Some algorithmic improvements of the loop cloud method

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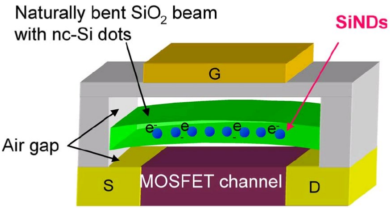
Outline

Nanotechnology at the University of Southampton, UK

- Southampton Nanofabrication Centre: `http://www.southampton-nanofab.com`
- ECS: Nano Group, ESD Group
- ORC: Nanophotonics, Metamaterials
- Engineering: nCATS, Tiny Technologies, Computational Engineering and Design

Example Devices

- Examples for NEMS designs where Casimir forces can be expected to become an important issue:
  - Ultrasensitive NEM mass sensors
    (functionalized vibrating transistor gate)
  - Non-volatile NEM memory elements
    (transistor gate beam bent upwards/downwards)
- Schematics:



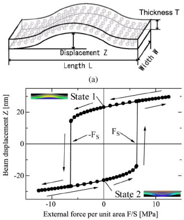


Diagram from: Mizuta, Tsuchiya, Oda et al., doi:10.1109/TED.2007.893811

Example Devices

- Miniaturization of CMOS may reach gate lengths $< 10\,\mathrm{nm}$ in this decade.
- Physical limitations to CMOS miniaturization.
- Operation speed of Nanoelectromechanical (NEMS) systems increases with minitaurization.
- Possible that buckling gate nonvolatile memory may supersede Flash RAM (but other technologies also in discussion).

Nanotechnology at the University of Southampton, UK

- Little previous activity/experience concerning research on Casimir Forces at UoS.
- We clearly see that understanding Casimir forces will become increasingly important for NEMS design.
- My involvement:
  - Member of the UoS Computational Engineering and Design Group
  - Background in Computational Field Theory;
    Other Research activities: Computational Micromagnetism; Quantum Gravity (supersymmetry-based).
  - EPSRC First Grant "Casimir Forces in Dynamic Geometries" since March 2011.
  - Establishing Links between Theoretical Physics and Engineering Sciences

Casimir Forces and Engineering Design

- For us: probably most promising present computational approach: employ F.D.-Theorem to re-write QFT expectation value in terms of imaginary frequency propagator (Rodriguez,Capasso,Johnson; MIT):

$$\langle T_{ij} \rangle_{\mathrm{QED}} \propto \partial\partial G_{\mathrm{Eucl.}}$$

- Computational techniques: FEM, linear equation solvers.
- Big advantage: Can realistically model optical material properties and arbitrary geometries!

Casimir Forces and Engineering Design

- Another computational approach: Worldline Numerics
  (Gies, Langfeld, Moyaerts)
- String theory inspired (Bern–Kosower Formalism).
- Setting:
  - Almost Free Quantum Field Theory: $\mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi + \frac{1}{2}V$
  - Only Interacion: external potential (models geometry): $V = V(x)$.
- So far: only "toy model" (Scalar photons; arbitrary geometry, but idealized behaviour only – no ω–dependent material properties.)
- Why is this interesting for Engineers? Three main reasons.

Casimir Forces and Engineering Design

- Reason 1: Potential to quickly give a crude estimate (Monte Carlo based)
- Reason 2: Worldline approach gives a very intuitive and accessible picture for quantum fluctuations.
  - Didactic uses in Education.
  - Helps to eliminate fundamental misunderstandings.
  - Easily accessible (conceptually and computationally).
- Reason 3:
  - Engineering is much about design optimization.
  - W.N. much more readily combined with computational engineering design optimization techniques than other computational approaches towards Casimir effect.
  - Will this ever play a major role? We don't know yet.

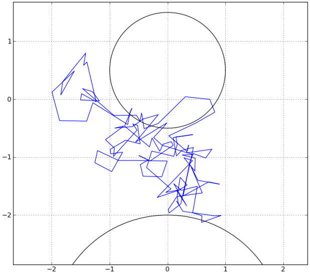
Worldline Numerics

- Idea: re–write Effective Action via Schwinger propertime formalism:

$$
\begin{aligned}
\Gamma[V] &= \frac{1}{2}\mathrm{Tr}\ln\frac{-\partial_\mu\partial^\mu + V}{-\partial_\mu\partial^\mu}\\
\ln(p/q) &\to \int_0^\infty \frac{dx}{x}\left(\exp(-px) - \exp(-qx)\right)\\
\Gamma_\Lambda[V] &= -\frac{1}{2}\frac{1}{(4\pi)^2}\int_{1/\Lambda^2}^\infty \frac{dT}{T^3}\int d^4x \left[\langle W_V[y;x,T]\rangle_y - 1\right]\\
\langle W_V[y;x,T]\rangle_y &= \frac{\int_{y\ \mathrm{c.l.}}\mathcal{D}y\, W_V[y;x,T]\, p[y]}{\int_{y\ \mathrm{c.l.}}\mathcal{D}y\, p[y]}\\
W_V[y;x,T] &= \exp\left(-T\int_{t=0}^{t=1} dt\ V(x+\sqrt{T}y(t))\right)\\
p[y] &= \exp\left(-\int_{t=0}^{t=1} dt\ \dot{y}(t)^2/4\right)
\end{aligned}
$$

Loop Clouds – Operational Procedure

- Discretize closed loops to polygonal paths with N vertices.
- Randomly generate loop ensemble with gaussian edge vector distribution.
- Re-scale each loop by factor s, with $\ln s$ equidistributed in $[\ln s_-; \ln s_+]$.



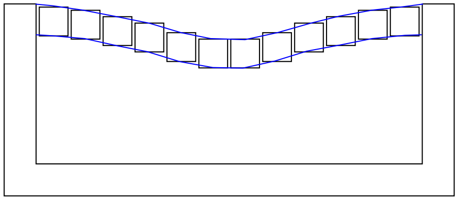
- Shift loops over geometry on raster.
- If loop intersects $N > 1$ different objects, increase total energy by $(1 - N)/s^4$.

Loop Clouds – Operational Procedure

- Important improvement: Work out ranges of re–scaling parameter s over which intersection behaviour does not change.
- $\Rightarrow$ *Analytic* dependence on geometry parameters (via scaling interval boundaries).
- Can work out forces on multiple (many!) objects in one go.
- Useful for shape optimization problems.
- Geometry deformations must be compatible with ∞ energy subtraction scheme:
  Either intruduce regulator Λ *or* restrict to shifts and rotations.

Loop Clouds – A Toy Problem

A toy optimization problem
Bending of a long beam under the influence of Casimir forces



Loop Clouds And Optimization

- Well known in Engineering Optimization
  (Not so well known among Physicists)
- If one has an *Algorithm A* computing an analytic function $f : \mathbb{R}^n \to \mathbb{R}$ that takes T seconds to execute, then there is a program transformation operation $A \mapsto A'$ that maps the program to a program computing $\mathrm{grad}\, f : \mathbb{R}^n \to \mathbb{R}^n$ that takes *no more than* $5T$ seconds.
- This works if:
  - There is enough memory to store all intermediate quantities used in the computation of $f(\vec{x})$,
  - plus enough memory to store one extra number each,
  - and if one can remember the full execution path.

Loop Clouds And Optimization

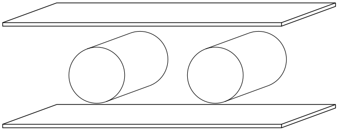
- Inherent advantage of Loop Cloud Method over $\Box^{-1}$ (solving sparse linear operator equations) methods:
  - Remembering all intermediate values may be quite impractical for iterative linear solvers (but is very easy for loop cloud method with pre–determined pseudo-random loop set: loops contribute individually).
  - When linear solver has converged, it may not actually have explored the problem sufficiently well to give a useful gradient.
- Relevant enough to justify investing time into developing Loop Cloud method towards general applicability? (Conceivable in the long run.)

Loop Clouds – Some Methodological Improvements

- Stratified sampling of loops rather than shifting C.O.M. over raster.
- Adaptive Sampling of loops: spend computational effort where it contributes most to improving statistics. No point in sampling many loops in places that do not contribute much.
- In almost symmetric toy geometries with cancellation of forces in opposing directions: sample over total collection of loops that is symmetric w.r.t. explicitly broken symmetry.
- "d loop" loop generation algorithm can be generalized...
  - to arbitrary number of loop points.
  - to not actually require to ever retain full loop in memory...
  - ...hence loop generation(1) on memory restricted cores (as in GPUs).
- (Paper soon on arXiv)

Some Calculations

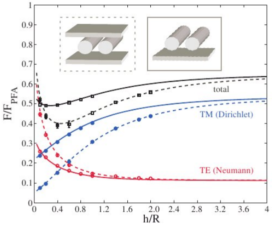
- Example: Cylinder/Cylinder/Plate/Plate geometry from `arXiv:0711.1987` (Rahi, Rodriguez, Emig, Jaffe, Johnson, Kardar).



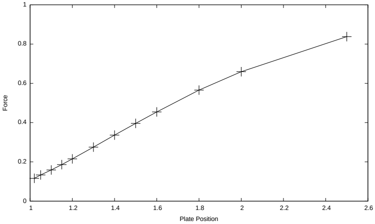
- Calculate force on cylinder using collection of loops that is symmetric w.r.t. two reflection planes through cylinder midpoint.

Some Calculations

- Scalar behaviour differs *qualitatively* from photon behaviour:



Photon case: `arXiv:0711.1987`



Scalar case

Some Calculations

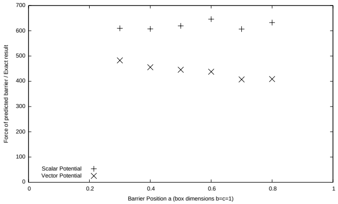
- Crucial problem of Worldline Numerics for Casimir forces: Scalar fields only!
- Unsolved problem: Photon/Conductor boundary conditions.
- Perhaps feasible: Photon/Superconductor: Photon gets effective mass due to coupling to scalar field that develops nonzero VEV ("Brout–Englert–Higgs Effect").
- For now (due to lack of better idea): Adventurous ansatz along the lines of "what may be simplest conceivable extension of W.N. that stands a chance of taking polarization into account?"
- Want: Free propagation in Vacuum, Conductor modeled as thin surface, Vector field with built–in "polarization", surfaces project out forbidden polarization.

Some Calculations

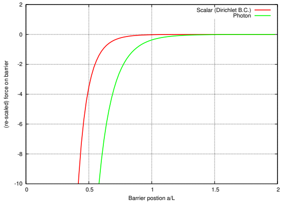
- Justification:
  - W.N. is toy model anyway.
  - Reasonable to ask: how do simplistic extensions/modifications behave? Can we maybe map these back to some QFT?

Some Calculations

- Some curious early data: Casimir piston geometry, W.N. vs. analytic result for scalars and "vector W.N." vs. analytic result for photons (arXiv:0705.0139 (Hertzberg, Jaffe, Kardar, Scardicchio):



Ratios W.N./analytic



Analytic result from arXiv:0705.0139

Conclusion

- Loop Cloud Method / Worldline Numerics certainly very interesting for didactic purposes.
- *Beyond that*: W.N. based approaches towards geometric optimization problems potentially more powerful than other Casimir Force methods.
- "Vector Worldline Numerics": Does this (or potentially a close relative) describe the behaviour of some QFT?