

# Errata for the MSc Thesis

## "A Space-Time Study of the Electron-Electron Interaction in High- $T_C$ Parent Compound La<sub>2</sub>CuO<sub>4</sub>: In Search of an Attractive Effective Interaction"

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### Section 3.3

An error was made when implementing  $\mathcal{I}_G^k(\mathbf{r}) = \mathcal{I}_G^{k(1)}(\mathbf{r}) + \mathcal{I}_G^{k(2)}(\mathbf{r}) + \mathcal{I}_G^{k(3)}(\mathbf{r})$ , which enter all  $\delta\rho$ ,  $W$  and  $U$  calculations in real-space. The calculation of component (1)-(3) was separated into three different subroutines. By mistake, in one of these, the smearing factor  $\alpha$  of the Ewald summation was locally defined differently than the global  $\alpha$  used for the other terms. This implied that the terms in the Ewald summation did not balance properly. Despite checking that  $W$  corresponded to old results in nickel, where the linear muffin-tin orbital method was used, this error escaped attention since this comparison was only made inside the nickel muffin-tin sphere, where the effect from  $\mathcal{I}_G^k(\mathbf{r})$  is small. Since this error affected both the results and conclusions, we provide corrected results together with a brief discussion in the appendix. Some conclusions remain unchanged, but some are different from before, as summarized in Table 1.

Table 1: Summary of the findings and conclusions in the appendix.

| Unchanged Findings/Conclusions   | New Findings/Conclusions  |
|--|---|
| The low-energy V 3d <sub>xy</sub> and Cu 3d <sub>x<sup>2</sup>-y<sup>2</sup></sub> orbitals dominate the real-space characteristics of $W$ in SrVO <sub>3</sub> and La <sub>2</sub> CuO <sub>4</sub> respectively. | $W$ , $U_1$ and $U_3$ are all short-ranged since unphysical screening and anti-screening in the interstitial region is no longer present. |
| In La <sub>2</sub> CuO <sub>4</sub> , $U_1$ displays attraction close to $\mathbf{r}'$ when put at the Cu site, but $U_3$ does not. The pd screening thus appears to cause the negative interaction.               | The magnitude of $W$ is very similar in SrVO <sub>3</sub> and La <sub>2</sub> CuO <sub>4</sub> .  |
| The pd screening has most of its weight at Cu.   | In the time-domain, $W$ starts of negative for all $\mathbf{r}, \mathbf{r}'$ combinations considered.                                     |
| The main attraction is found in the first temporal oscillation, where all frequency components add up constructively.  | $W(t)$ is unstable against the choice of local orbitals for $t \lesssim 1$ femtosecond.   |

*Note:* Only a subset of the most essential and important results, entering the conclusion of the thesis, are presented in their modified form in this errata. In other words, the conclusions of the study can be verified or changed entirely based on what is presented here. For the less important subset of results, which is not presented, the changes can be understood qualitatively by extrapolating main features. The linear density response function  $R$  remains the same as before, since this does not contain  $\mathcal{I}_G^k$ . The induced charge density  $\delta\rho$  and the screened interaction  $W$  (and  $U$ ), however, depend linearly and quadratically on  $\mathcal{I}_G^k$  respectively. The former is not presented here since it was not the central quantity of the study. But the reduced weight of  $W$  in the interstitial region indicates that also  $\delta\rho$  is affected accordingly. Further, in the time-domain,  $W$  is here only presented for fixed  $\mathbf{r}$  and  $\mathbf{r}'$ . The combined space-time plots in the thesis did not add to the conclusion and were merely included to illustrate the power of the numerical implementation. The interested reader is encouraged to read the future publication, which also will focus on the space-time screening in cuprates.

## Appendix

The static  $W$  in  $\text{SrVO}_3$  and  $\text{La}_2\text{CuO}_4$  are presented in Fig. 1 and 2 respectively. Note that the color map is discontinuous at a value of 0, to more easily see where the interaction is attractive and repulsive.  $W$  goes to 0 more rapidly in both compounds than the old results suggested. Also, with  $\mathbf{r}'$  put far from any atom, no significant attraction is found closeby, contrary to what the wrong results yielded, especially for  $\text{La}_2\text{CuO}_4$ . The amount of attraction does therefore not appear to be more pronounced in  $\text{La}_2\text{CuO}_4$  than in  $\text{SrVO}_3$ , quite opposite to what was concluded in the thesis.

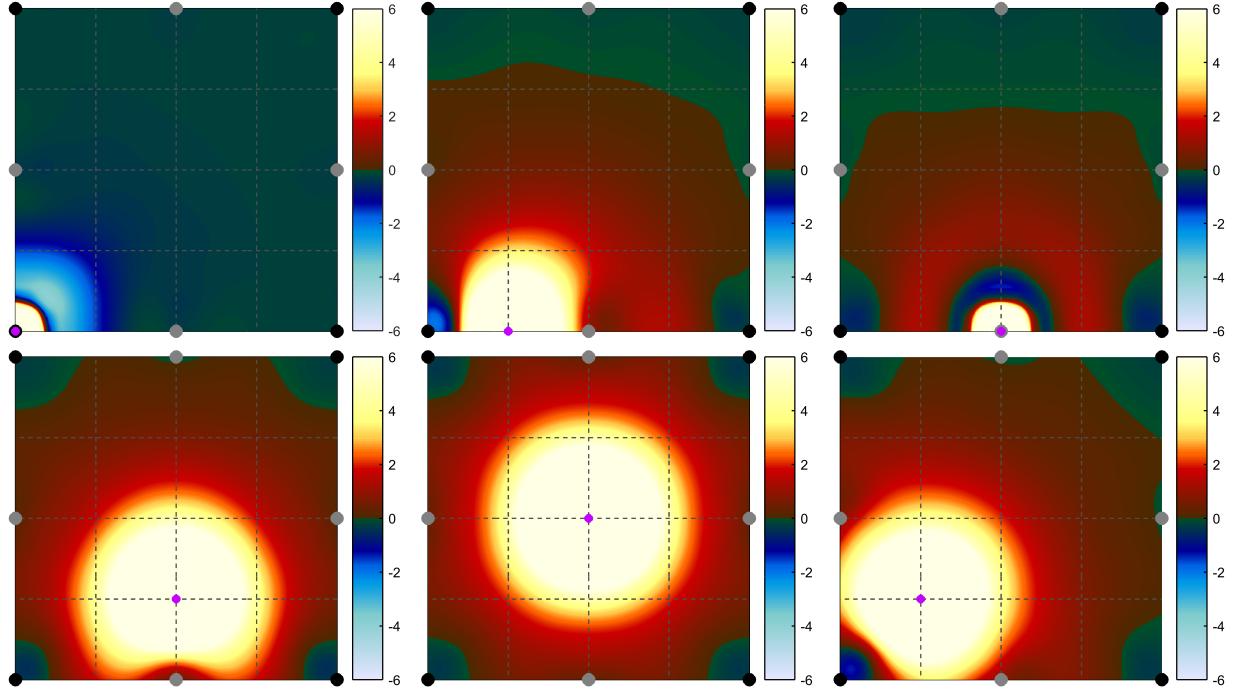


Figure 1:  $W(\mathbf{r}, \mathbf{r}'; \omega = 0)$  in the  $\text{VO}_2$  plane of  $\text{SrVO}_3$  (unit: eV). Black and grey points mark V and O atoms respectively. The test charge (purple point) is put at six different  $\mathbf{r}'$ .

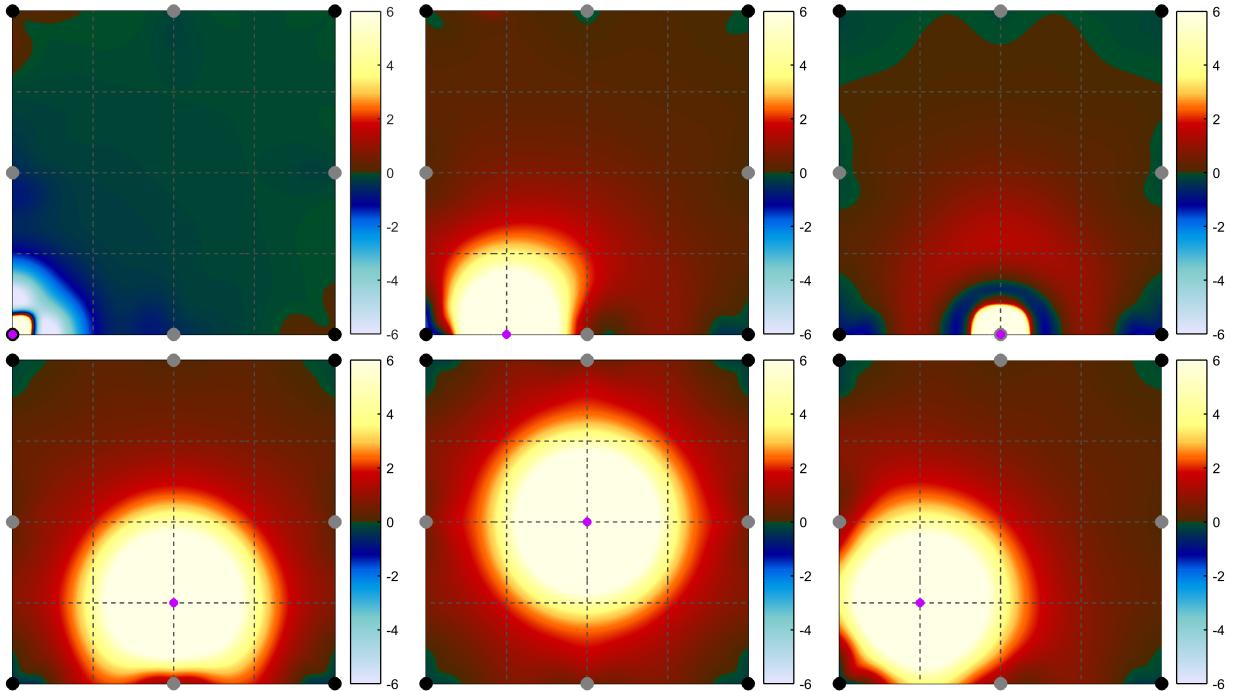


Figure 2:  $W(\mathbf{r}, \mathbf{r}'; \omega = 0)$  in the  $\text{CuO}_2$  plane of  $\text{La}_2\text{CuO}_4$  (unit: eV). Black and grey points mark the Cu and O atoms respectively. The test charge (purple point) is put at six different  $\mathbf{r}'$ .

$U_1$  and  $U_3$  in  $\text{La}_2\text{CuO}_4$  are further shown in Fig. 3 and 4. Just like for  $W$ , the screening in the interstitial region is reduced compared to the wrong results, which here implies that both  $U_1$  and  $U_3$  are positive there. As was found in the thesis,  $U_1$  is negative close to the Cu atom if  $\mathbf{r}'$  is put there, while  $U_3$  is not. But this observation is now more interesting, since no other attraction is present in the interstitial region. We therefore conclude, just like in the thesis, that it is the pd-screening that causes a negative interaction at the Cu site.

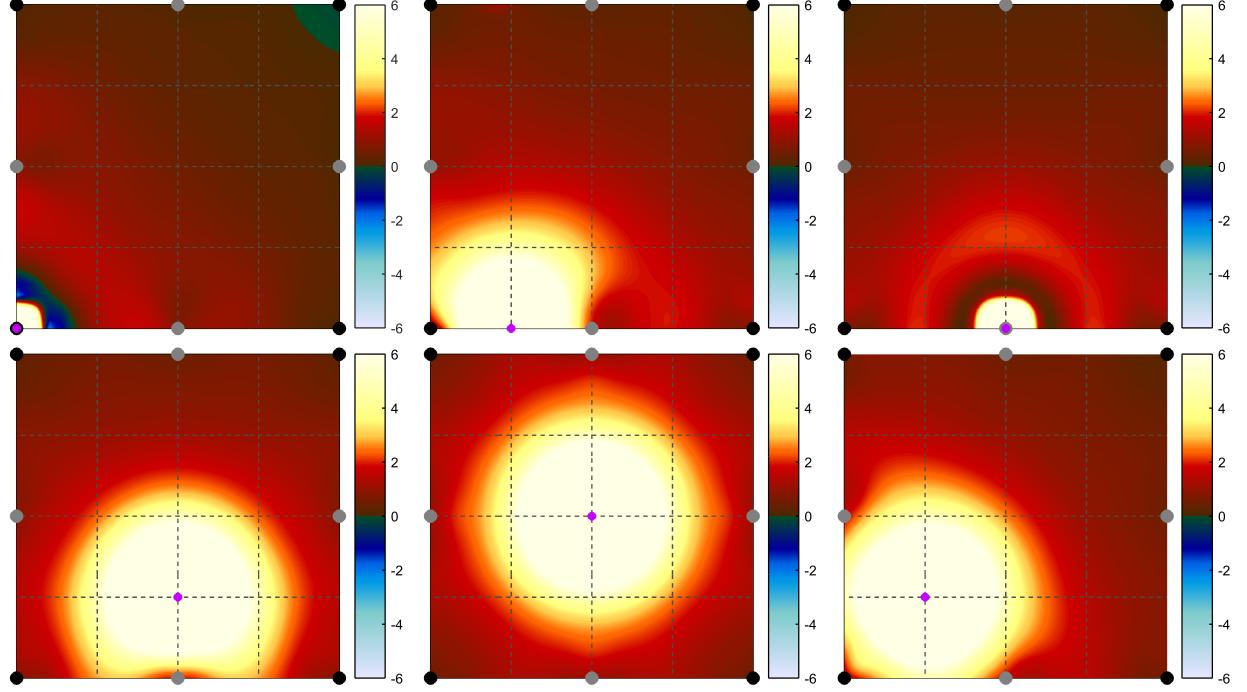


Figure 3:  $U_1(\mathbf{r}, \mathbf{r}'; \omega = 0)$  of the 1-band model in the  $\text{CuO}_2$  plane of  $\text{La}_2\text{CuO}_4$  (unit: eV). Black and grey points mark the Cu and O atoms respectively. The test charge (purple point) is put at six different  $\mathbf{r}'$ .

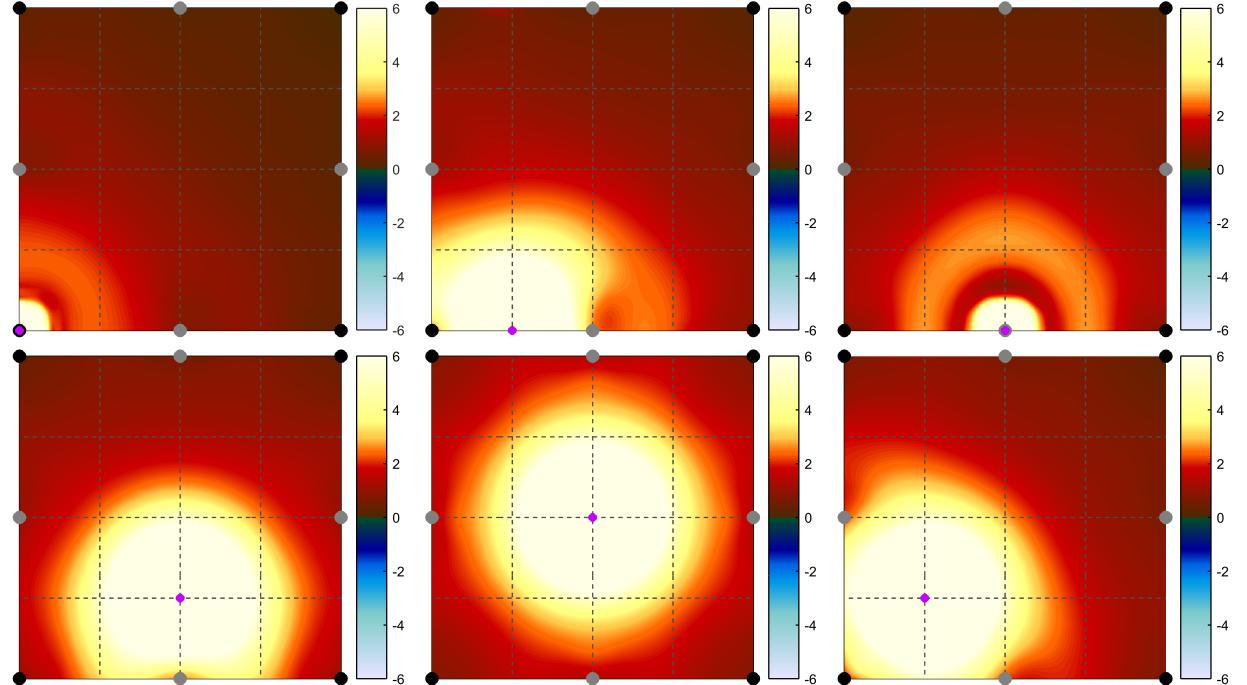


Figure 4:  $U_3(\mathbf{r}, \mathbf{r}'; \omega = 0)$  of the 3-band model in the  $\text{CuO}_2$  plane of  $\text{La}_2\text{CuO}_4$  (unit: eV). Black and grey points mark the Cu and O atoms respectively. The test charge (purple point) is put at six different  $\mathbf{r}'$ .

The dd screening ( $W - U_1$ ) and pd screening ( $U_1 - U_3$ ) in  $\text{La}_2\text{CuO}_4$  is presented in Fig. 5 and 6. The wrong results gave large regions of positive values for both channels far from  $\mathbf{r}'$ . We here see however that the channels are predominantly negative in the first unit cell. Naturally, the dd screening is mainly localized at the Cu site, just like was concluded from the wrong results. More interestingly, also the pd screening has most of its weight at the Cu site, again in accordance with the earlier results.

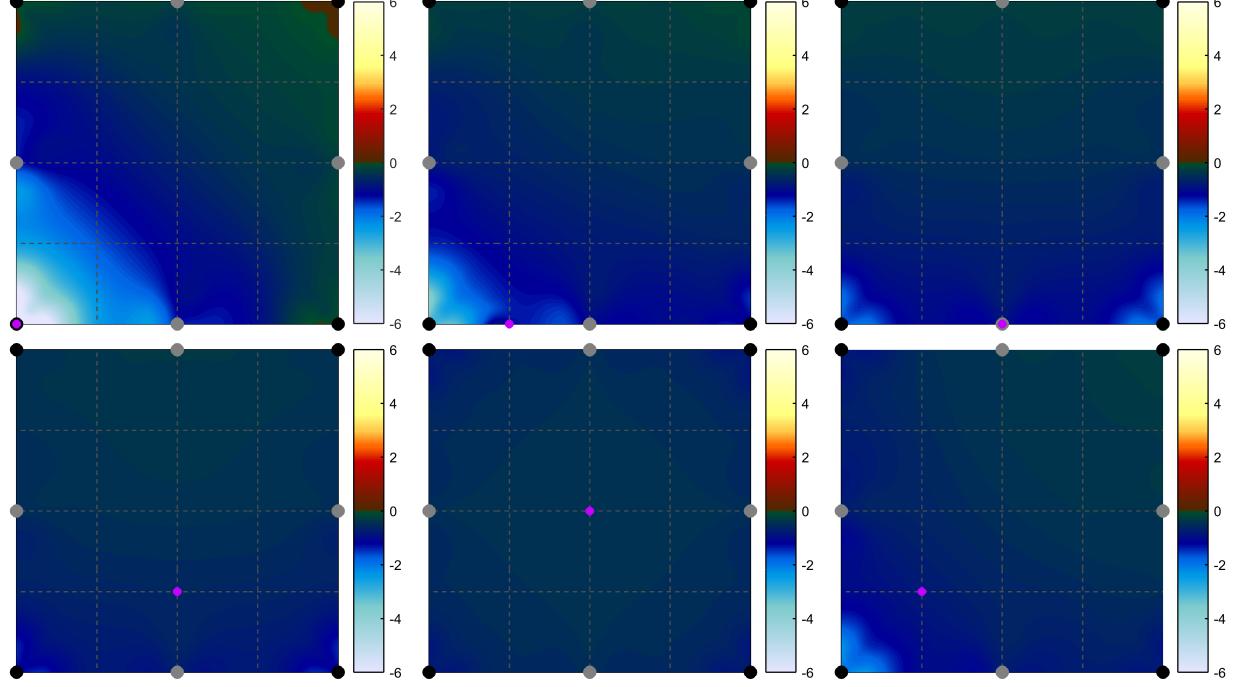


Figure 5: dd screening ( $W(\mathbf{r}, \mathbf{r}'; \omega = 0) - U_1(\mathbf{r}, \mathbf{r}'; \omega = 0)$ ) in the  $\text{CuO}_2$  plane of  $\text{La}_2\text{CuO}_4$  (unit: eV). Black and grey points mark the Cu and O atoms respectively. The test charge (purple point) is put at six different  $\mathbf{r}'$ .

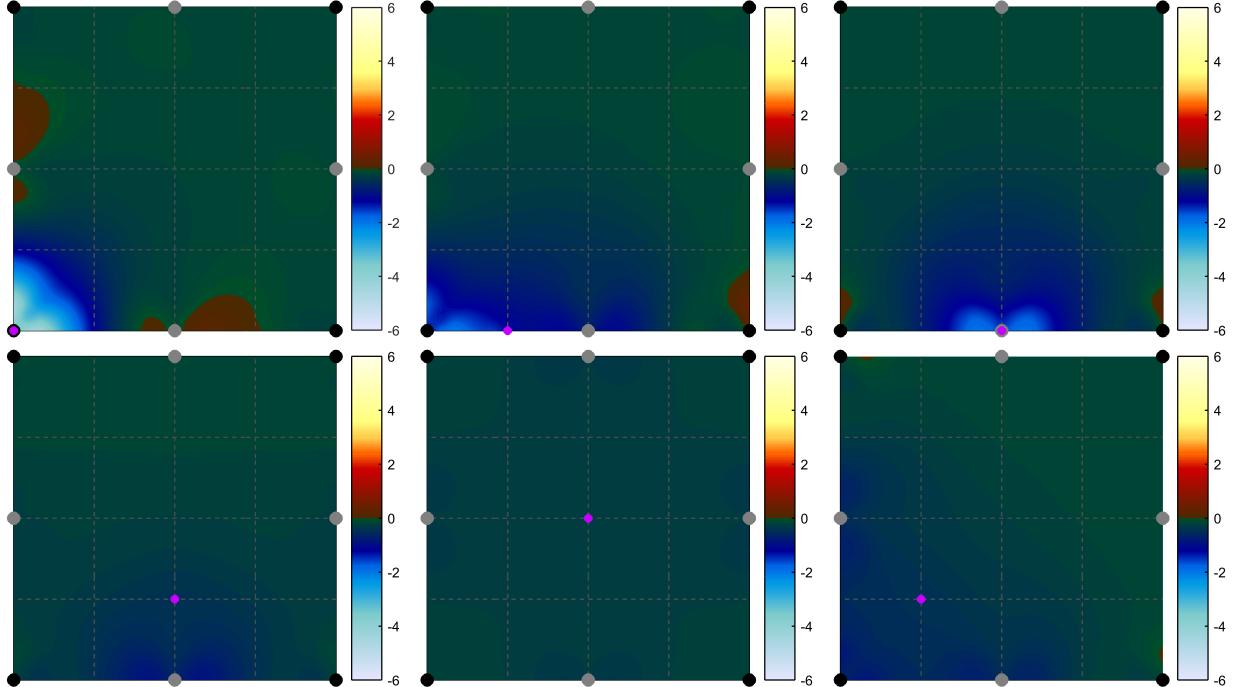


Figure 6: pd screening ( $U_1(\mathbf{r}, \mathbf{r}'; \omega = 0) - U_3(\mathbf{r}, \mathbf{r}'; \omega = 0)$ ) in the  $\text{CuO}_2$  plane of  $\text{La}_2\text{CuO}_4$  (unit: eV). Black and grey points mark the Cu and O atoms respectively. The test charge (purple point) is put at six different  $\mathbf{r}'$ .

Finally,  $W(t)$  in  $\text{La}_2\text{CuO}_4$  is presented in Fig. 7. Contrary to the earlier findings,  $W$  starts off negative for all  $\mathbf{r}, \mathbf{r}'$  combinations. But just like was concluded before, the main attraction is found in the first temporal oscillation. For this reason, we concluded in the thesis that  $W(\omega = 0)$ , which is the time-integral of  $W(t)$ , is mainly affected by the first few oscillations. But this cannot be the case since  $W(\omega = 0)$ , contrary to the short-time  $W$ , is essentially unaffected by the choice of local orbitals.  $W(t)$  is only stable against this choice for  $t$  larger than approximately one femtosecond. A detailed analysis of the long-time screening is thereby necessary to understand the low-energy physics. The common view that a dynamical picture is required to explain the pairing in the cuprates does however indicate that the short-time screening is relevant. It is therefore unfortunate that this is the limit in which the results are unstable.

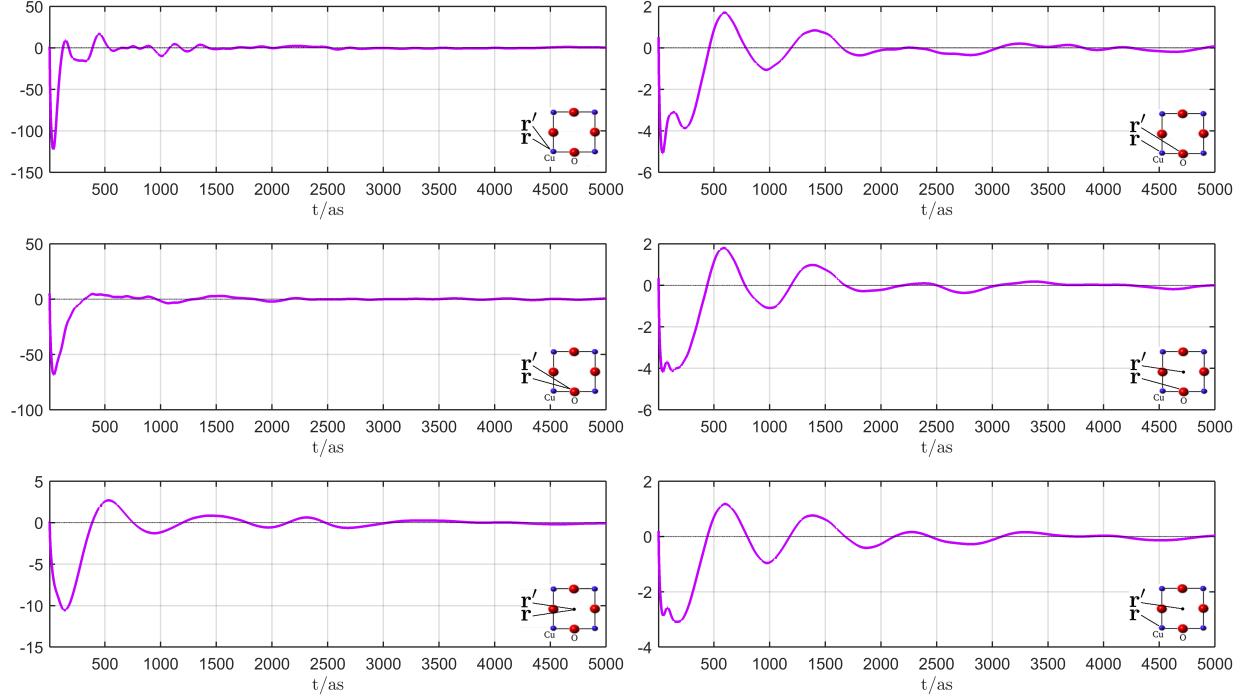


Figure 7:  $W(\mathbf{r}, \mathbf{r}'; t)$  in the  $\text{CuO}_2$  plane of  $\text{La}_2\text{CuO}_4$  (unit: eV/152.26as), with  $\mathbf{r}$  and  $\mathbf{r}'$  marked in each subfigure. Blue and red points mark the Cu and O atoms respectively.  $t' = 0$ .