



Niraj Nepal <tug11655@temple.edu>

structure factor: figures and codes

4 messages

Adrienn Ruzsinszky <tuf27796@temple.edu>
To: Niraj Kumar Nepal <tug11655@temple.edu>

Wed, Feb 5, 2020 at 7:26 PM

Hi Niraj,

I am attaching the material that we discussed today.

The excel file has now five new tabs: the three structure_factor_Q's show the spectral analysis for $r_s=4$ with all methods and just for the three NEOs. The same analysis with the NEOs is repeated for Cs.The two int_structure_factors are the integrated S quantities (xc and correlation energies) for $r_s=4$ and Cs. These last figures correspond to Figure 2 in John's wavevector analysis paper.

In my notation NEOxc means that we use the x from RPA and c beyond RPA from NEO.

I am attaching the corresponding codes.(in the integrated S, I am closing the contour for the integral along the imaginary axis taking the real part of khi).

The last attachment is John's paper about the charge density waves.

Good night for now,
Adrienn

Adrienn Ruzsinszky
Associate Professor of Physics
Department of Physics
Temple University
[1925 N. 12th St.](#)
[Philadelphia, PA 19122-1801](#)
<https://sites.temple.edu/aruzsinszky/about/>

4 attachments**plasmon_disp.xlsx**
570K**plasmon_disp_complex_strucf.f**
32K**plasmon_disp_complex_strucfq.f**
33K**Perdew_et_al-1980-physica_status_solidi_(b).pdf**
612K

Adrienn Ruzsinszky <tuf27796@temple.edu>
To: Niraj Kumar Nepal <tug11655@temple.edu>

Wed, Feb 5, 2020 at 7:47 PM

For $r_s=4$, the "low-density" NEO c should be 0.43 not 0.44. I forgot to correct it in some of the figures.
For Cs $c=0.44$.

Adrienn

Adrienn Ruzsinszky
Associate Professor of Physics

2/5/2020

Temple University Mail - structure factor: figures and codes

Department of Physics
Temple University
[1925 N. 12th St.](#)
[Philadelphia, PA 19122-1801](#)
<https://sites.temple.edu/aruzsinszky/about/>

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Adrienn Ruzsinszky <tuf27796@temple.edu>
To: Niraj Kumar Nepal <tug11655@temple.edu>

Wed, Feb 5, 2020 at 7:49 PM

Ooops, it is correct, sorry,
Cs NEO c=0.43. Everything is correct as it is.
I am getting a little sleepy...

Adrienn Ruzsinszky
Associate Professor of Physics
Department of Physics
Temple University
[1925 N. 12th St.](#)
[Philadelphia, PA 19122-1801](#)
<https://sites.temple.edu/aruzsinszky/about/>

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Niraj Nepal <tug11655@temple.edu>
To: Adrienn Ruzsinszky <tuf27796@temple.edu>

Wed, Feb 5, 2020 at 8:01 PM

Hi Adrienn,

Thanks, I will look into it.

Best,
Niraj

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