



# Hartree-Fock Stability

## Applications to the Homogeneous Electron Gas

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# Background Information

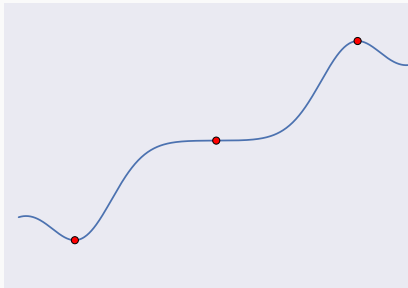
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# Levels of Hartree-Fock Theory

Method	Spinorbital	DoF	Eigenfunction of
Restricted	$\chi_j^\alpha(\vec{r}, \sigma) = \sum_{i=1}^N c_{ij} \phi_i(\vec{r}) \alpha(\sigma)$ $\chi_j^\beta(\vec{r}, \sigma) = \sum_{i=1}^N c_{ij} \phi_i(\vec{r}) \beta(\sigma)$	N/2	$\hat{S}^2, \hat{S}_z$
Unrestricted	$\chi_j^\alpha(\vec{r}, \sigma) = \sum_{i=1}^N c_{ij}^\alpha \phi_i(\vec{r}) \alpha(\sigma)$ $\chi_j^\beta(\vec{r}, \sigma) = \sum_{i=1}^N c_{ij}^\beta \phi_i(\vec{r}) \beta(\sigma)$	N	$\hat{S}_z$
General	$\chi_j(\vec{r}, \sigma) = \sum_{i=1}^N [c_{ij}^\alpha \phi_i(\vec{r}) \alpha(\sigma) + c_{ij}^\beta \phi_i(\vec{r}) \beta(\sigma)]$	2N	Neither

# Restricted Minimization

- Hartee-Fock SCF guarantees only stationary energy w.r.t. change in orbitals
- The solution may be a maximum, minimum or saddle point

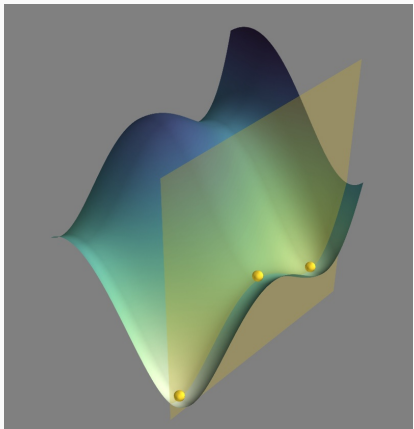


# Restricted Minimization

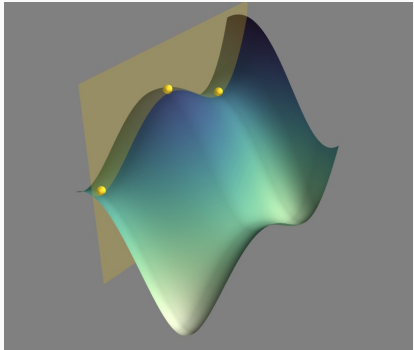
- Hartree-Fock SCF guarantees only stationary energy w.r.t. change in orbitals
- The solution may be a maximum, minimum or saddle point
  - *Within the constrained space*



# Restricted Minimization

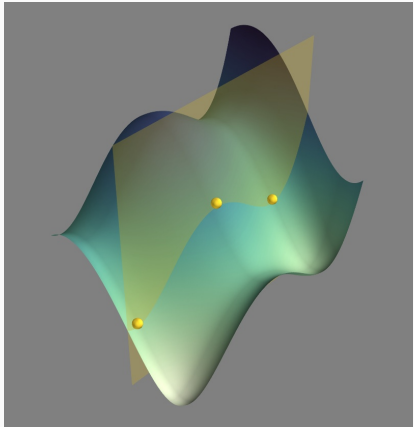


# Restricted Minimization





# Restricted Minimization



# Titleformats

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**metropolis** supports 4 different titleformats:

- Regular
- SMALLCAPS
- ALLSMALLCAPS
- ALLCAPS

They can either be set at once for every title type or individually.

This frame uses the `smallcaps` titleformat.

## Potential Problems

Be aware, that not every font supports small caps. If for example you typeset your presentation with pdfTeX and the Computer Modern Sans Serif font, every text in smallcaps will be typeset with the Computer Modern Serif font instead.

This frame uses the `allsmallcaps` titleformat.

### Potential problems

As this titleformat also uses smallcaps you face the same problems as with the `smallcaps` titleformat. Additionally this format can cause some other problems. Please refer to the documentation if you consider using it.

As a rule of thumb: Just use it for plaintext-only titles.

This frame uses the `allcaps` titleformat.

## Potential Problems

This titleformat is not as problematic as the `allsmallcaps` format, but basically suffers from the same deficiencies. So please have a look at the documentation if you want to use it.

# Elements

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The theme provides sensible defaults to  
`\emph{emphasize}` text, `\alert{accent}` parts  
or show `\textbf{bold}` results.

becomes

The theme provides sensible defaults to *emphasize* text, **accent** parts or  
show **bold** results.



# Font feature test

- Regular
- *Italic*
- SMALLCAPS
- **Bold**
- **Bold Italic**
- **Bold SmallCaps**
- Monospace
- *Monospace Italic*
- Monospace Bold
- *Monospace Bold Italic*

## Items

- Milk
- Eggs
- Potatos

## Enumerations

1. First,
2. Second and
3. Last.

## Descriptions

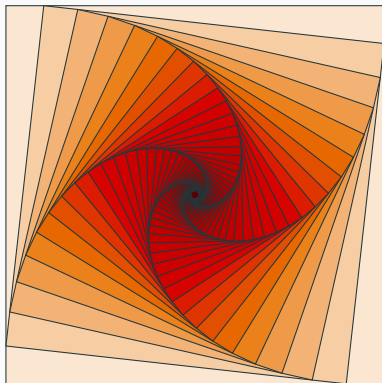
**PowerPoint** Meeh.  
**Beamer** Yeeeha.

- This is important

- This is important
- Now this

- This is important
- Now this
- And now this

- This is really important
- Now this
- And now this



**Figure 1:** Rotated square from texample.net.

**Table 1:** Largest cities in the world (source: Wikipedia)

City	Population
Mexico City	20,116,842
Shanghai	19,210,000
Peking	15,796,450
Istanbul	14,160,467



# Blocks

Three different block environments are pre-defined and may be styled with an optional background color.

## Default

Block content.

## Alert

Block content.

## Example

Block content.

## Default

Block content.

## Alert

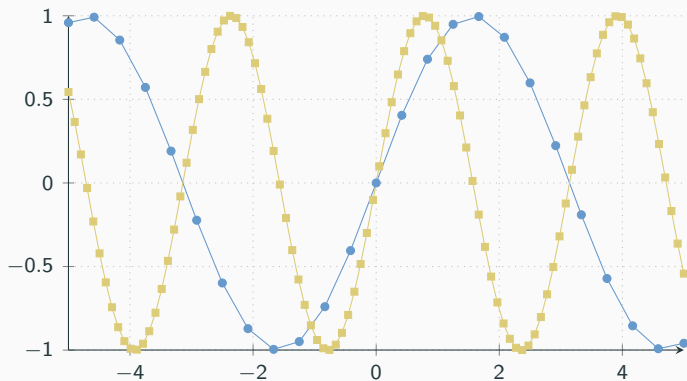
Block content.

## Example

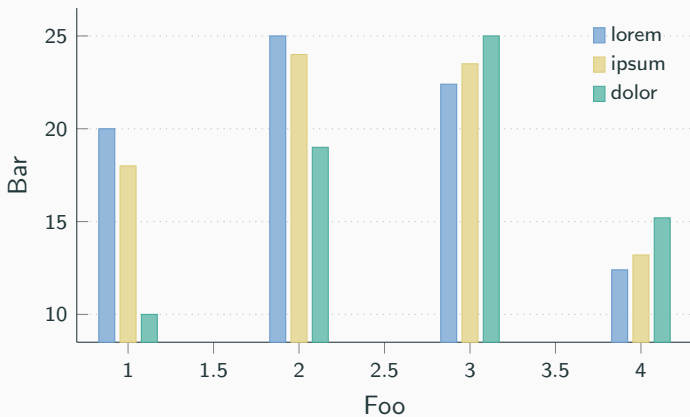
Block content.

$$e = \lim_{n \rightarrow \infty} \left(1 + \frac{1}{n}\right)^n$$

# Line plots



## Bar charts



*Veni, Vidi, Vici*

**metropolis** defines a custom beamer template to add a text to the footer. It can be set via

```
\setbeamertemplate{frame footer}{My custom footer}
```

Some references to showcase `[allowframebreaks]` `[?, ?, ?, ?, ?]`

## Conclusion

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# Summary

Get the source of this theme and the demo presentation from

`github.com/matze/mtheme`

The theme *itself* is licensed under a Creative Commons Attribution-ShareAlike 4.0 International License.



**Questions?**

# Backup slides

Sometimes, it is useful to add slides at the end of your presentation to refer to during audience questions.

The best way to do this is to include the `appendixnumberbeamer` package in your preamble and call `\appendix` before your backup slides.

**metropolis** will automatically turn off slide numbering and progress bars for slides in the appendix.

## References I