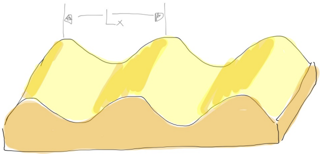
Casimir Energies for Surface Relief Gratings

C-Method in Casimir Calculations



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Outline

Given the wave equation

$$\big(-\nabla^2 + \zeta^2 + \mathcal{V}^1 + \mathcal{V}^2 \big) f = 0$$

With two disjoint potentials

$$\sup \mathcal{V}^i = \Omega_i \qquad \mathcal{T}^i = \mathcal{V}^i (1 + \mathcal{G}_0 \mathcal{V}^i)^{-1}$$

The Casimir interaction energy can be written

$$E = \frac{1}{4\pi} \int \mathrm{d}\zeta \ \operatorname{Tr} \ln \left(1 - \mathcal{T}^1 \mathcal{G}_0 \mathcal{T}^2 \mathcal{G}_0 \right)$$

The trace is over the spatial coordinates

$$E = \frac{1}{4\pi}\int \mathrm{d}\zeta \;\, \mathrm{Tr}\ln\left(1 - \mathcal{T}^1\mathcal{G}_0\mathcal{T}^2\mathcal{G}_0\right)$$

The spatial integrals can be done explicitly by expanding the Green's function

$$\mathcal{G}(x, x') = \sum_\alpha \phi_\alpha^{\mathrm{in}}(x)\phi_\alpha^{\mathrm{out}}(x') \qquad x \in \Omega_1, x' \in \Omega_2$$

and then defining translation and scattering matrices

$$\phi_\alpha^{\mathrm{out}}(x_1) = \sum_\beta \mathbb{U}_{\alpha\beta}\phi_\beta^{\mathrm{in}}(x_2) \qquad\qquad \mathbb{T}_{\alpha\beta} = \int \mathrm{d}x \phi_\beta^{\mathrm{in}}(x)\mathcal{T}\phi_\alpha^{\mathrm{in}}(x)$$

The trace in the new form is over separation constants

$$E = \frac{1}{4\pi}\int \mathrm{d}\zeta \;\, \mathrm{Tr}\ln\left(1 - \mathbb{T}^1\mathbb{U}\mathbb{T}^2\mathbb{U}\right)$$

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and then defining translation and scattering matrices

$$\phi_\alpha^{\text{out}}(x_1) = \sum_\beta \mathbb{U}_{\alpha\beta} \phi_\beta^{\text{in}}(x_2) \qquad \left(\phi_\alpha^{\text{in}}(x) + \sum_\beta \mathbb{T}_{\alpha\beta} \phi_\beta^{\text{out}}(x)\right)\Big|_{x \in \delta\Omega} = 0$$

The trace in the new form is over separation constants

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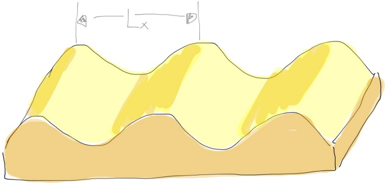


For a 1-D periodic system the free wave equation becomes

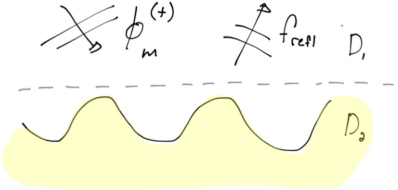
$$\left(-\partial_x^2 - \partial_z^2 + \kappa^2\right) f(x,z) = 0$$

The basis functions are plane waves

$$\phi_m^{(\pm)}(x,z) = \exp\left(\imath \mathbf{K}_m x \pm \sqrt{\kappa^2 + \mathbf{K}_m^2}\, z\right)$$

where the wave vector has been replaced with a Bloch wave vector

$$k_\perp \to \mathbf{K}_m, \quad \mathbf{K}_m = k_\perp + \mathbf{G}_m, \quad \mathbf{G}_m = \frac{2\pi m}{L_x}$$



The field can be written in a Rayleigh expansion

$$f = \phi_m^{(+)} + \sum_{m'} \mathbb{R}_{mm'} \phi_{m'}^{(-)}$$

The scattering matrix is exponentially suppressed for large m

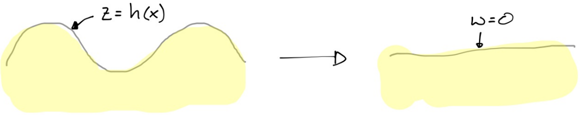
$$\mathbb{U} = \exp\left(-\sqrt{\kappa^2 + \mathbf{K}_m^2}\; d \right)$$

The Casimir interaction energy between two periodic structures is

$$\frac{E}{L_y} = \frac{1}{8\pi^2} \int_0^\infty \kappa \mathrm{d}\kappa \int_{-\pi/L_x}^{\pi/L_x} \mathrm{d}k_x \ln\det\left(1 - \mathbb{R}^1 \mathbb{U} \mathbb{R}^2 \mathbb{U}\right)$$

The C method

- Numerical method for calculating Rayleigh coefficients
- Established method from E&M grating theory
- Specialized for surface relief gratings



Begins with a change in variables

$$\{u, v, w\} = \{x, y, z - h(x)\}$$

The partial derivative is

$$\partial_x^2 \to \left(\partial_u - (\partial_u h)\partial_w\right)^2.$$

Expand the height profile and field in a Fourier and Block series

$$h(u) = \sum_m e^{\imath \mathbf{G}_m u} h_m$$

$$f(u, w) = \sum_m e^{\imath \mathbf{K}_m u} f_m(w)$$

Define the following vectors and matrices

$$\big(\mathbf{f}(w)\big)_m = f_m(w)$$

$$(\underline{\mathbf{K}})_{m,m'} = \delta_{m,m'} \mathbf{K}_m.$$

$$(\underline{\mathbf{Gh}})_{m,m'} = \mathbf{G}_{(m-m')} h_{(m-m')}.$$

Separate the Fourier modes - The wave equations becomes a system of ODEs

$$\left((\underline{\mathbf{K}} - \underline{\mathbf{Gh}} \partial_w)^2 - \underline{\mathbf{I}} \partial_w^2 + \underline{\mathbf{I}} \kappa^2 \right) \cdot \mathbf{f}(w) = 0$$

Proceeding in the standard method

$$\mathbf{f}(w) = \mathbf{V} e^{\lambda w}$$

yields an quadratic eigenvalue problem

$$\lambda_q^2 \underline{\mathbf{A}}_2 \cdot \mathbf{V}_q + \lambda_q \underline{\mathbf{A}}_1 \cdot \mathbf{V}_q + \underline{\mathbf{A}}_0 \mathbf{V}_q = 0.$$

A quick note about the quadratic eigenvalue problem

- For an $N \times N$ matrix there will be $2N$ eigenvalues
- A general solution to the wave equation can be written

$$f(u,w) = \sum_m e^{\imath \mathbf{K}_m u} \sum_q c_q \left(\mathbf{V}_q\right)_m e^{\lambda_q w}$$

- The eigenvalues will separate into two sets

$$\{\lambda_+ | \text{ All } \lambda_q \text{ such that } \Re(\lambda_q) > 0\}$$

$$\{\lambda_- | \text{ All } \lambda_q \text{ such that } \Re(\lambda_q) < 0\}$$

Assume Dirichlet boundary conditions on the field

$$f_{\rm tot}(u,0) = 0$$

The field is written in terms on an incident wave and a reflected field

$$f_{\rm tot}(u,w) = \phi_m^{(+)}(u,w) + f_{\rm refl}(u,w)$$

The incident wave and be rewritten in the $\{u, w\}$ coordinates

$$\begin{aligned}\phi_m^{(\pm)}(u,w) &= e^{\imath \mathbf{K}_m u \pm \widetilde{\lambda}_m (w + h(u))} \\ &= \sum_{m'} e^{\imath \mathbf{K}_{m'} u} \mathcal{L}_m^{m'(\pm)} e^{\pm \widetilde{\lambda}_m w}\end{aligned}$$

where

$$\mathcal{L}_m^{m'(\pm)} = \int \mathrm{d}u e^{-\imath \mathbf{G}_{m'-m} u \pm \tilde{\lambda}_m h(u)} \quad \text{and} \quad \tilde{\lambda}_m = \sqrt{\kappa^2 + \mathbf{K}_m^2}$$

Assume Dirichlet boundary conditions on the field

$$f_{\mathrm{tot}}(u,0)=0$$

The field is written in terms on an incident wave and a reflected field

$$f_{\mathrm{tot}}(u,w)=\phi_m^{(+)}(u,w)+f_{\mathrm{refl}}(u,w)$$

The reflected wave is written with eigenvalue from $\{\lambda_-\}$

$$f_{\mathrm{refl}}(u,w)=\sum_{m'} e^{\imath \mathbf{K}_{m'} u} \sum_{q\in\{\lambda_-\}} c_{mq}\left(\mathbf{V}_q\right)_{m'} e^{\lambda_q w},$$

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The reflected wave is written with eigenvalue from $\{\lambda_-\}$

$$f_{\text{refl}}(u,w) = \sum_{m'} e^{\imath \mathbf{K}_{m'} u} \sum_{q\in\{\lambda_-\}} c_{mq} \left(\mathbf{V}_q\right)_{m'} e^{\lambda_q w},$$

The boundary condition yields a linear system of equation for c_{mq}

$$\sum_{q\in\{\lambda_-\}} c_{mq} \left(\mathbf{V}_q\right)_{m'} = -\mathcal{L}_m^{m'(+)}$$

The Rayleigh coefficients can by comparing the Rayleigh expansion

$$f_{\mathrm{refl}}(u,w) = \sum_{m''} \mathbb{R}_{mm''} \phi^{(-)}_{m'}(u,w)$$

With the eigenvector expansion

$$f_{\mathrm{refl}}(u,w) = \sum_{m'} e^{\imath \mathbf{K}_{m'} u} \sum_{q \in \{\lambda_-\}} c_{mq} \left(\mathbf{V}_q\right)_{m'} e^{\lambda_q w},$$

For all q where we can make the identification

$$\lambda_q \approx -\sqrt{\kappa^2 + \mathbf{K}^2_{m''}} \quad \text{and} \quad \left(\mathbf{V}_q\right)_{m'} \propto \mathcal{L}^{m'(-)}_{m''}$$

The Rayleigh coefficients are

$$\mathbb{R}_{mm''} = c_{mq} \frac{\left(V_m\right)_m}{\mathcal{L}^{m(-)}_m}$$

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$$f_{\text{refl}}(u,w) = \sum_{m'} e^{\imath \mathbf{K}_{m'} u} \sum_{m''} \mathbb{R}_{mm''} \mathcal{L}_{m''}^{m'(-)} e^{-\widetilde{\lambda}_{m''} w}$$

With the eigenvector expansion

$$f_{\text{refl}}(u,w) = \sum_{m'} e^{\imath \mathbf{K}_{m'} u} \sum_{q \in \{\lambda_-\}} c_{mq} \left(\mathbf{V}_q\right)_{m'} e^{\lambda_q w},$$

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The Rayleigh coefficients are

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Function RayleighCoefficient(κ, k_x, $h(x)$, N)

- Form $N \times N$ matrices for eigenvalue problem
- Solve eigenvalue problem
- Use eigenvectors to solve boundary conditions for c_{mq}
- Find all indices q where eigenvalues match expected
- Return matched indices $\{q\}$, and Rayleigh Coefficients

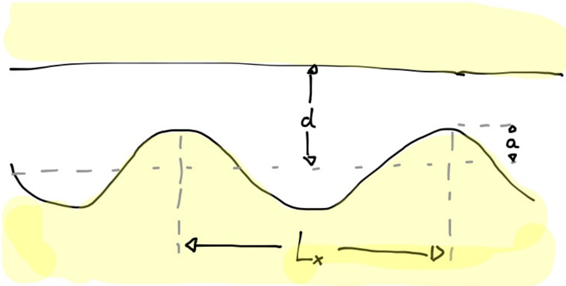
Function LogDet(κ, k_x, $h(x)$, d, N)

- $(\{q\}, \mathbb{R})$ = RaylieghCoefficient
- Use $\{q\}$ to calculates $\mathbb{U}$
- Form $\mathbb{N} = \left(\underline{\mathbf{I}} - \mathbb{R}\mathbb{U}\right)$
- Take $\ln \det \mathbb{N}$

Function Ecas($h(x)$, d, N)

- Numerically Integrate LogDet over κ and k_x

The test system is a sinusoidal grating and a flat plate



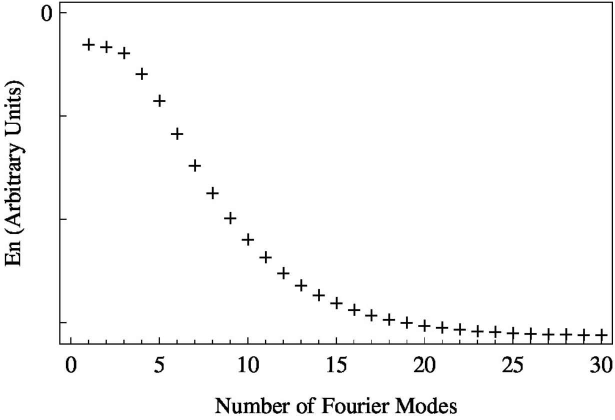
Three parameters:

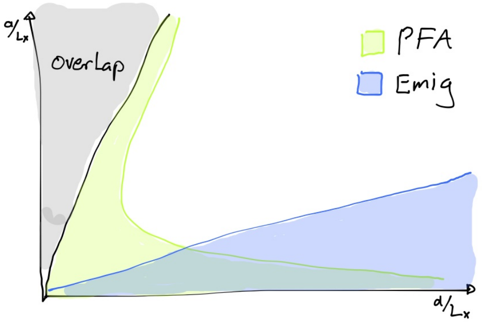
- Amplitude a
- Average separation d
- Wavelength L_x

Two dimensionless paramters:

- a/L_x
- d/L_x

The energy should converge exponentially as the number of Fourier modes kept is increased





There are two analytic approximations to compare to

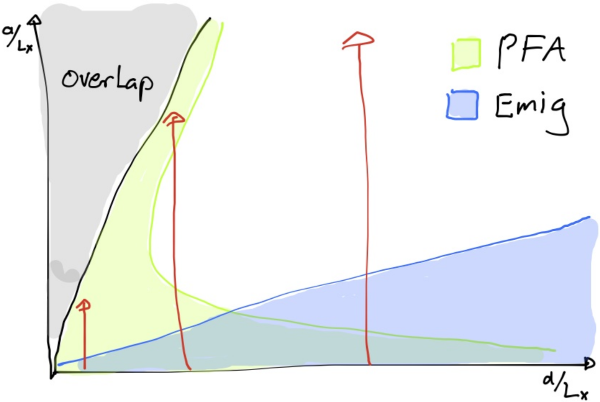
The Proximity Force Approximation

$$\frac{E_{\text{PFA}}}{L_y L_x} = -\frac{\pi^2}{1440} \frac{2d^2 + a^2}{2(d^2 - a^2)^{5/2}}.$$

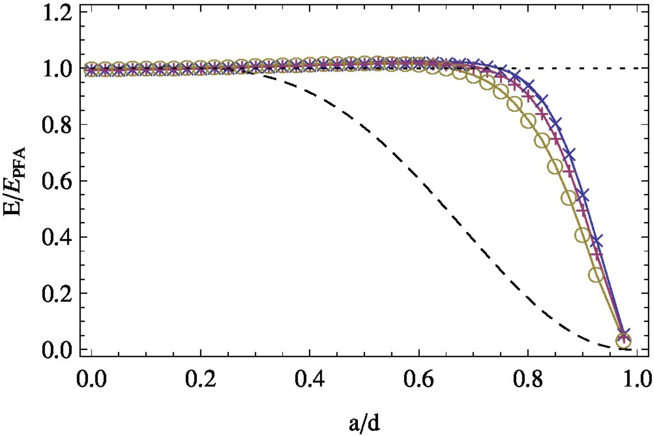
Emig's perturbative approximation

$$\frac{E_{\text{Emig}}}{L_y L_x} = -\frac{\pi^2}{1440} \frac{1}{d^3} - \frac{a^2}{d^5} G_{TM}\left(\frac{d}{L_x}\right).$$

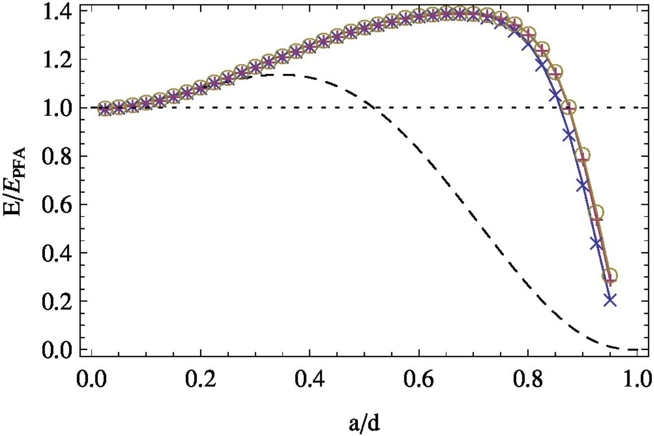
The following plots follow the red paths through parameters space



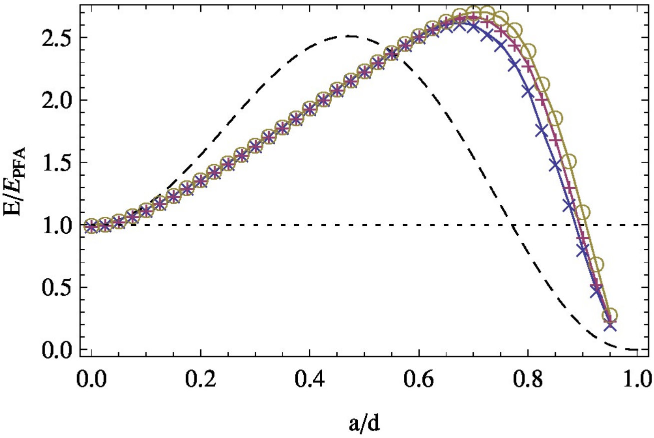
$d/L_x = 0.1$



$d/L_x = 0.5$



$d/L_x = 2.0$



For small amplitudes ($h(x)$ small) it is possible to solve the eigenvalue problem perturbatively.

$$\lambda_q^2(\underline{\mathbf{I}} - \underline{\mathbf{B}}_2)\mathbf{V}_q + \lambda_q \underline{\mathbf{B}}_1 \mathbf{V}_q - \underline{\mathbf{A}}_0 \mathbf{V}_q = 0$$

The matrices are

$$\begin{aligned} B_2 &= \underline{\mathbf{Gh}} \cdot \underline{\mathbf{Gh}} && \mathcal{O}(h^2) \\ B_1 &= (\underline{\mathbf{K}} \cdot \underline{\mathbf{Gh}} + \underline{\mathbf{Gh}} \cdot \underline{\mathbf{K}}) && \mathcal{O}(h) \\ A_0 &= (\underline{\mathbf{I}}\kappa^2 + \underline{\mathbf{K}} \cdot \underline{\mathbf{K}}) && \mathcal{O}(1) \end{aligned}$$

Following standard perturbation theory

$$\lambda = \sum_i \lambda^{(i)} \quad \text{and} \quad \mathbf{V} = \sum_i \mathbf{V}^{(i)}$$

where the superscript $^{(i)}$ denotes the order of the expression.

Perturbative Expansion

$$\lambda_q^{(0)} = -\sqrt{\kappa^2 + \mathbf{K}_q^2}$$

$$\lambda_q^{(1)} = \mathbf{K}_q \mathbf{G}_0 h_0$$

$$\lambda_q^{(2)} = \lambda_q^{(0)} \mathbf{K}_q \sum_m |h_{m-q}|^2 \mathbf{G}_{m-q}$$

$$\left(\mathbf{V}_q^{(0)}\right)_m = \delta_{qm}$$

$$\left(\mathbf{V}_q^{(1)}\right)_m = \lambda_q^{(0)} h_{m-q}$$

$$\left(\mathbf{V}_q^{(2)}\right)_m = \frac{(\lambda_q^{(0)})^2}{2} \sum_{m'} h_{m-m'} h_{m'-q} -$$

$$\frac{(\lambda_q^{(0)})^2}{2} \sum_{m'} h_{m-m'} h_{m'-q} \frac{\mathbf{G}_{m+q-2m'}}{\mathbf{G}_{m-q}}$$

Rayleigh Expansion

$$-\widetilde{\lambda}_m = -\sqrt{\kappa^2 + \mathbf{K}_m^2}$$

$$\mathcal{L}_m^{m'(\pm)} = \sum_i \mathcal{L}_m^{m'(\pm)(i)}$$

$$\mathcal{L}_m^{m'(\pm)(i)} = \frac{(\mp\lambda_m^{(0)})^i}{i!} \int \mathrm{d}u \; e^{-\imath \mathbf{G}_{m'-m} u} h^i(u)$$

$$\mathcal{L}_m^{m'(\pm)(0)} = \delta_{mm'}$$

$$\mathcal{L}_m^{m'(\pm)(1)} = \mp\lambda_m^{(0)} h_{m'-m}$$

$$\mathcal{L}_m^{m'(\pm)(2)} = \frac{(\lambda_m^{(0)})^2}{2} \sum_{m''} h_{m'-m''} h_{m''-m}$$

In the large N limit the perturbative solution (through second order) matches the Rayleigh expansion.
We can now proceed using only the Rayleigh expansion

$$\sum_{m''} \mathbb{R}_{mm''} \mathcal{L}_{m''}^{m'(-)} = -\mathcal{L}_{m}^{m'(+)}$$

This is equivalent to the Rayleigh hypothesis? The first few reflection coefficients are

$$\mathbb{R}_{mm'}^{(0)} = -\delta_{mm'}$$
$$\mathbb{R}_{mm'}^{(1)} = 2\lambda_m^{(0)} h_{m'-m}$$
$$\mathbb{R}_{mm'}^{(2)} = 2\lambda_m^{(0)} \sum_{m''} \lambda_{m''}^{(0)} h_{m'-m''} h_{m''-m}$$

The zeroth order term gives the Casimir energy for flat plates

$$\frac{E^{(0)}}{L_y L_x} = -\frac{\pi^2}{1440}\frac{1}{d^3}$$

The first correction only depends on the average h_0

$$\frac{E^{(1)}}{L_y L_x} = -\frac{\pi^2}{480}\frac{h_0}{d^4}$$

The second term depends explicitly on radio d/L_x

$$\frac{E^{(2)}}{L_y L_x} = -\frac{\pi^2}{240}\sum_m \frac{|h_m|^2}{d^5} J(4\pi m d/L_x)$$

This is NOT the same expression from Emig (and Prachi).

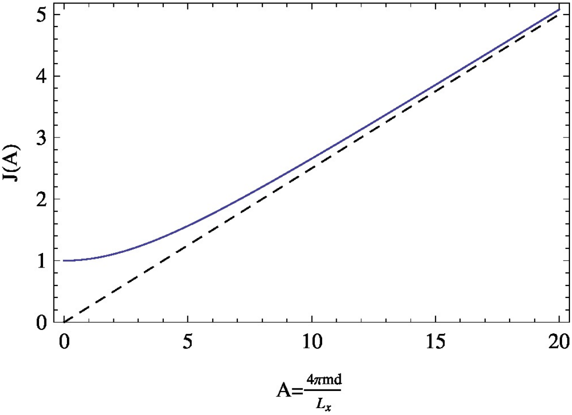
The J function is explicitly given by

$$J(A) = \frac{15}{4\pi^4} \int_0^\infty \mathrm{d}z \frac{z^2 e^{-z}}{1 - e^{-z}} \int_{-1}^{1} \mathrm{d}x \frac{\sqrt{z^2 + A^2 + 2zAx}}{1 - e^{-\sqrt{z^2+A^2+2zAx}}}$$

$$J(0) = 1$$

$$J(x) \sim x/4$$

For Large x



Conclusions

- Scattering method allows us to leverage existing techniques (such as the C method) for Casimir calculations
- I get converged results for a wide range of parameters
- Perturbatively the C method is equivalent the Rayleigh hypothesis
- I do not agree with Emig's approximation either numerically or perturbatively

I would like to thank Kim, Prachi, Elom, and Nima for letting me discuss this work when it was first starting. I would also like to thank Steve for inviting me and hosting this conference.