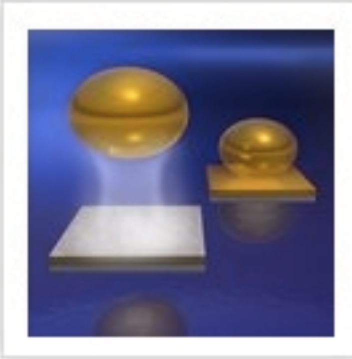

Casimir Effects in Graphene Systems

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Bo E. Sernelius, EPL, **95** (2011) 57003.

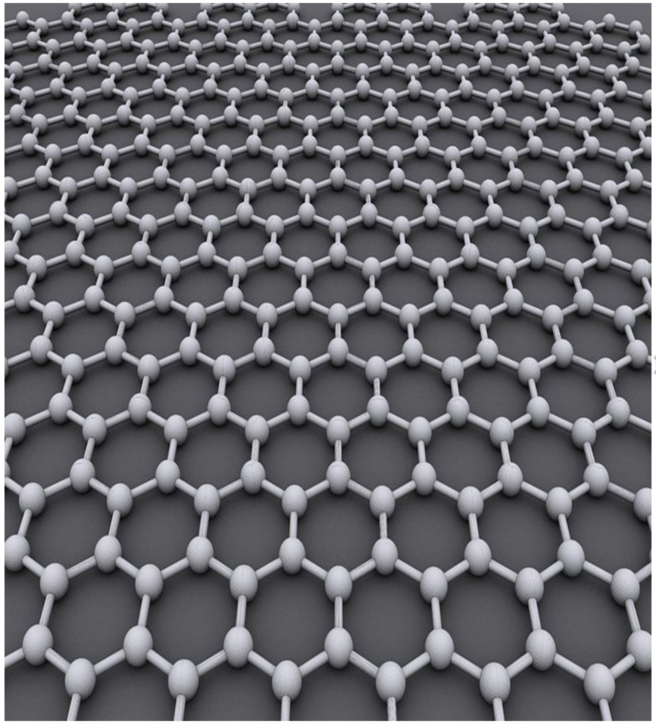
Short abstract:

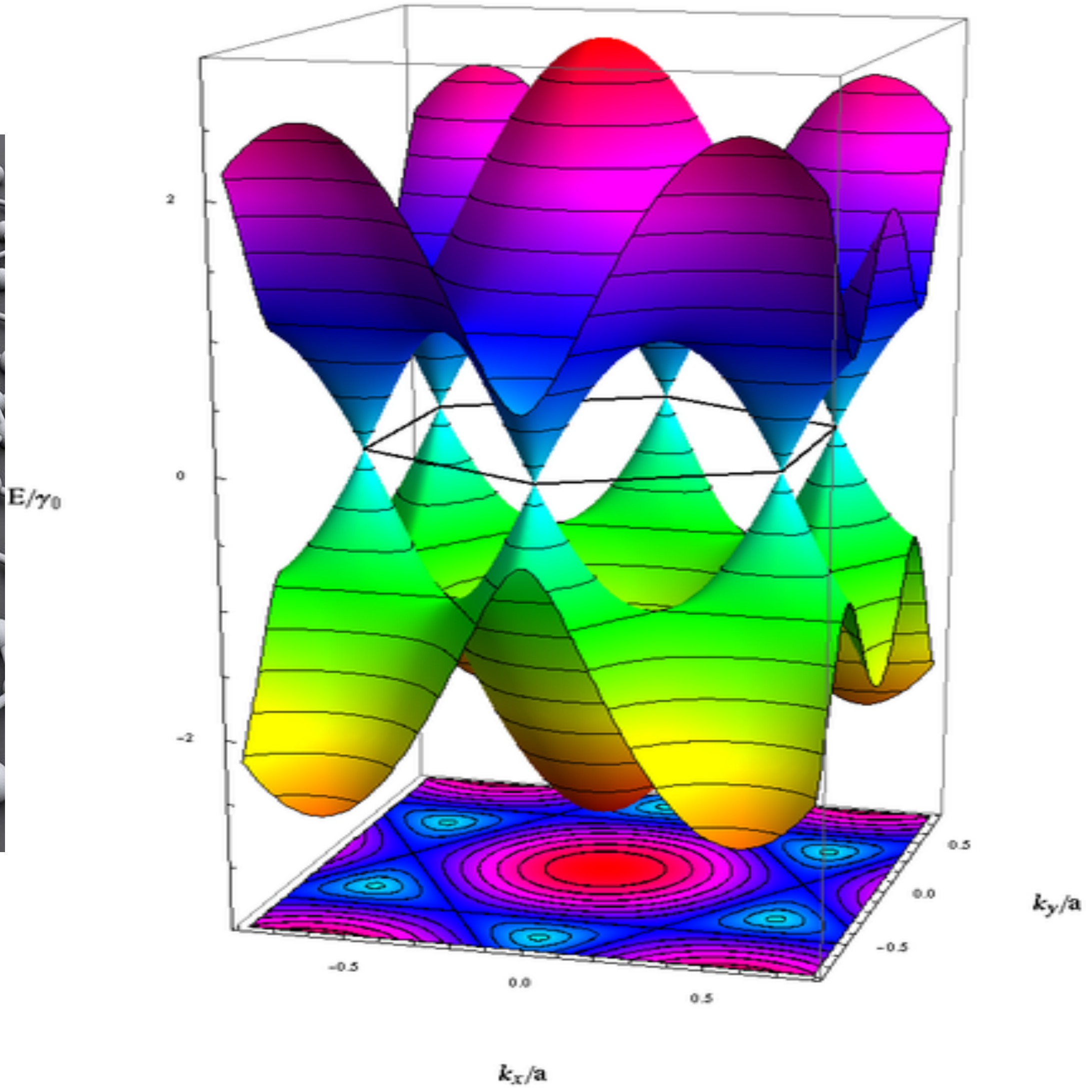
- We derive and calculate the Casimir interaction between two doped or undoped Graphene sheets at zero temperature.
- We derive the Casimir interaction between a doped or undoped Graphene sheet and a substrate. We calculate the interaction for a gold substrate.
- We find a separation dependence that differs from that predicted by Langbein.

Outline of the talk

- Brief description of Graphene, its band structure and dielectric function.
- Brief description of the van der Waals and Casimir interaction.
- Expected distance dependence of the interaction.
- How to derive the interaction.
- Results
- Summary and conclusions

Brief description of Graphene, its band structure and dielectric function





Figures from Wikipedia

Dielectric function of virgin Graphene

$$\varepsilon(\mathbf{q},\omega) = 1 - v^{2D}(q)\chi(\mathbf{q},\omega) = 1 + \alpha(\mathbf{q},\omega) = 1 + \frac{\pi e^2}{2\hbar}\frac{q}{\sqrt{v^2 q^2 - \omega^2}};$$

$$\varepsilon'(\mathbf{q},\omega) = 1 - v^{2D}(q)\chi'(\mathbf{q},\omega) = 1 + \alpha'(\mathbf{q},\omega) = 1 + \frac{\pi e^2}{2\hbar}\frac{q}{\sqrt{v^2 q^2 + \omega^2}};$$

$$v^{2D}(q) = 2\pi e^2 / q$$

Dielectric function for doped Graphene

$$\chi'(\mathbf{q},\omega)=\chi(\mathbf{q},i\omega)=$$

$$=-D_0\left\{1+\frac{x^2}{4\sqrt{y^2+x^2}}\left[\pi-\operatorname{atan}\left(\frac{2\left\{\left[x^2\left(y^2-1\right)+\left(y^2+1\right)^2\right]^2+\left(2yx^2\right)^2\right\}^{1/4}\sin\left\{\frac{1}{2}\operatorname{atan}\left[\frac{2yx^2}{x^2\left(y^2-1\right)+\left(y^2+1\right)^2}\right]\right\}}{\sqrt{\left(x^2+y^2-1\right)^2+(2y)^2}-\left(y^2+1\right)}\right)\right.\right.$$

$$\left.\left.-\frac{\sqrt{-2x^2\left(y^2-1\right)-2\left(y^4-6y^2+1\right)+2\left(y^2+1\right)\sqrt{x^4+2x^2\left(y^2-1\right)+\left(y^2+1\right)^2}}}{x^2}\right]\right\};\quad 0\le\operatorname{atan}<\pi$$

$$D_0=\frac{gE_F}{2\pi(\hbar v)^2}=\frac{gk_F^2}{2\pi E_F}=\frac{gn}{2E_F}=\sqrt{\frac{gn}{\pi\hbar^2v^2}}$$ (Density of states at the Fermi level).

$$E^{\pm}=\pm v\hbar k;\quad E_F=\hbar v k_F$$

$$x=q/2k_F;\quad y=\hbar\omega/2E_F$$

$$\alpha(\mathbf{q},i\omega)=-\frac{2\pi e^2}{q}\chi(\mathbf{q},i\omega)$$

Brief description of the van der Waals and Casimir interaction

- The vdW and Casimir interaction energy is the shift of the total zero-point energy of the system when interaction is turned on.

- For planar structures it can be written as

$$E = \hbar \int \frac{d^2 q}{(2\pi)^2} \int_0^\infty \frac{d\omega}{2\pi} \ln\left[f_{\mathbf{q}}(i\omega) \right],$$

where

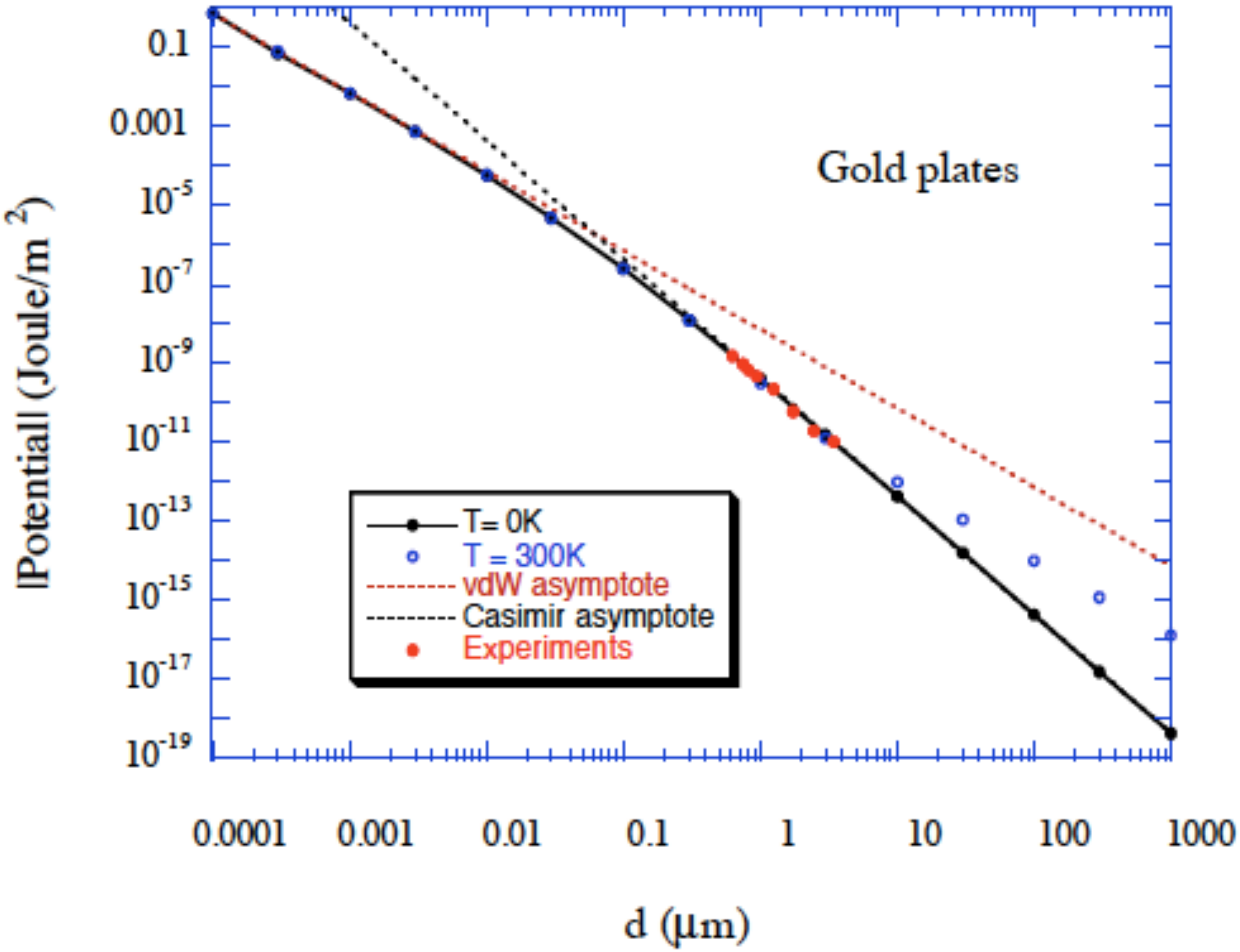
$$f_{\mathbf{q}}\left(\omega_{\mathbf{q}}\right) = 0$$

is the condition for electromagnetic normal modes

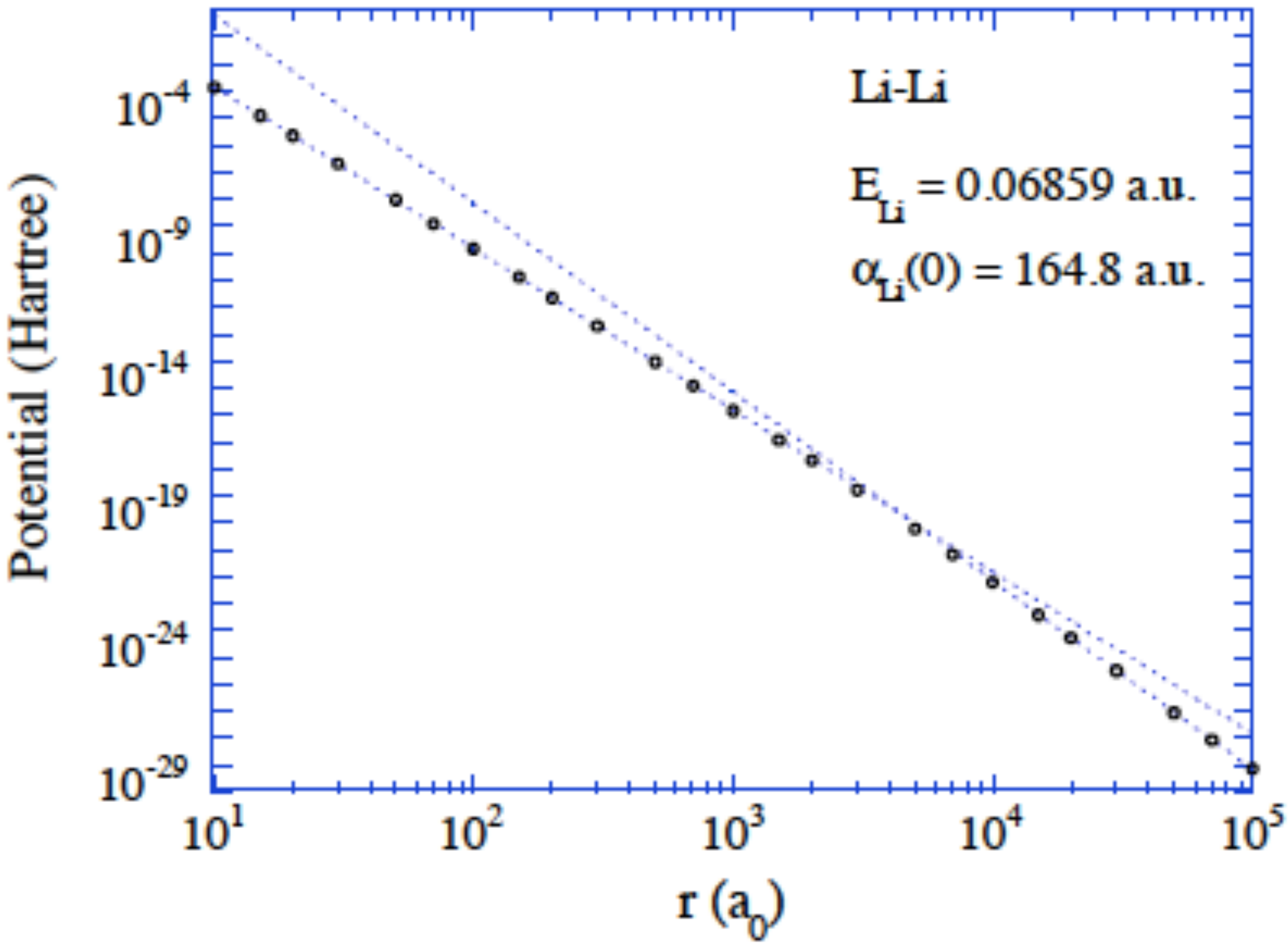
Van der Waals versus Casimir

- The van der Waals result is obtained if one neglects retardation effects, i.e. lets the speed of light be infinite.
- Keeping the finite speed of light results in van der Waals interaction for small separations and Casimir interaction at large.
- On a log-log plot of energy versus separation the ordinary behavior is that there are two asymptotes, the vdW and Casimir asymptotes.
- They are both straight lines that cross at a certain separation. The full result follows the vdW asymptote for small separations, then makes a smooth transition to the Casimir asymptote and follows that for large separations. The Casimir asymptote has a steeper negative slope.
- Graphene has a very odd behavior: The two asymptotes have the same slope and the vdW asymptote never crosses the Casimir asymptote. The retardation effects are negligible.

Two gold half spaces



Two lithium atoms



Expected distance dependence of the interaction.

- One way to find fast results for the van der Waals and Casimir interactions between objects of various shapes is to sum over pair interactions.

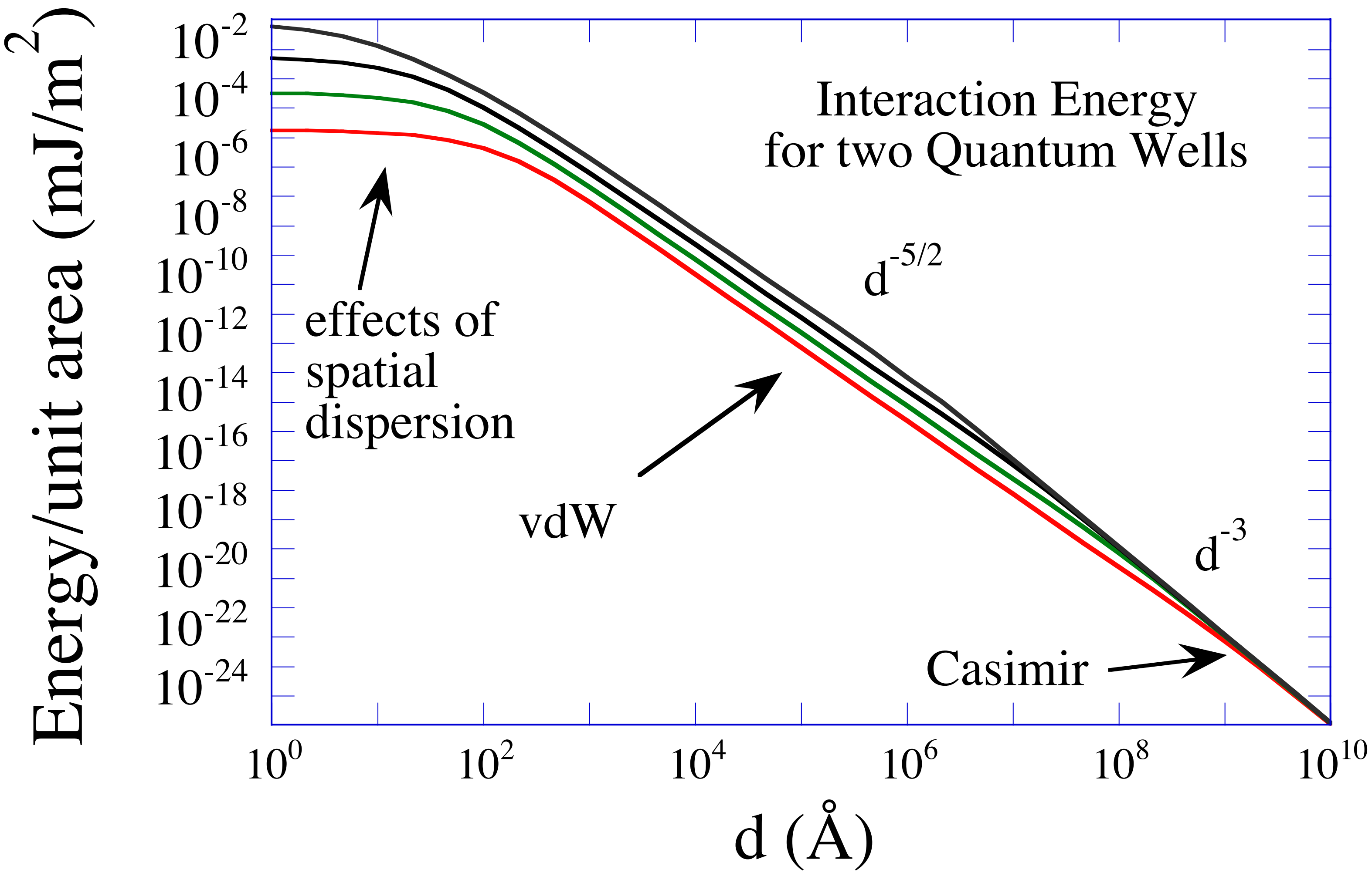
- According to Langbein* one finds the correct separation dependence but the overall strength is not always right.

*[Langbein D., *Theory of Van der Waals Attraction*, in Springer Tracts Mod. Phys., Vol. 72 (Springer, New York) 1974]

Langbein predictions

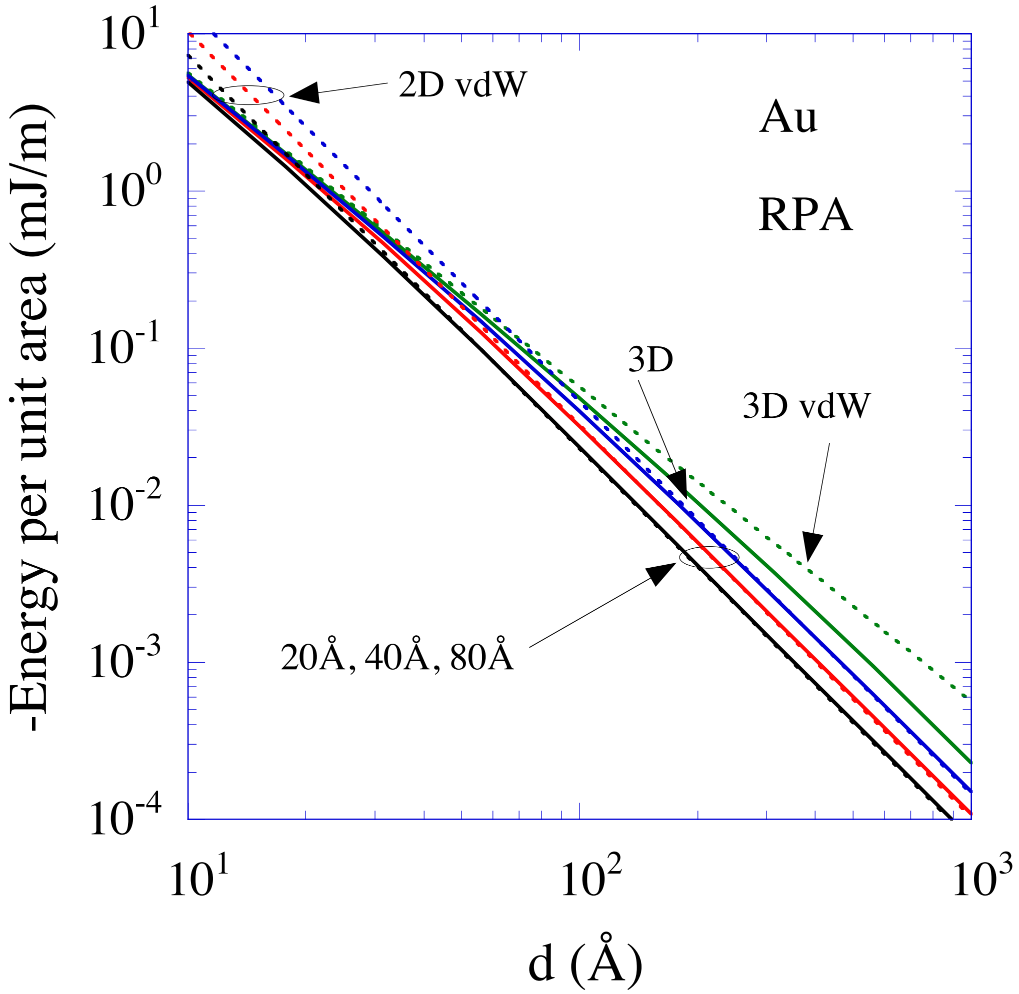
Langbein	Van der Waals	Casimir
Half space – half space	d^{-2}	d^{-3}
Film-half space	d^{-3}	d^{-4}
Film-film	d^{-4}	d^{-5}

Two 2D metal films



Bo E. Sernelius and P. Björk, Phys. Rev. B **57**, 6592 (1998)

Two thin metal films



M. Boström and Bo E. Sernelius, Phys. Rev. B **61**, 2204 (2000)

- Thus we found that the Langbein prediction failed for two 2D metallic films.

- We further found that it failed for two thin metal films.

- Will it work for two graphene sheets?

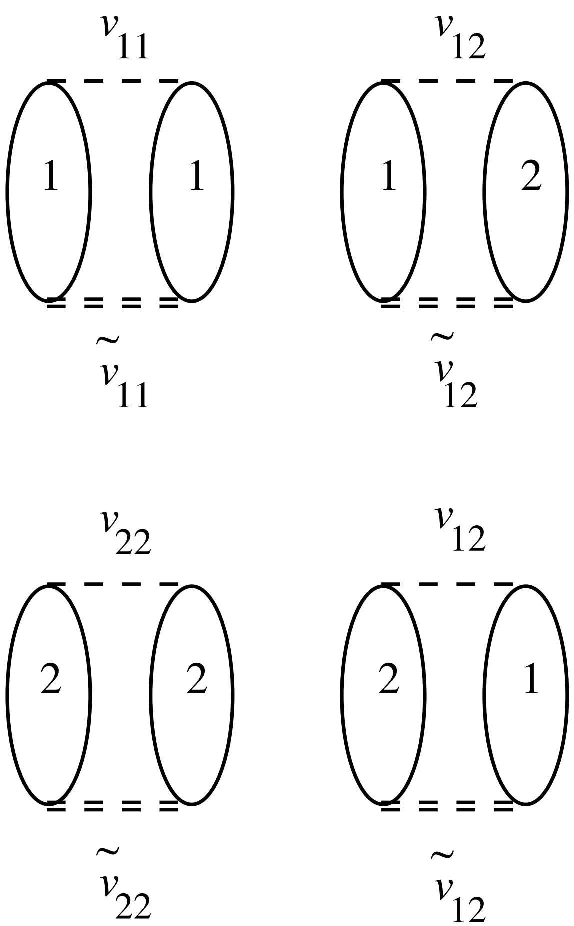
How to derive the interaction.

- This can be done in different ways

- One is to use many-body theory and use Feynman diagrams.

- One is to use the electromagnetic normal modes

For 2D-sheets the interaction is the inter-sheet correlation-energy



Sernelius and Björk, *Phys. Rev. B*, **57** 6592 (1998)

Result

$$E_c(d) = \frac{\hbar}{(2\pi)^2} \int_0^{\infty} \int_0^{\infty} d\omega \, dq q \ln \left\{ 1 - e^{-2qd} \left[\frac{\alpha'(q,\omega)}{1+\alpha'(q,\omega)} \right]^2 \right\}$$

Normal mode derivation

- Let us assume that we have an induced carrier distribution, $\rho_1(\mathbf{q},\omega)$ in sheet number 1
- This gives rise to the potential $v(\mathbf{q},\omega) = v^{2D}(q)\rho_1(\mathbf{q},\omega)$ in sheet number 1,

  and $\exp(-qd)v^{2D}(q)\rho_1(\mathbf{q},\omega)$ in sheet number 2.
- The resulting potential in sheet 2 after screening by the carriers is $\exp(-qd)v^{2D}(q)\rho_1(\mathbf{q},\omega)/\left[1+\alpha(\mathbf{q},\omega)\right]$

- This gives rise to an induced carrier distribution in sheet 2,

$$\rho_2(\mathbf{q},\omega)=\chi(\mathbf{q},\omega)e^{-qd}v^{2D}(q)\frac{\rho_1(\mathbf{q},\omega)}{\left[1+\alpha(\mathbf{q},\omega)\right]}.$$

In complete analogy, this carrier distribution in sheet 2 gives rise to a carrier distribution in sheet 1

$$\rho_1(\mathbf{q},\omega)=\chi(\mathbf{q},\omega)e^{-qd}v^{2D}(q)\frac{\rho_2(\mathbf{q},\omega)}{\left[1+\alpha(\mathbf{q},\omega)\right]}.$$

The mode condition

- To find the condition for self-sustained fields, normal modes, we let this induced carrier density in sheet 1 be the carrier density we started from. This leads to

$$1 - e^{-2qd}\left[\frac{\alpha(\mathbf{q},\omega)}{1+\alpha(\mathbf{q},\omega)}\right]^2 = 0$$

Two parallel 2D sheets

$$E_c(d) = \frac{\hbar}{(2\pi)^2} \int_0^{\infty}\int_0^{\infty} d\omega\, dq q \ln\left\{1 - e^{-2qd}\left[\frac{\alpha'(q,\omega)}{1+\alpha'(q,\omega)}\right]^2\right\}$$

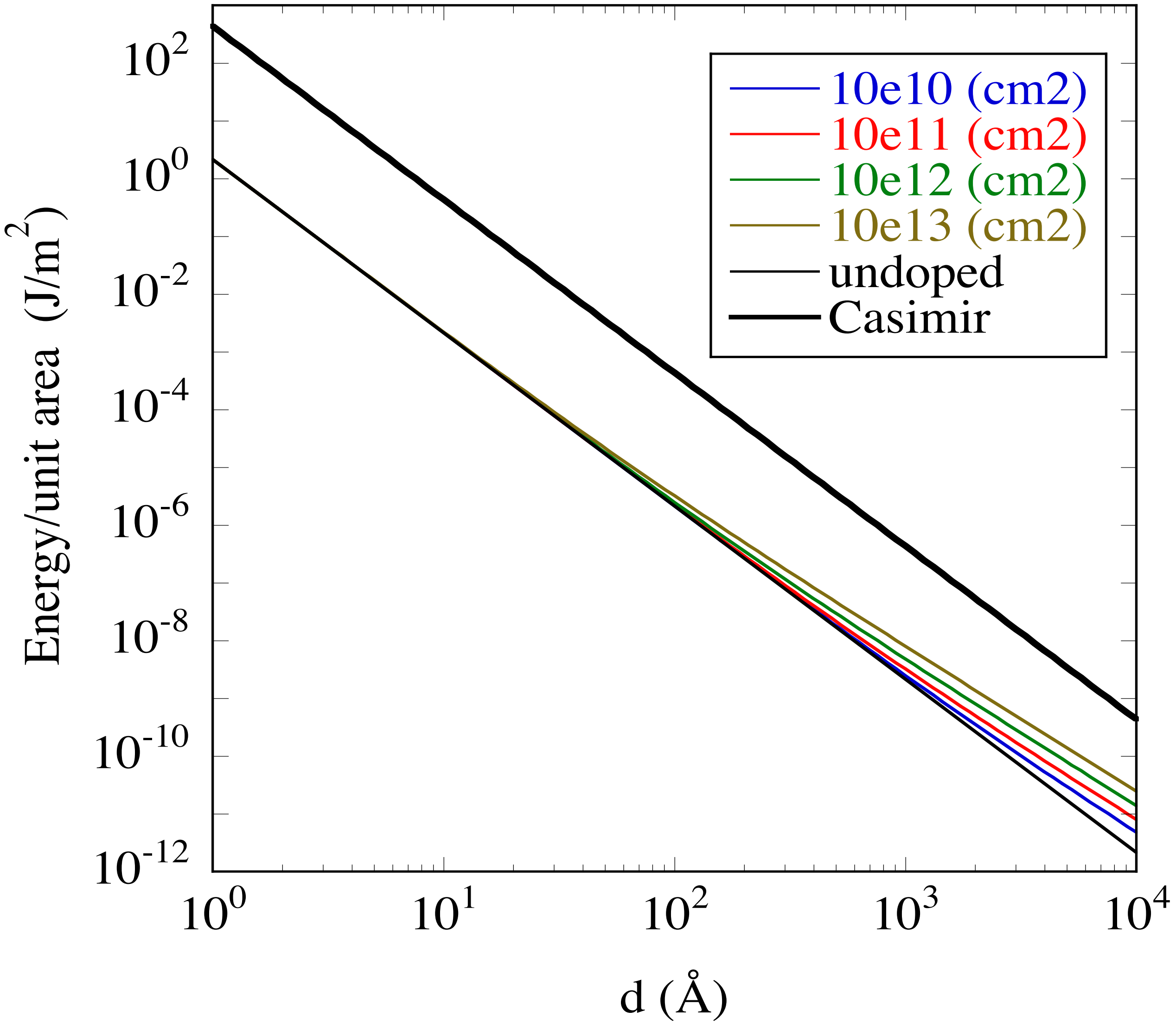
Undoped Graphene

$$\alpha'(\mathbf{q},\omega)=\frac{\pi e^2}{2\hbar}\frac{q}{\sqrt{v^2q^2+\omega^2}}\rightarrow\alpha'\left(\frac{\mathbf{q}}{d},\frac{\omega}{d}\right)=\alpha'(\mathbf{q},\omega)$$

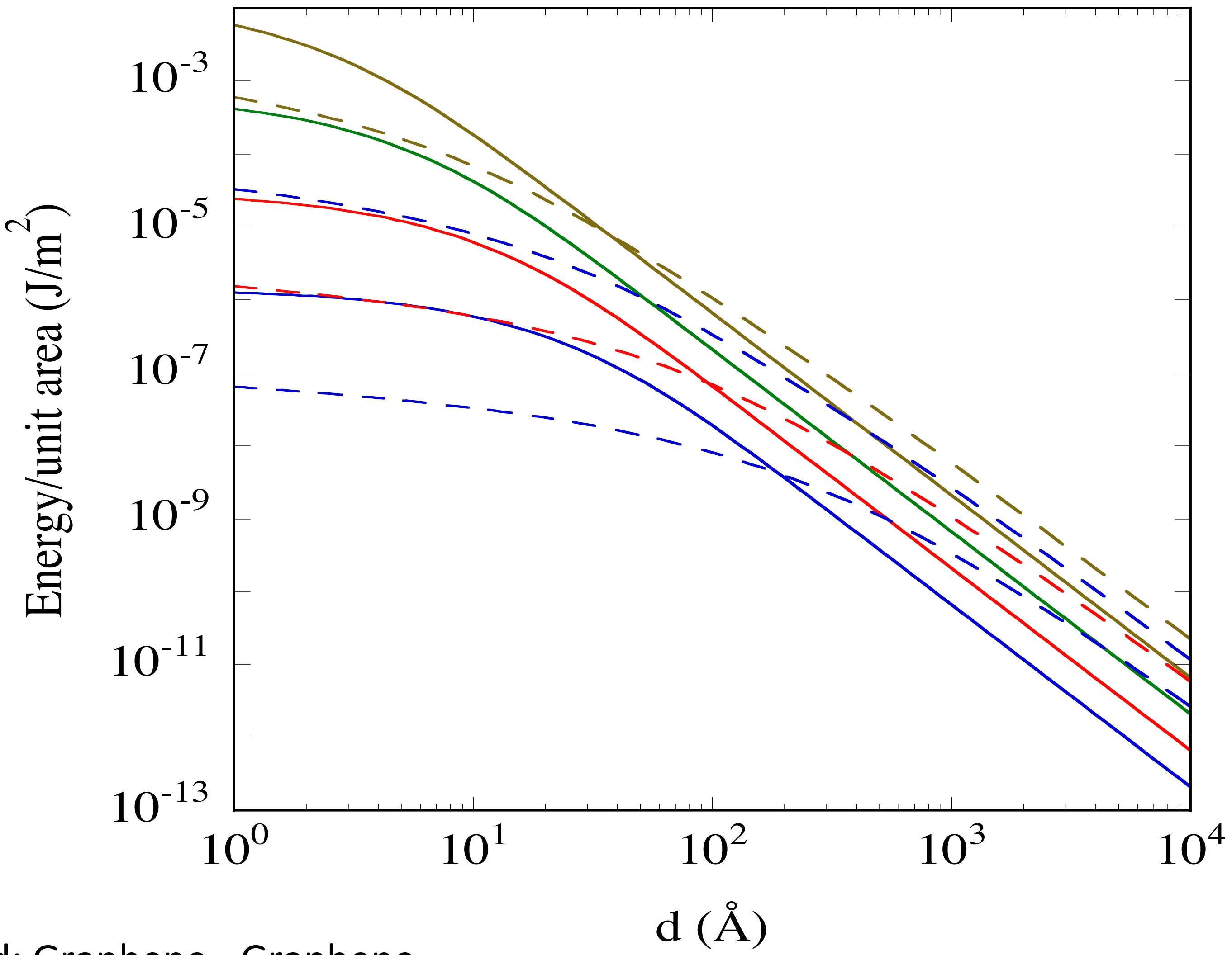
$$\downarrow$$

$$E_c(d)=\frac{\hbar}{(2\pi)^2 d^3}\int_0^\infty\int_0^\infty d\omega\, dq q \ln\left\{1-e^{-2q}\left[\frac{\alpha'(q,\omega)}{1+\alpha'(q,\omega)}\right]^2\right\}\propto\frac{1}{d^3}$$

Graphene-Graphene interaction



Contribution from the doping carriers



Dashed: Graphene - Graphene
Solid: 2D – 2D

"Saturation" due to spatial Dispersion.

One 2D sheet parallel to a substrate

- Now we start from a mirror charge in the substrate: $\rho_1(\mathbf{q},\omega)$
- This gives rise to an induced charge density in the 2D sheet

$$\rho_2(\mathbf{q},\omega) = \chi(\mathbf{q},\omega)e^{-2qd}v^{2D}(q)\frac{\rho_1(\mathbf{q},\omega)}{\left[1+\alpha(\mathbf{q},\omega)\right]}.$$

Note the distance is now $2d$. The mirror charge is at a distance d from the surface.

The mode condition

- This charge density gives rise to an image charge density

$$\rho_1(\mathbf{q},\omega) = -\rho_2(\mathbf{q},\omega)\frac{\varepsilon_s(\omega)-1}{\varepsilon_s(\omega)+1}$$

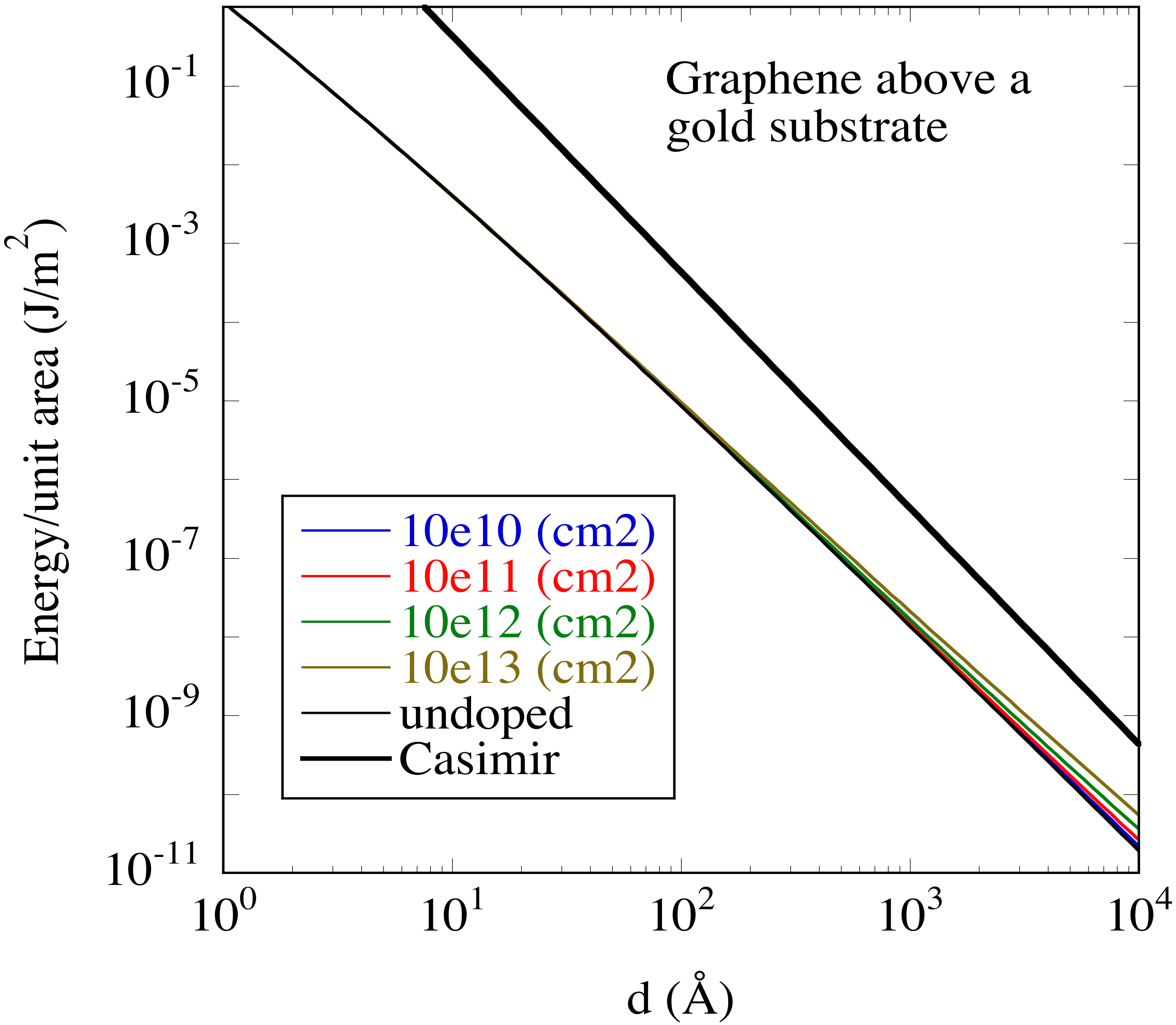
Letting this be the image charge we started from gives

$$1 - e^{-2qd}\frac{\alpha(\mathbf{q},\omega)}{1+\alpha(\mathbf{q},\omega)}\frac{\varepsilon_s(\omega)-1}{\varepsilon_s(\omega)+1} = 0.$$

One 2D sheet parallel to a substrate

$$E_c(d) = \frac{\hbar}{(2\pi)^2} \int_0^\infty \int_0^\infty d\omega\, dq q \ln\left\{1 - e^{-2qd}\left[\frac{\alpha'(q,\omega)}{1+\alpha'(q,\omega)} \frac{\varepsilon_s'(\omega)-1}{\varepsilon_s'(\omega)+1}\right]\right\}$$

Graphene — Gold-substrate interaction



Predictions and outcome

Langbein	Van der Waals	Casimir
Half space – half space	d^{-2}	d^{-3}
Film-half space	d^{-3}	d^{-4}
Film-film	d^{-4}	d^{-5}
2D metal – metal half space	$d^{-5/2}$ [a]	d^{-3}
2D metal – 2D metal	$d^{-5/2}$ [a][b]	d^{-3} [b]
Graphene – metal half space	No pure power law [c]	d^{-3}
Graphene – graphene	d^{-3} [c],[d]	d^{-3}
Doped	$d^{-5/2}$ [c]	d^{-3}

(a) Boström and Sernelius, *Phys. Rev. B*, **61** 2204 (2000).
(b) Sernelius and Björk, *Phys. Rev. B*, **57** 6592 (1998).
(c) Bo E. Sernelius, EPL, **95** (2011) 57003. (Present)
(d) Predicted by Dobson et al., *Phys. Rev. Lett.*, **96** 073201 (2006).

Summary and conclusions

- We have derived the non-retarded Casimir interaction (van der Waals interaction) between two free standing graphene sheets. Numerical results were presented for undoped and for doped graphene. We found a d^{-3} dependence for the undoped case and a $d^{-5/2}$ dependence for the doped at large separations.

- We furthermore derived the interaction between a graphene sheet and a substrate. Numerical results were presented for a doped and undoped graphene sheet above a gold substrate.
  We found no simple power law.

- To be noted is that there were no signs of spatial dispersion effects in the undoped graphene geometries.