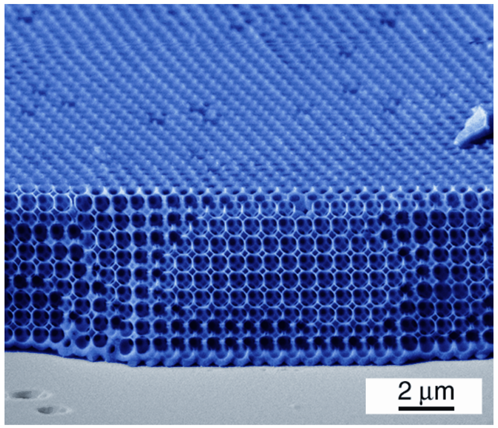
unusual effects, novel devices

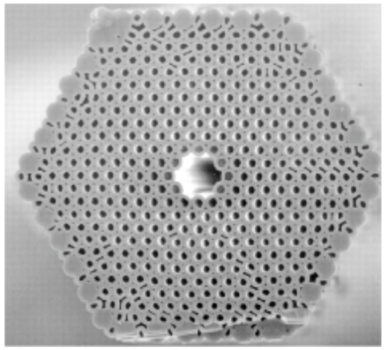
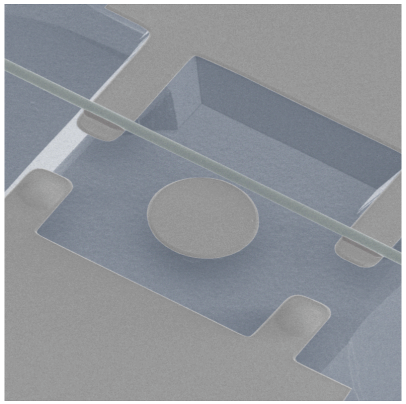
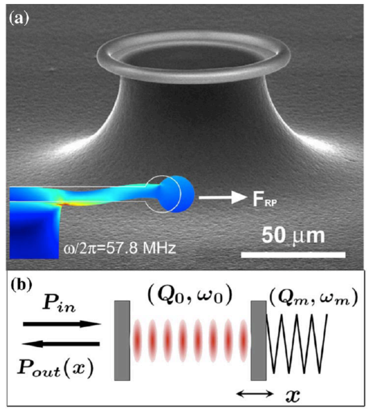
Ways forward
(2007–Present)

- Problem: how to practically evaluate forces in arbitrary cases.

- Many semi-analytic approaches in last 5–10 years
  [Emig/Jaffe/Kardar/Rahi, Lambrecht/Marachevsky, …]

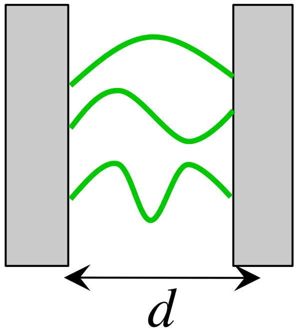
- Another approach: exploit mature, scalable methods from classical EM
  [Rodriguez/McCauley/Reid/White/Johnson]



How to relate quantum fluctuations to classical nanophotonics?

Fluctuation–Dissipation Theorem



Goal: compute electromagnetic fluctuation-induced forces

current fluctuations ⇔ EM field fluctuations

total energy

$$U = \int_0^\infty d\omega \int_V d^3\mathbf{x} \langle U(\mathbf{x},\omega) \rangle$$

energy density $\langle U(\mathbf{x}) \rangle_\omega \sim \sum_i \langle E_i(\mathbf{x})^2 \rangle_\omega$

force

$$F_i = \int_0^\infty d\omega \oiint_S \sum_j \langle T \rangle_{ij} \, dS_j$$

stress tensor $\langle T(\mathbf{x},\omega) \rangle_{ij} \sim \varepsilon(\mathbf{x},\omega) \left[\langle E_i E_j \rangle_\omega - \frac{1}{2} \delta_{ij} \langle E_i E_i \rangle_\omega \right]$

Fluctuation-Dissipation Theorem

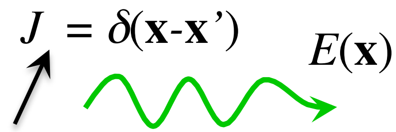
$$\langle E_i(\mathbf{x}) E_j(\mathbf{x}') \rangle_\omega = \hbar \omega^2 \, \mathrm{Im} G_{ij}(\omega, \mathbf{x} - \mathbf{x}')$$

$$\langle H_i(\mathbf{x}) H_j(\mathbf{x}') \rangle_\omega = -\hbar \omega^2 (\nabla\times)_{il} (\nabla\times)_{jm} \, \mathrm{Im} G_{lm}(\omega, \mathbf{x} - \mathbf{x}')$$

classical “photon” Green’s function

$$\left[\nabla \times \nabla \times - \omega^2 \varepsilon(\mathbf{x},\omega) \right] G_{ij}(\omega, \mathbf{x} - \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}') \hat{e}_j$$

electric response to current source



Computing Green's Functions

Solve Maxwell's equations in a localized basis:

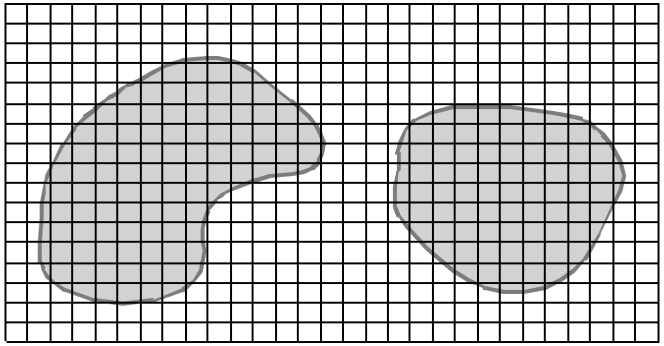
standard problem in classical electromagnetism!

solving some PDEs:

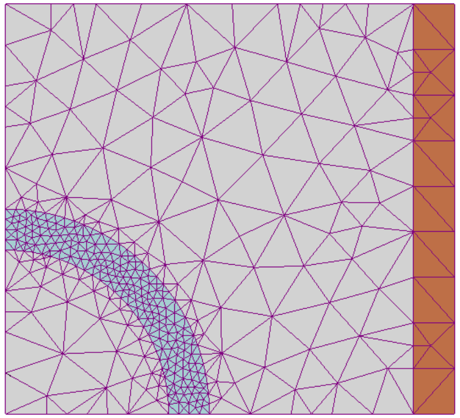
$$\frac{\partial \mu \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\frac{\partial \varepsilon \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}$$

finite difference

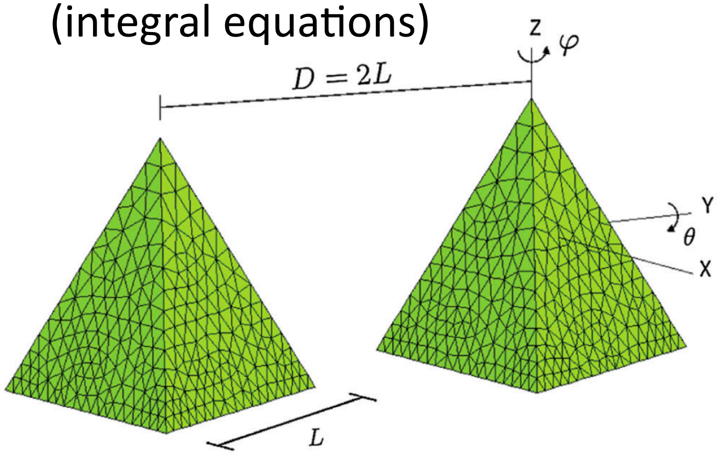


finite element

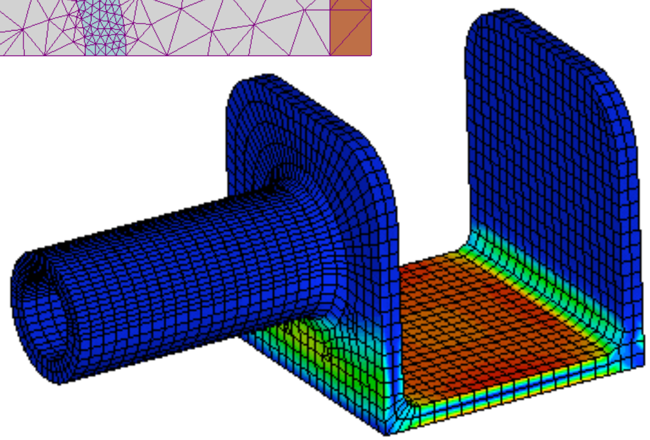


choice of basis functions
(depends on problem)
– ultimately, solving linear eq.

boundary element methods
(integral equations)



[H. Reid, Jacob White (MIT)]

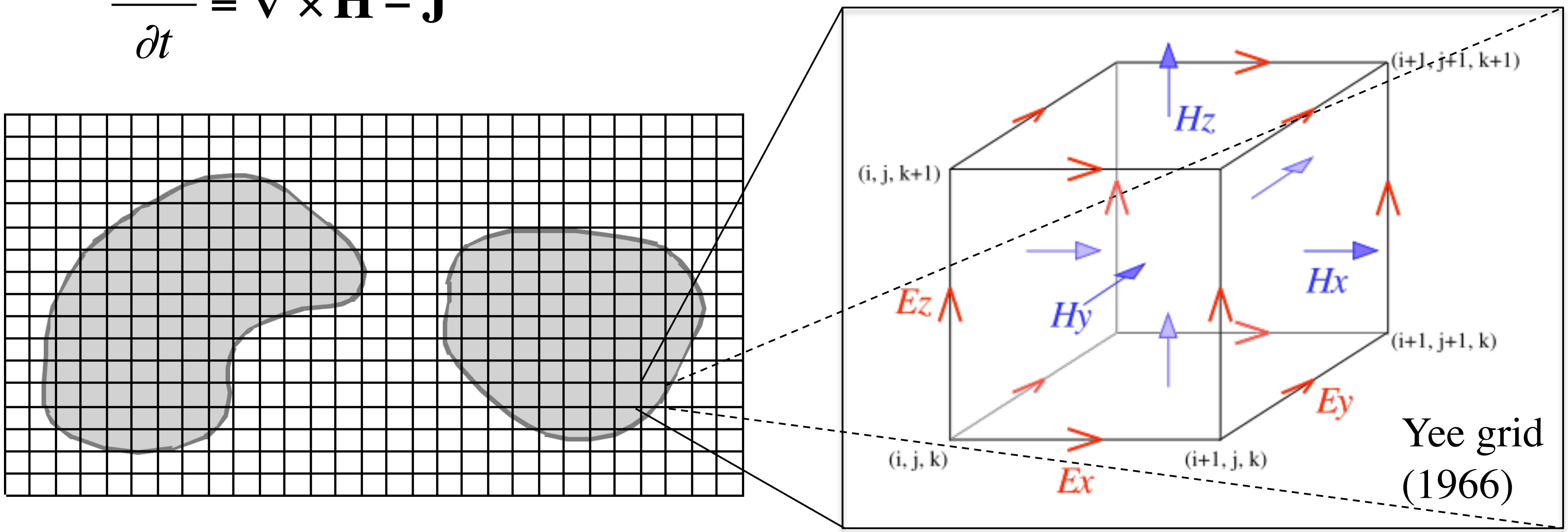


Green's Functions via finite differences

$$\frac{\partial \mu \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\frac{\partial \varepsilon \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}$$

$$derivatives \rightarrow \quad \frac{\partial f(x,t)}{\partial x} = \frac{f_{n+1}^{m} - f_{n-1}^{m}}{2\Delta x}$$



Decoupling Maxwell's equations [**J** = δ(**x**-**x**')]

$$\left[\nabla \times \nabla \times -\omega^2 \varepsilon\right] G_{ij}(\omega, \mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')\hat{e}_j$$

Linear matrix equation

$$A\mathbf{x} = b$$

Casimir Energy Density

U = trace of Green's function

= integral of mean energy density

by fluctuation-dissipation theorem

[e.g. Tomas, *PRA* (2002)]

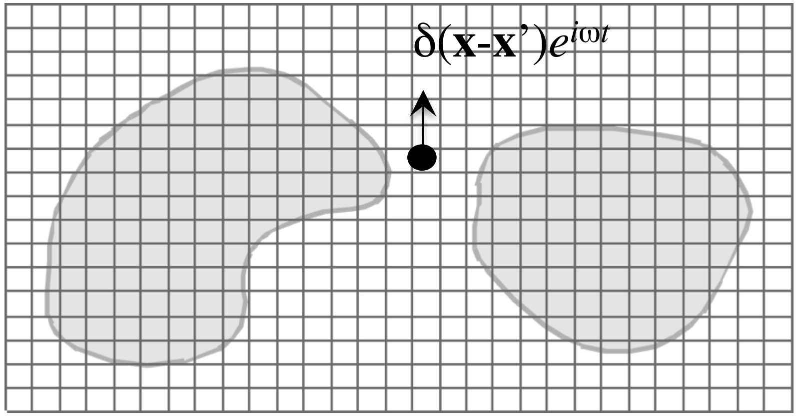
$$\sim \int_0^\infty dw \iiint_{\text{volume}} d^3\mathbf{x} \frac{d(w^2\varepsilon)}{dw} \left\langle \mathbf{E}(\mathbf{x})^2 \right\rangle$$

= Green's function

= **E** at **x** from current at **x**

= solving one linear system

$$A\mathbf{x} = b$$



—at every point in space (pixel) and at every frequency ω, solve for the Green's function

(employ direct or iterative solvers, depending on system size)

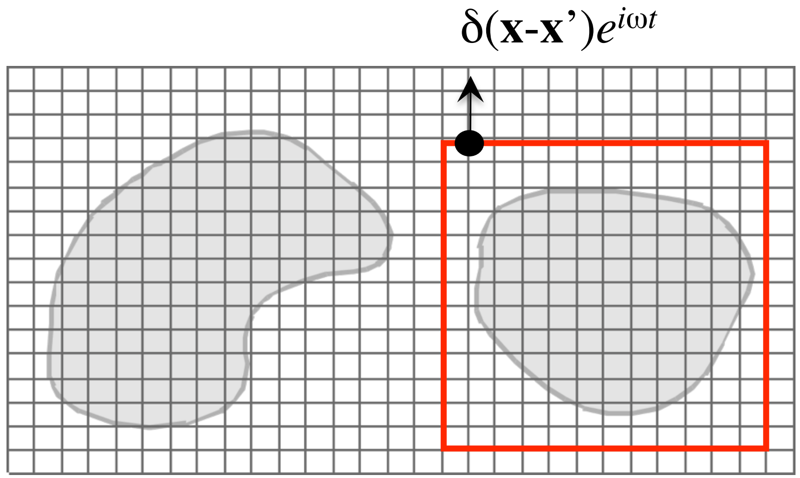
N degrees of freedom,
solving Green's = O(*N*) time
[e.g. via multigrid method]
need at *every* **x** (*N* points)
= $O(N^2)$ time

Casimir Stress Tensor

want **force**, not energy

stress tensor method

$$F = \int_0^\infty d\omega \oiint_S \langle \overleftrightarrow{T} \rangle \cdot d\vec{A}$$



surface surrounding body *S*

stress tensor $\sim \langle \mathbf{E}^2 \rangle + \langle \mathbf{H}^2 \rangle$ terms

= Green's function

evaluated only on the surface

<< *N* times

<< O(N^2) work

O($N^{2-1/d}$) … (actually, can do better with additional tricks)

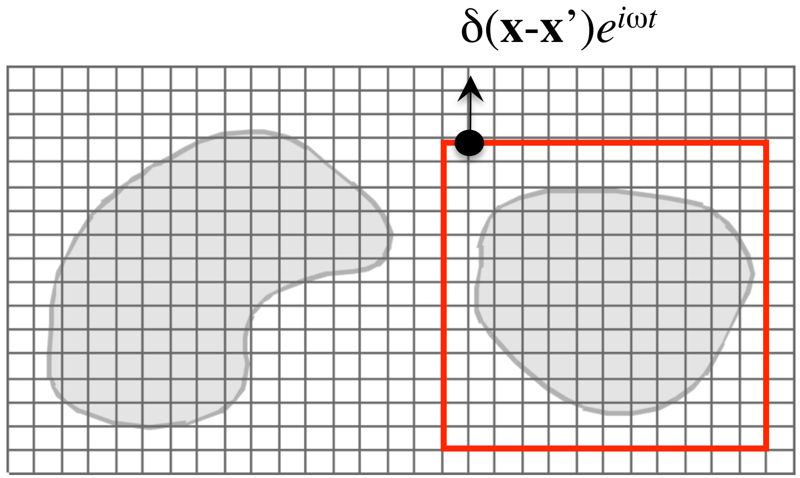
are we done yet?

Problems with real frequency

stress tensor method

$$F = \int_0^\infty d\omega \oiint_S \langle \overleftrightarrow{T} \rangle \cdot d\vec{A}$$

$$\langle T \rangle \propto \langle E^2 \rangle + \langle B^2 \rangle$$



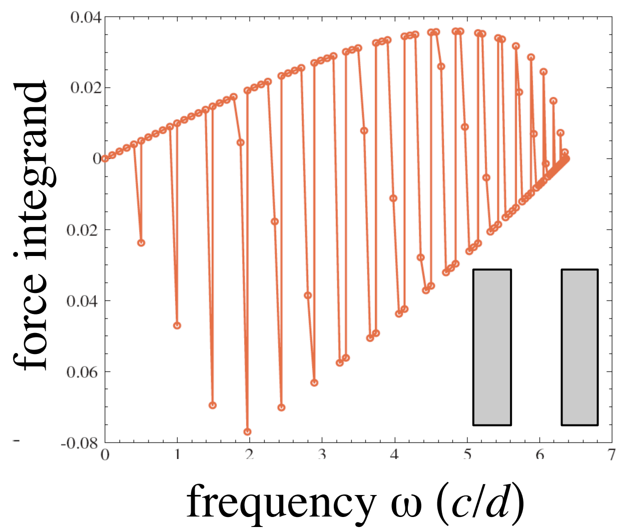
surface surrounding body S

Casimir integrand $f(\omega)$

(after surface, spatial integration)

$$F = \int_0^\infty d\omega\, f(\omega)$$

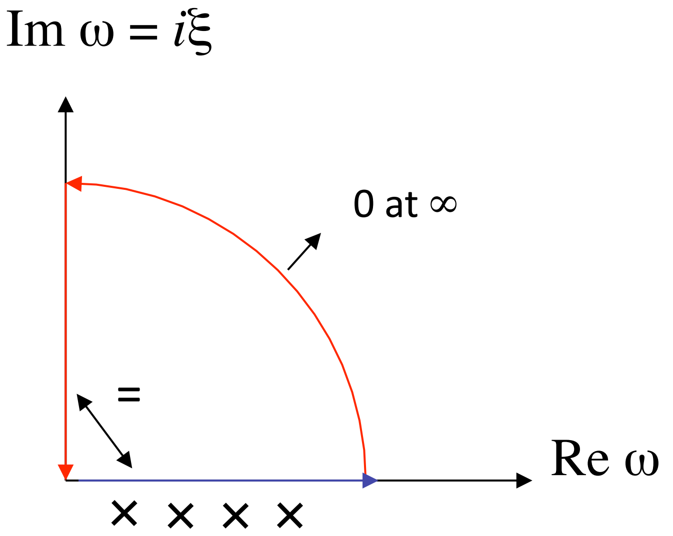
turns out $f(\omega)$ is ill-behaved…



- wildly oscillatory
- contributions up to Nyquist frequency

- comes from wave interference & resonances…

Complex frequency: Wick rotation



causality ⇒ poles only in lower-half plane

vacuum Green's function:

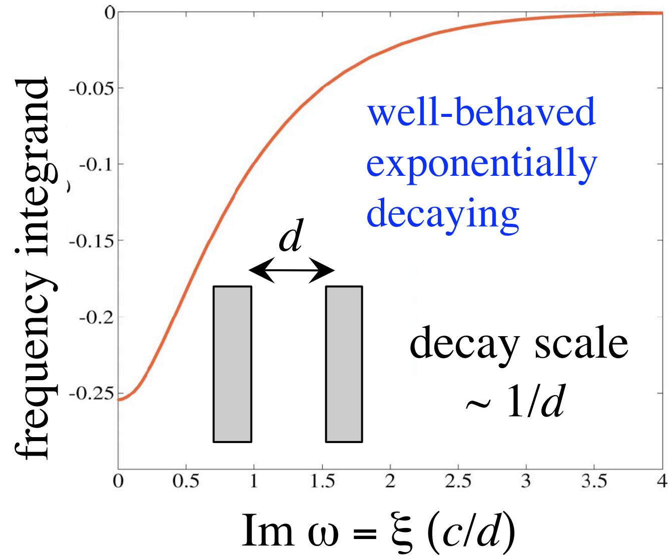
$$G_\omega \sim \frac{e^{i\omega r/c}}{r} \rightarrow G_{i\xi} \sim \frac{e^{-\xi r/c}}{r}$$

exponentially decaying
non-oscillatory
no resonance/interference

Wick rotation *(contour integration)*:

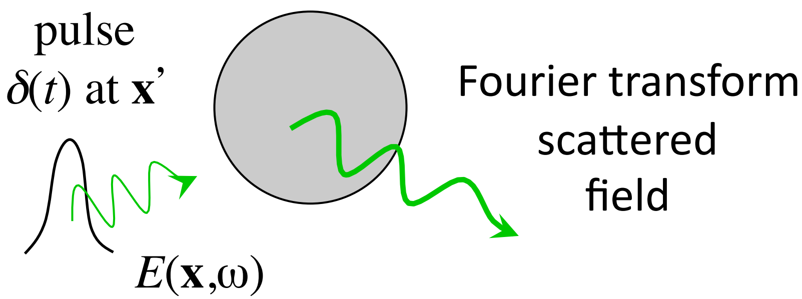
real ω to imaginary ω → *i*ξ

— move contour away from poles



Time domain

want response integrated over many frequencies:



time domain equivalent…

$$\frac{\partial \mu \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\frac{\partial \varepsilon \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}$$

time-evolve ME → **E** in response to $J = \delta(t)\delta(\mathbf{x}-\mathbf{x}')$

Why?

Entire frequency response in a single shot

FDTD solvers widespread (off the shelf), highly efficient, and extremely versatile
e.g. *anisotropic dielectrics, many boundary conditions, highly parallelizable*

[Rodriguez, McCauley *et al*. *PRA* **80** 012115 (2009)]
[McCauley, Rodriguez *et al*. *PRA* **81** 012119 (2010)]

MEEP: http://ab-initio.mit.edu/wiki/index.php/Meep

however…there's a wrinkle…

Wick Rotation?

Green's function inverts: $\nabla \times \nabla \times - \omega^2 \varepsilon(\omega, x)$

ω and ε only appear together!

complex contour deformation

⇒ change from ω to $\omega f(\omega)$ is
equivalent to changing material to $f(\omega)^2 \varepsilon(\omega f(\omega), x)$
(+ Jacobian factor in frequency integral)

Can get all the advantages of complex-frequency but for real frequency/time with transformed materials

Wick Rotations in the Time Domain

Wick rotations

$$\omega \to i\xi$$

⇔

Gain media

$$\varepsilon \to -\varepsilon$$

exponentially growing solutions
if negative at **all** *frequencies*

Try different contour?

$$\omega \to \xi\sqrt{1+\frac{i\sigma}{\xi}} \quad \Leftrightarrow \quad \left(1+\frac{i\sigma}{\xi}\right)\varepsilon$$

= conductive medium

time domain: real-frequency response in dispersive medium

$$\frac{\partial \mu \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\frac{\partial \varepsilon \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \sigma\varepsilon\mathbf{E} - \mathbf{J}$$

most off-the-shelf FDTD software
already supports conductive media

[Rodriguez, McCauley *et al*. *PNAS* **106** 6883 (2010)]

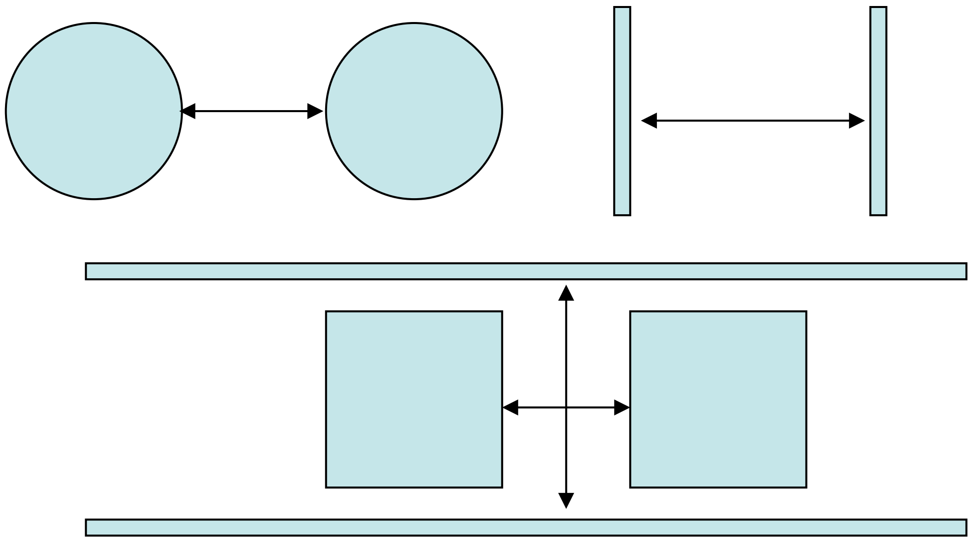
… many interesting things to compute …

… almost any geometry you can imagine is unstudied …

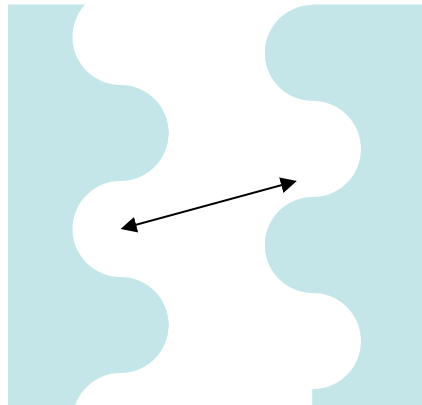
What about repulsive forces?

Theorem:
[Kenneth, 2006]

in a mirror-symmetric
metal/dielectric [$\varepsilon(iw) \geq 1$] structure,
the Casimir force is always attractive



… but what about
asymmetric structures?

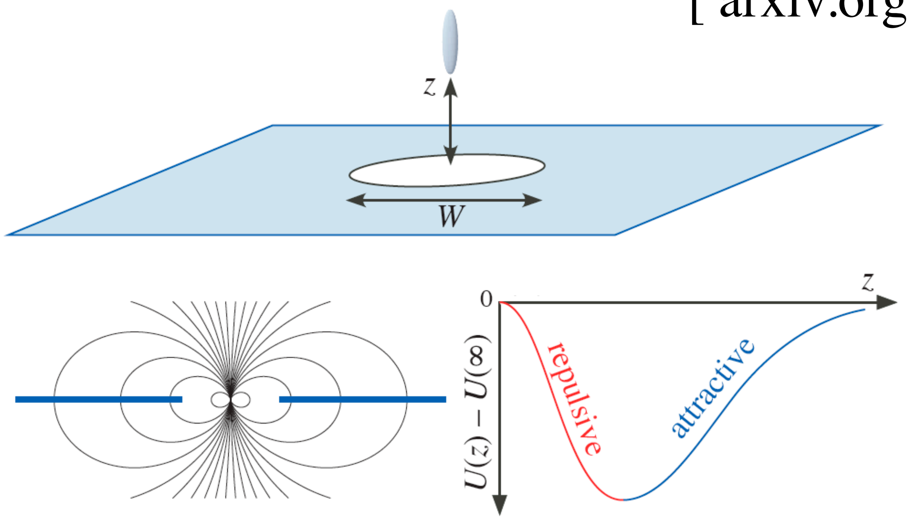


lots of interesting
structures, e.g. with
lateral forces,
even Casimir "ratchets"

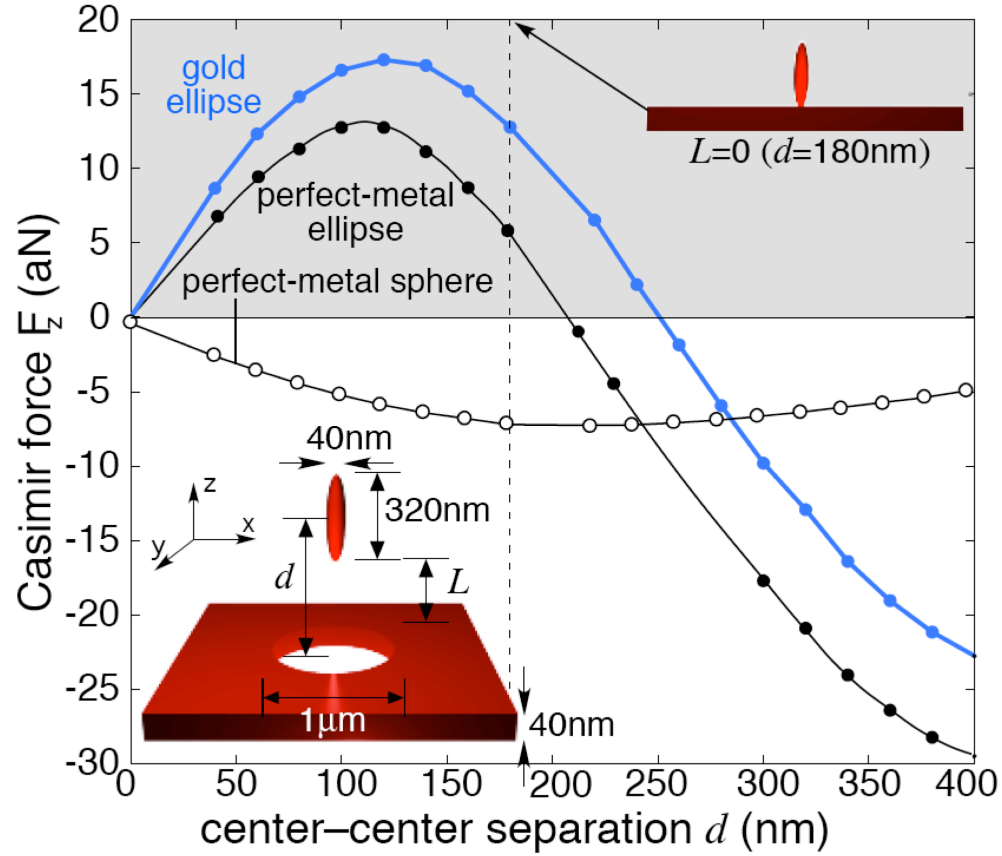
[Emig, arXiv
cond-mat/0701641 (2007)]

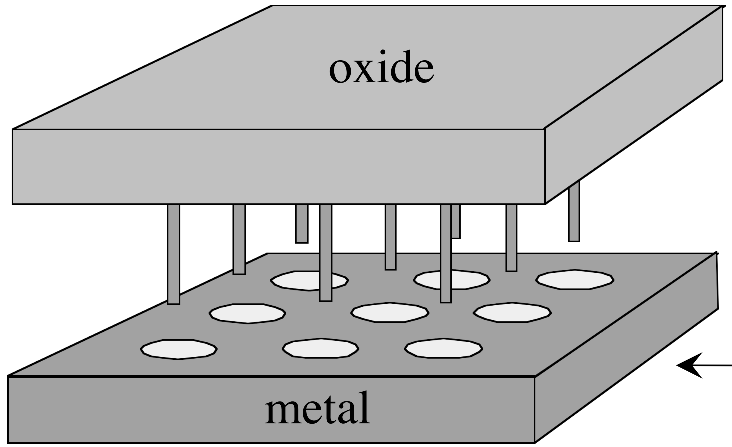
True Casimir Repulsion Between Metallic Objects in Vacuum

[arxiv.org:1003.3487]



field lines do not interact with plate





array of pillars on oxide:
still a repulsive force

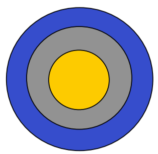
Casimir Forces in Fluids

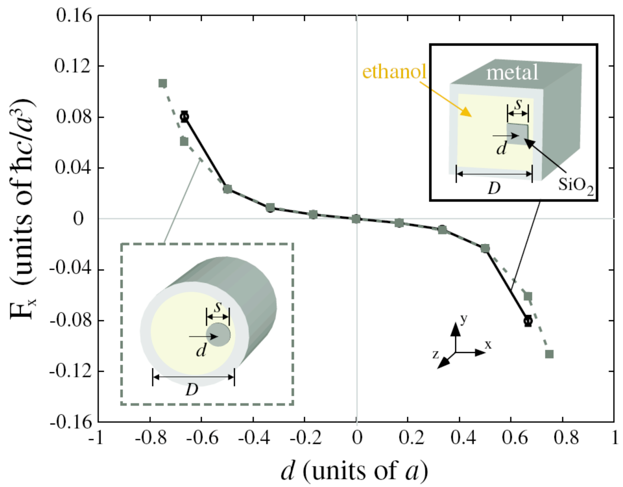
Repulsive forces
(between dielectrics in fluids)

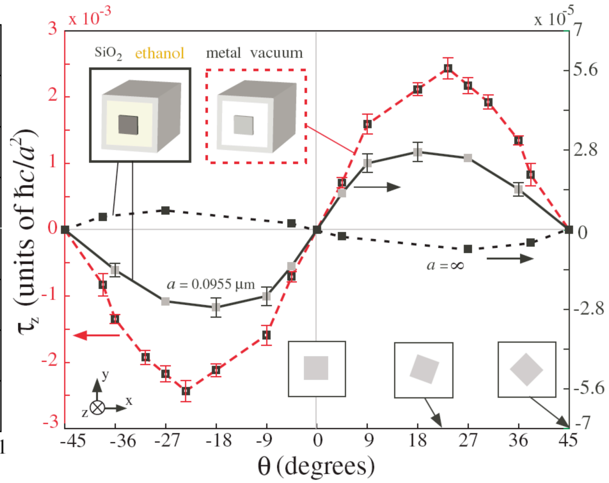
Known: dielectric configuration satisfying
$\varepsilon_\alpha(i\xi) \leq \varepsilon_{fluid}(i\xi) \leq \varepsilon_\beta(i\xi)$ then Casimir force repulsive
[Dzyaloschinski, Lifshitz, Pitaevskii, 1956]

eccentric geometries

geometry-enabled in-plane suspension
— preferred orientation (torque calculations)

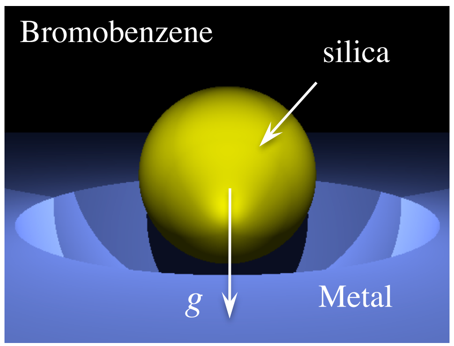


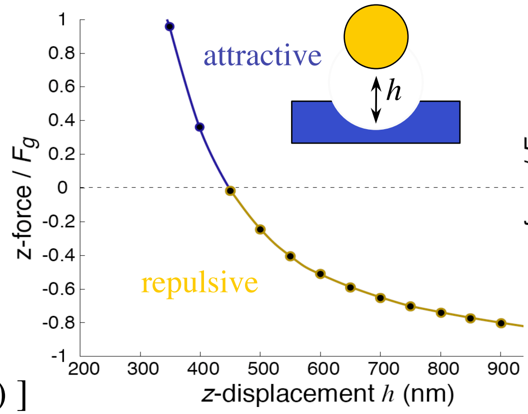


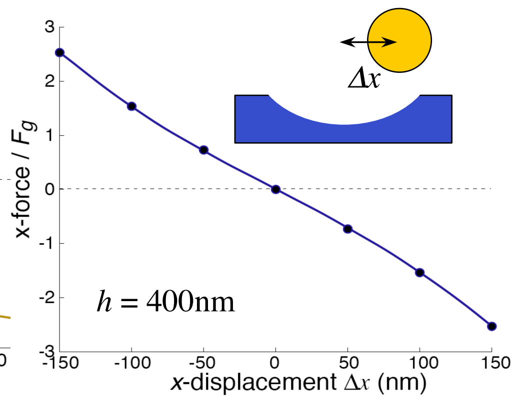


[A. W. Rodriguez, J. Munday, *et. al.* *PRL* **101** 190404 (2008)]

gravity and geometry



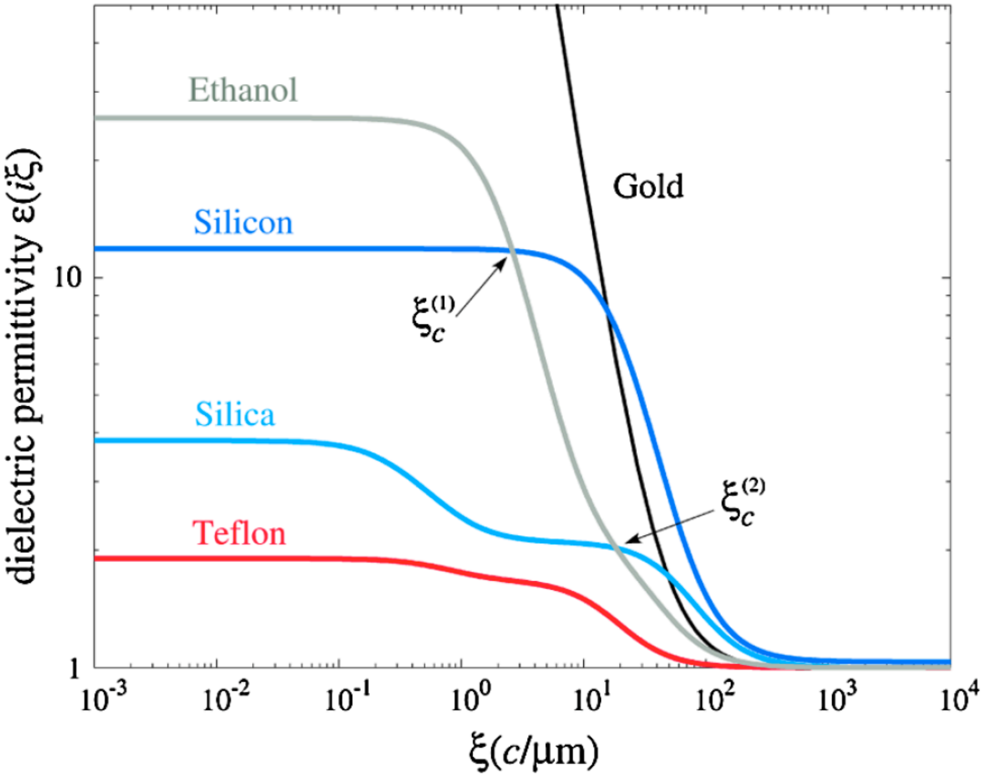


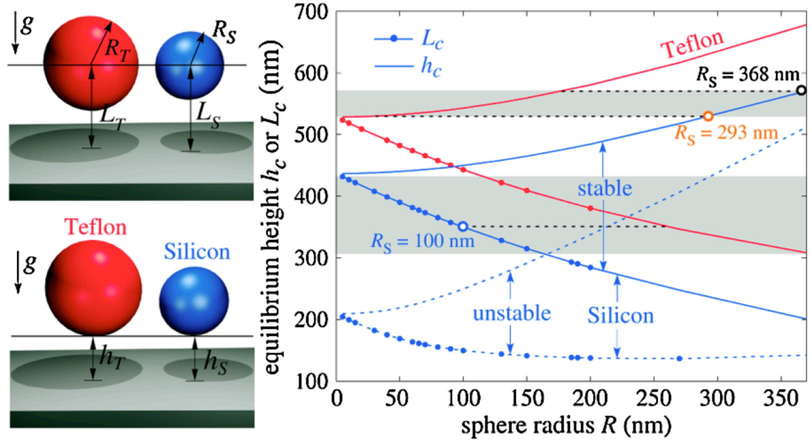


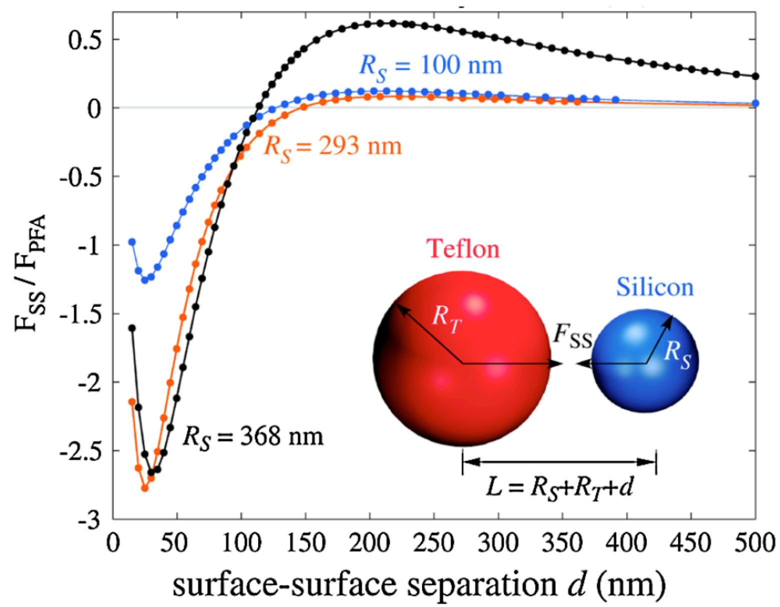
[A. McCauley, A. W. Rodriguez, *PRA* **97** 160401 (2008)]

Stable non-touching bonding

nanoparticle diclusters







[A. W. Rodriguez, A. McCauley, *et. al. PRL* **104** 160402 (2010)]

finis

[papers: http://math.mit.edu/~stevenj

students/postdocs: A. Rodriguez, A. McCauley, H. Reid

collaborators: F. Capasso & M. Loncar (Harvard),
J. White & R. Jaffe & M. Kardar (MIT),
T. Emig (Köln), D. Dalvit (LANL)]

- MEMS devices + nanophotonics opening new regimes of optical-force interactions/devices & many problems are relatively unexplored.

- In electromagnetism, where powerful off-the-shelf solvers are widely available, fine details of computations are often less important than how you formulate the problem