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Erratum: "Anomalous propagators and the particle–particle channel: Bethe–Salpeter equation" [J. Chem. Phys. 162, 134105 (2005)] FREE

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The authors would like to point out an error in Eq. (54) of Ref. 1. The expression of the hh–hh GW effective dynamic kernel matrix elements is

$$\begin{aligned} \mathrm{i}\tilde{\Xi}^{\mathrm{pp},GW}_{ij,kl}(-\omega) = \langle ij||kl\rangle &+ \frac{1}{2}\sum_{\mu} \frac{M_{ik,\mu}M_{lj,\mu} - M_{jk,\mu}M_{li,\mu}}{\omega - (-\epsilon_j - \epsilon_l + \Omega_\mu - \mathrm{i}\eta)} \\ &+ \frac{1}{2}\sum_{\mu} \frac{M_{ki,\mu}M_{jl,\mu} - M_{kj,\mu}M_{il,\mu}}{\omega - (-\epsilon_i - \epsilon_k + \Omega_\mu - \mathrm{i}\eta)} \\ &+ \frac{1}{2}\sum_{\mu} \frac{M_{ik,\mu}M_{lj,\mu} - M_{jk,\mu}M_{li,\mu}}{\omega - (-\epsilon_i - \epsilon_l + \Omega_\mu - \mathrm{i}\eta)} \\ &+ \frac{1}{2}\sum_{\mu} \frac{M_{ki,\mu}M_{jl,\mu} - M_{kj,\mu}M_{il,\mu}}{\omega - (-\epsilon_j - \epsilon_k + \Omega_\mu - \mathrm{i}\eta)}. \end{aligned} \quad (1)$$

Note that this expression was correct in the original supplementary material, but the factor 1/2 was missing in the main text.[1]

In this correction, we update the results obtained for the dynamic ppBSE@GW correction and presented in Table II and Fig. 6 of the original manuscript, as a wrong factor 1/2 was found in the implementation. The new results are listed in Table I and shown graphically in Fig. 1. This shows that the effect of the dynamics is actually to worsen the results with respect to the ppBSE@GW static kernel approximation. Therefore, the good performance of the latter is the result of a fortuitous error cancellation. The magnitude of the dynamic kernel is too large, and this would be mitigated by higher-order terms in the kernel.

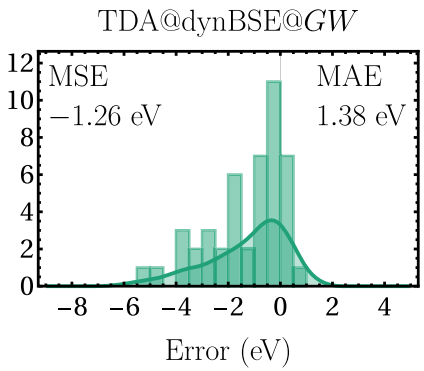

FIG. 1. Histogram of the errors (with respect to FCI) for the singlet and triplet principal DIPs of 23 small molecules in the aug-cc-pVTZ basis set computed at the pp-BSE level using the dynamic GW kernel within the TDA (TDA@dynBSE@GW) using $\eta = 0.1E_\mathrm{h}$.

TABLE I. DIPs (in eV) toward the singlet and triplet dication ground states in the aug-cc-pVTZ basis set computed at the pp-BSE level using the dynamic *GW* kernel within the TDA (TDA@dynBSE@*GW*) using $\eta = 0.1E_h$. The renormalization factor associated with the dynamic correction is reported in parentheses.

	TDA@dynBSE@*GW*	
Molecule	Singlet DIPs	Triplet DIPs
H_2O	38.31(0.73)	38.73(0.78)
HF	46.93(0.71)	45.35(0.76)
Ne	60.71(0.74)	58.75(0.79)
CH_4	38.73(0.89)	38.23(0.90)
NH_3	33.33(0.83)	37.64(0.89)
CO	40.99(0.86)	41.33(0.95)
N_2	43.65(0.93)	43.63(0.89)
BF	32.45(0.96)	38.08(0.99)
LiF	34.59(0.92)	33.56(0.79)
BeO	28.33(0.86)	27.64(0.77)
BN	32.64(0.82)	31.89(0.82)
C_2	35.44(0.84)	34.68(0.85)
CS	33.40(0.92)	32.99(0.93)
LiCl	28.92(0.87)	28.06(0.84)
F_2	44.80(0.98)	44.17(0.96)
H_2S	30.24(0.87)	32.20(0.91)
PH_3	30.29(0.88)	32.31(0.95)
HCl	35.64(0.84)	34.64(0.86)
Ar	43.00(0.84)	41.83(0.87)
SiH_4	33.26(0.97)	33.11(0.97)
CH_2O	32.51(0.90)	35.03(0.87)
CO_2	38.10(0.95)	37.49(0.95)
BH_3	36.32(0.92)	35.32(0.94)
MSE	−1.59	−0.92
MAE	1.73	1.03
RMSE	2.30	1.49
SDE	1.70	1.19
Min	−5.41	−3.78
Max	0.84	0.47

REFERENCE

[1] A. Marie, P. Romaniello, X. Blase, and P.-F. Loos, "Anomalous propagators and the particle–particle channel: Bethe–Salpeter equation," J. Chem. Phys. **162**, 134105 (2025).