

## GROMACS - Bug #396

### nan in g\_anaeig entropy because of sqr instead of dsqr

02/11/2010 09:46 AM - Jochen Hub

|  |                                  |
|--|----------------------------------|
| <b>Status:</b> Closed  |                                  |
| <b>Priority:</b> Normal  |                                  |
| <b>Assignee:</b> Erik Lindahl                                      |                                  |
| <b>Category:</b> analysis tools                                    |                                  |
| <b>Target version:</b> 4.0   |                                  |
| <b>Affected version - extra info:</b>                              | <b>Difficulty:</b> uncategorized |
| <b>Affected version:</b>   |                                  |
| <b>Description</b>   |                                  |
| The line   |                                  |
| <pre>kteh = kt*exp(2.0)/sqr(hbar)*AMU*sqr(NANO);</pre>             |                                  |
| in the calc_entropy_schlitter routine in gmx_anaeig.c should be    |                                  |
| <pre>kteh = kt*exp(2.0)/dsqr(hbar)*AMU*dsqr(NANO);</pre>           |                                  |
| Otherwise the kteh is nan since sqr(hbar) = 0 in single precision. |                                  |
| Cheers,  |                                  |
| Jochen   |                                  |

### History

#1 - 06/02/2010 07:40 PM - David van der Spoel

Fixed by writing out the square.