Yerong – here is what you wrote:

- 08/11

Isn't there another factor b^2 here?

$$X = [\delta - (v_H^2 - v_C^2)] \cdot \frac{\delta}{|\vec{v}_H + \vec{v}_C|^2} \cdot \frac{1}{b^2 r^2 - (\vec{b} \cdot \vec{r})^2} \times b^2 = \frac{\delta^2}{\left|\vec{v}_H + \vec{v}_C\right|^2}$$

For safety in evolutions, we'd better keep X negative. As shown in Eqs.(10) the last two terms are positive so $\boxed{\delta - (v_H^2 - v_C^2) = 2\Delta/m - (v_H^2 - v_C^2) \text{ dominates.}}$ It is found in tests that $v_H^2 - v_C^2$ sometimes touches the ground of 3(in L-J reduced units), so if $\boxed{W}$ were set to be 480 in this case, for instance, we would soon find errors in the data. One may insist on a W which is much smaller than 60 to enable inputs with larger amplitudes for the simple reason that large imposes converge much faster. However, this proves unnecessary: it has been shown in Muller-Plathe's method that validity of linear response theory breaks down for large variation with $W = 15$, which is parallel to the impose with $\dot{e} = 10.120$ in our theory. So even if, with lower W and larger input amplitude, there is nothing wrong with the calculation of vector $\vec{w}$, it is meaningless to do calculations of this kind without the validity of linear response theory. It is been tested that $W = 60$ does not work for $\dot{e} = 10.120$, therefore, our choice of W seems quite reasonable.

I see your point that X has to be negative for reasonable Δ. For some reason, I always thought it was positive. This means α is also negative. Are you saying that this is all OK? I am not quite understanding you here. Could you please remind me what is W?