Supporting Information for Monte Carlo Second- and Third-Order Many-Body Green's Function Methods with Frequency-Dependent, Non-Diagonal Self-Energy

Alexander E. Doran and So Hirata*

Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA

E-mail: sohirata@illinois.edu

1 Integrand of the third-order self-energy

The integrand of the third-order self-energy is

$$f_{pq}^{(3)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, \mathbf{r}_5, \mathbf{r}_6, \tau_1, \tau_2, \omega) = \sum_{n=1}^{84} f_{pq}^{(3:n)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, \mathbf{r}_5, \mathbf{r}_6, \tau_1, \tau_2, \omega), \tag{1}$$

where

$$f_{pq}^{(3:n)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, \mathbf{r}_5, \mathbf{r}_6, \tau_1, \tau_2, \omega) = \frac{\bar{f}_{pq}^{(3:n)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4, \mathbf{r}_5, \mathbf{r}_6, \tau_1, \tau_2, \omega)}{r_{12} r_{34} r_{56}} \tag{2}$$

and r_{12} is the distance between $\mathbf{r}_1$ and $\mathbf{r}_2$. The terms, $\bar{f}_{pq}^{(3:n)}$, with the arguments omitted for brevity are

$$\bar{f}_{pq}^{(3:1)} = -G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1{+}\tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_3, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1{-}\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_1)e^{-\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:2)} = G^{+}(\mathbf{r}_2, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_6, \tau_1)G^{+}(\mathbf{r}_4, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_1)e^{-\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:3)} = -G^{+}(\mathbf{r}_2, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_1)e^{-\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:4)} = -G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_4, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_2, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_1)e^{-\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:5)} = 2G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_1)e^{-\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:6)} = -2G^{+}(\mathbf{r}_2, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_1)e^{-\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:7)} = 2G^{+}(\mathbf{r}_2, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_3, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_1)e^{-\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:8)} = 2G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_4, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_1)e^{-\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:9)} = 2G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_3, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_2, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_1)e^{-\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:10)} = -4G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_3, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_1)e^{-\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:11)} = G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_3)e^{\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:12)} = -G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_3, -\tau_1)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_3)e^{\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:13)} = G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_2, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_3, -\tau_1)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_3)e^{\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:14)} = G^{+}(\mathbf{r}_1, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_3)e^{\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:15)} = -2G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_3)e^{\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:16)} = 2G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_3)e^{\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:17)} = -2G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_2, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_3)e^{\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:18)} = -2G^{+}(\mathbf{r}_1, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_3)e^{\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:19)} = -2G^{+}(\mathbf{r}_1, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_2, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_3)e^{\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:20)} = 4G^{+}(\mathbf{r}_1, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_3)e^{\omega\tau_2},$$

$$\bar{f}_{pq}^{(3:21)} = -G^{+}(\mathbf{r}_2,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_4,-\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1-\tau_2)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_1)e^{-\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:22)} = G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1+\tau_2)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_4,-\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_3,-\tau_1)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_1)e^{-\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:23)} = -G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_2,-\tau_1-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_3,-\tau_1)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_1)e^{-\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:24)} = -G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_3,-\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_1,-\tau_1-\tau_2)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_1)e^{-\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:25)} = -2G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1+\tau_2)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_3,-\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_1)e^{-\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:26)} = 2G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_3,-\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1-\tau_2)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_1)e^{-\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:27)} = 2G^{+}(\mathbf{r}_2,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_2,-\tau_1-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_1)e^{-\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:28)} = 2G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_3,-\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_1,-\tau_1-\tau_2)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_1)e^{-\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:29)} = 2G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_1,-\tau_1-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_3,-\tau_1)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_1)e^{-\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:30)} = -4G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_1,-\tau_1-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_3,-\tau_1)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_1)e^{-\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:31)} = G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1+\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_5,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^{*}(\mathrm{r}_1)\phi_q(\mathrm{r}_5)e^{\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:32)} = -G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_6,\tau_1)G^{+}(\mathbf{r}_4,\mathbf{r}_5,\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1-\tau_2)\phi_p^{*}(\mathrm{r}_1)\phi_q(\mathrm{r}_5)e^{\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:33)} = G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_5,\tau_1+\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^{*}(\mathrm{r}_1)\phi_q(\mathrm{r}_5)e^{\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:34)} = G^{+}(\mathbf{r}_1,\mathbf{r}_6,\tau_1+\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_5,\tau_1)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^{*}(\mathrm{r}_1)\phi_q(\mathrm{r}_5)e^{\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:35)} = 2G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_5,\tau_1)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1-\tau_2)\phi_p^{*}(\mathrm{r}_1)\phi_q(\mathrm{r}_5)e^{\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:36)} = -2G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1+\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_5,\tau_1)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^{*}(\mathrm{r}_1)\phi_q(\mathrm{r}_5)e^{\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:37)} = -2G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_5,\tau_1+\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^{*}(\mathrm{r}_1)\phi_q(\mathrm{r}_5)e^{\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:38)} = -2G^{+}(\mathbf{r}_1,\mathbf{r}_6,\tau_1+\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_5,\tau_1)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_3,-\tau_1)\phi_p^{*}(\mathrm{r}_1)\phi_q(\mathrm{r}_5)e^{\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:39)} = -2G^{+}(\mathbf{r}_1,\mathbf{r}_5,\tau_1+\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_3,-\tau_1)\phi_p^{*}(\mathrm{r}_1)\phi_q(\mathrm{r}_5)e^{\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:40)} = 4G^{+}(\mathbf{r}_1,\mathbf{r}_5,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_3,-\tau_1)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_5)e^{\omega(\tau_1+\tau_2)},$$

$$\bar{f}_{pq}^{(3:41)} = -G^{+}(\mathbf{r}_1,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1{+}\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_1,-\tau_1{-}\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_3,-\tau_1)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_3)e^{-\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:42)} = G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_5,\mathbf{r}_2,-\tau_1{-}\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_1,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_3)e^{-\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:43)} = -G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1{+}\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_4,-\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_1,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_3)e^{-\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:44)} = -G^{+}(\mathbf{r}_1,\mathbf{r}_6,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_3,\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_1,-\tau_1{-}\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_3)e^{-\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:45)} = 2G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1{+}\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_1,-\tau_1{-}\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_3)e^{-\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:46)} = -2G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_5,\mathbf{r}_1,-\tau_1{-}\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_3)e^{-\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:47)} = 2G^{+}(\mathbf{r}_1,\mathbf{r}_6,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_1,-\tau_1{-}\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_3,-\tau_1)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_3)e^{-\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:48)} = 2G^{+}(\mathbf{r}_1,\mathbf{r}_3,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1{+}\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_4,-\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_3)e^{-\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:49)} = 2G^{+}(\mathbf{r}_1,\mathbf{r}_6,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_3,-\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_3)e^{-\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:50)} = -4G^{+}(\mathbf{r}_1,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1{+}\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_5,\mathbf{r}_3,-\tau_1)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_3)e^{-\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:51)} = G^{+}(\mathbf{r}_1,\mathbf{r}_5,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_4,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_5)e^{\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:52)} = -G^{+}(\mathbf{r}_1,\mathbf{r}_6,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_5,\tau_1{+}\tau_2)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_5)e^{\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:53)} = G^{+}(\mathbf{r}_1,\mathbf{r}_6,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_5,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_5)e^{\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:54)} = G^{+}(\mathbf{r}_1,\mathbf{r}_5,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_1,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_5)e^{\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:55)} = -2G^{+}(\mathbf{r}_1,\mathbf{r}_5,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_5)e^{\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:56)} = 2G^{+}(\mathbf{r}_1,\mathbf{r}_5,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1{+}\tau_2)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_4,-\tau_1)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_5)e^{\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:57)} = -2G^{+}(\mathbf{r}_1,\mathbf{r}_5,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_3,\mathbf{r}_6,\tau_1)G^{-}(\mathbf{r}_4,\mathbf{r}_2,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_1,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_5)e^{\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:58)} = -2G^{+}(\mathbf{r}_1,\mathbf{r}_4,\tau_2)G^{+}(\mathbf{r}_2,\mathbf{r}_6,\tau_1{+}\tau_2)G^{+}(\mathbf{r}_4,\mathbf{r}_5,\tau_1)G^{-}(\mathbf{r}_3,\mathbf{r}_1,-\tau_2)G^{-}(\mathbf{r}_6,\mathbf{r}_2,-\tau_1{-}\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_5)e^{\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:59)} = -2G^{+}(\mathbf{r}_1, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_1, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_5)e^{\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:60)} = 4G^{+}(\mathbf{r}_1, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_4, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_5)e^{\omega\tau_1},$$

$$\bar{f}_{pq}^{(3:61)} = 2G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1 + \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_3, -\tau_1)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_1),$$

$$\bar{f}_{pq}^{(3:62)} = -2G^{+}(\mathbf{r}_2, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_6, \tau_1)G^{+}(\mathbf{r}_4, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1 - \tau_2)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_1),$$

$$\bar{f}_{pq}^{(3:63)} = -4G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1 + \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_1),$$

$$\bar{f}_{pq}^{(3:64)} = 4G^{+}(\mathbf{r}_2, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1 - \tau_2)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_1),$$

$$\bar{f}_{pq}^{(3:65)} = -2G^{+}(\mathbf{r}_1, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_2, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_1, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_3),$$

$$\bar{f}_{pq}^{(3:66)} = 2G^{+}(\mathbf{r}_1, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_5, \tau_1+\tau_2)G^{-}(\mathbf{r}_4, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_3),$$

$$\bar{f}_{pq}^{(3:67)} = -4G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{-}(\mathbf{r}_4, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_3),$$

$$\bar{f}_{pq}^{(3:68)} = 4G^{+}(\mathbf{r}_1, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_3),$$

$$\bar{f}_{pq}^{(3:69)} = 2G^{+}(\mathbf{r}_1, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1 + \tau_2)G^{-}(\mathbf{r}_3, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_4, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_5),$$

$$\bar{f}_{pq}^{(3:70)} = -2G^{+}(\mathbf{r}_1, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_3, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1 - \tau_2)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_5),$$

$$\bar{f}_{pq}^{(3:71)} = -4G^{+}(\mathbf{r}_1, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1 + \tau_2)G^{-}(\mathbf{r}_3, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_5),$$

$$\bar{f}_{pq}^{(3:72)} = 4G^{+}(\mathbf{r}_1, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_3, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1 - \tau_2)\phi_p^*(\mathrm{r}_5)\phi_q(\mathrm{r}_5),$$

$$\bar{f}_{pq}^{(3:73)} = -G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1 + \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_2),$$

$$\bar{f}_{pq}^{(3:74)} = G^{+}(\mathbf{r}_1, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1 - \tau_2)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_2),$$

$$\bar{f}_{pq}^{(3:75)} = 2G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1 + \tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_3, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_2),$$

$$\bar{f}_{pq}^{(3:76)} = -2G^{+}(\mathbf{r}_1, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1 - \tau_2)\phi_p^*(\mathrm{r}_1)\phi_q(\mathrm{r}_2),$$

$$\bar{f}_{pq}^{(3:77)} = -G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{-}(\mathbf{r}_3, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_2, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_4, -\tau_1)\phi_p^*(\mathrm{r}_3)\phi_q(\mathrm{r}_4),$$

$$\bar{f}_{pq}^{(3:78)} = G^{+}(\mathbf{r}_1, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^{*}(\mathrm{r}_3)\phi_q(\mathrm{r}_4),$$

$$\bar{f}_{pq}^{(3:79)} = 2G^{+}(\mathbf{r}_1, \mathbf{r}_5, \tau_1+\tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{-}(\mathbf{r}_3, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^{*}(\mathrm{r}_3)\phi_q(\mathrm{r}_4),$$

$$\bar{f}_{pq}^{(3:80)} = -2G^{+}(\mathbf{r}_1, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1+\tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_5, \tau_1)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1-\tau_2)G^{-}(\mathbf{r}_6, \mathbf{r}_2, -\tau_1-\tau_2)\phi_p^{*}(\mathrm{r}_3)\phi_q(\mathrm{r}_4),$$

$$\bar{f}_{pq}^{(3:81)} = G^{+}(\mathbf{r}_1, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_4, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_3, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1 - \tau_2)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_6),$$

$$\bar{f}_{pq}^{(3:82)} = -G^{+}(\mathbf{r}_1, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1 + \tau_2)G^{-}(\mathbf{r}_3, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_3, -\tau_1)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_6),$$

$$\bar{f}_{pq}^{(3:83)} = -2G^{+}(\mathbf{r}_1, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_4, \tau_2)G^{+}(\mathbf{r}_3, \mathbf{r}_6, \tau_1)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_1, -\tau_1 - \tau_2)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_6),$$

$$\bar{f}_{pq}^{(3:84)} = 2G^{+}(\mathbf{r}_1, \mathbf{r}_3, \tau_2)G^{+}(\mathbf{r}_2, \mathbf{r}_6, \tau_1 + \tau_2)G^{-}(\mathbf{r}_3, \mathbf{r}_1, -\tau_2)G^{-}(\mathbf{r}_4, \mathbf{r}_2, -\tau_2)G^{-}(\mathbf{r}_5, \mathbf{r}_4, -\tau_1)\phi_p^{*}(\mathrm{r}_5)\phi_q(\mathrm{r}_6).$$

2 Data for Table 4 of the Main Text

Table 1: The number of Monte Carlo steps, variances (in E_h^2), and total simulation times (in seconds) of the MC-GF3 calculations used in Table 4.

τ-Integration[a]	Molecule	Formula	n_{ele}[b]	N_{MC}[c]	Time	σ^2[d]
MC	Methane	CH_4	10	19393536	$1.393 \cdot 10^5$	$8.634 \cdot 10^{-1}$
MC	Propane	C_3H_8	26	1577984	$1.243 \cdot 10^4$	$5.536 \cdot 10^1$
MC	Benzene	C_6H_6	42	17617920	$1.400 \cdot 10^5$	$2.773 \cdot 10^2$
MC	Nonane	C_9H_{20}	74	1571840	$1.239 \cdot 10^4$	$5.189 \cdot 10^3$
MC	Decane	$C_{10}H_{22}$	82	1555456	$1.237 \cdot 10^4$	$6.280 \cdot 10^3$
MC	Pentacene	$C_{22}H_{14}$	146	17075200	$1.400 \cdot 10^5$	$8.417 \cdot 10^4$
Quadrature	Methane	CH_4	10	40960	$1.295 \cdot 10^5$	$4.442 \cdot 10^{-1}$
Quadrature	Propane	C_3H_8	26	35840	$1.175 \cdot 10^5$	$1.788 \cdot 10^1$
Quadrature	Benzene	C_6H_6	42	38912	$1.293 \cdot 10^5$	$8.336 \cdot 10^1$
Quadrature	Nonane	C_9H_{20}	74	56320	$1.804 \cdot 10^5$	$1.647 \cdot 10^3$
Quadrature	Decane	$C_{10}H_{22}$	82	71680	$2.351 \cdot 10^5$	$3.176 \cdot 10^3$
Quadrature	Pentacene	$C_{22}H_{14}$	146	56320	$1.879 \cdot 10^5$	$1.173 \cdot 10^4$

[a]'MC' stands for the direct Monte Carlo integration, while 'quadrature' a 21-point Gauss–Kronrod quadrature.
[b]The number of electrons.
[c]The number of Monte Carlo steps.
[d]Variance of the diagonal element of the third-order self-energy matrix associated with the HOMO.

3 Data for Figures 5 and 6 of the Main Text

Table 2: The variances (in E_{h}^2) of the MC-GF3/aug-cc-pVDZ calculations used in Figures 5 and 6.

Molecule	Formula	$n_{\mathrm{ele}}{}^a$	$N_{\mathrm{MC}}{}^b$	σ^2 (diagonal)^c	σ^2 (non-diagonal)^d
Methane	CH_4	10	6745088	$8.679 \cdot 10^{-1}$	$1.477 \cdot 10^{0}$
Acetylene	C_2H_2	14	6673408	$1.066 \cdot 10^{0}$	$1.417 \cdot 10^{0}$
Ethylene	C_2H_4	16	6650880	$4.200 \cdot 10^{0}$	$4.502 \cdot 10^{0}$
Ethane	C_2H_6	18	5740544	$1.442 \cdot 10^{1}$	$2.690 \cdot 10^{1}$
Butadiyne	C_4H_2	26	5728256	$1.088 \cdot 10^{1}$	$1.722 \cdot 10^{1}$
Propane	C_3H_8	26	5671936	$5.724 \cdot 10^{1}$	$6.691 \cdot 10^{1}$
Butadiene	C_4H_6	30	5680128	$6.190 \cdot 10^{1}$	$9.359 \cdot 10^{1}$
Butane	C_4H_{10}	34	5598208	$1.708 \cdot 10^{2}$	$2.052 \cdot 10^{2}$
Pentane	C_5H_{12}	42	5531648	$4.223 \cdot 10^{2}$	$5.330 \cdot 10^{2}$
Benzene	C_6H_6	42	5657600	$2.570 \cdot 10^{2}$	$8.888 \cdot 10^{3}$
Hexatriene	C_6H_8	44	5564416	$4.189 \cdot 10^{2}$	$1.076 \cdot 10^{3}$
Hexane	C_6H_{14}	50	6178816	$1.137 \cdot 10^{3}$	$2.096 \cdot 10^{3}$
Heptane	C_7H_{16}	58	6102016	$1.796 \cdot 10^{3}$	$3.306 \cdot 10^{3}$
Octane	C_8H_{18}	66	5965824	$3.173 \cdot 10^{3}$	$1.208 \cdot 10^{4}$
Napthalene	$C_{10}H_8$	68	6147072	$2.076 \cdot 10^{3}$	$7.139 \cdot 10^{3}$
Nonane	C_9H_{20}	74	5856256	$5.153 \cdot 10^{3}$	$2.692 \cdot 10^{4}$
Decane	$C_{10}H_{22}$	82	5769216	$9.502 \cdot 10^{3}$	$4.667 \cdot 10^{4}$
Anthracene	$C_{14}H_{10}$	94	5892096	$9.582 \cdot 10^{3}$	$7.081 \cdot 10^{4}$
Naphthacene	$C_{18}H_{12}$	120	5569536	$2.501 \cdot 10^{4}$	$3.293 \cdot 10^{5}$
Pentacene	$C_{22}H_{14}$	146	5328896	$1.114 \cdot 10^{5}$	$7.458 \cdot 10^{6}$

[a]The number of electrons.

[b]The number of Monte Carlo steps.

[c]Variance of the binding energy of the HOMO within the diagonal, frequency-independent approximation.

[d]Variance of the binding energy of the HOMO within the frequency-independent approximation.

Table 3: The same as Table 2, but with the aug-cc-pVTZ basis set.

Molecule	Formula	n_{ele} [a]	N_{MC} [b]	σ^2 (diagonal) [c]	σ^2 (non-diagonal) [d]
Methane	CH_4	10	5783552	$8.371 \cdot 10^0$	$2.230 \cdot 10^1$
Acetylene	C_2H_2	14	7341056	$1.061 \cdot 10^1$	$1.406 \cdot 10^1$
Ethylene	C_2H_4	16	7264256	$4.010 \cdot 10^1$	$4.812 \cdot 10^1$
Ethane	C_2H_6	18	7151616	$1.006 \cdot 10^2$	$1.224 \cdot 10^2$
Butadiyne	C_4H_2	26	7207936	$6.601 \cdot 10^1$	$3.517 \cdot 10^2$
Propane	C_3H_8	26	6890496	$1.320 \cdot 10^3$	$2.871 \cdot 10^3$
Butadiene	C_4H_6	30	6868992	$6.291 \cdot 10^2$	$1.055 \cdot 10^3$
Butane	C_4H_{10}	34	6649856	$1.724 \cdot 10^3$	$3.744 \cdot 10^3$
n-Pentane	C_5H_{12}	42	6409216	$7.221 \cdot 10^3$	$1.322 \cdot 10^4$
Benzene	C_6H_6	42	5254144	$2.328 \cdot 10^3$	$6.264 \cdot 10^3$
Hexatriene	C_6H_8	44	6598656	$2.745 \cdot 10^3$	$7.579 \cdot 10^3$
Hexane	C_6H_{14}	50	6907904	$9.220 \cdot 10^3$	$1.126 \cdot 10^5$
n-Heptane	C_7H_{16}	58	6601728	$1.434 \cdot 10^4$	$6.014 \cdot 10^4$
n-Octane	C_8H_{18}	66	6304768	$2.988 \cdot 10^4$	$1.753 \cdot 10^5$
Napthalene	$C_{10}H_8$	68	6832128	$1.796 \cdot 10^4$	$1.421 \cdot 10^5$
Nonane	C_9H_{20}	74	6037504	$4.470 \cdot 10^4$	$2.403 \cdot 10^5$
n-Decane	$C_{10}H_{22}$	82	5585920	$5.422 \cdot 10^4$	$6.886 \cdot 10^5$
Anthracene	$C_{14}H_{10}$	94	6159360	$9.449 \cdot 10^4$	$1.553 \cdot 10^6$
Naphthacene	$C_{18}H_{12}$	120	5321728	$2.879 \cdot 10^5$	$1.048 \cdot 10^7$
Pentacene	$C_{22}H_{14}$	146	3533824	$1.147 \cdot 10^6$	$6.014 \cdot 10^7$

[a] The number of electrons.

[b] The number of Monte Carlo steps.

[c] Variance of the binding energy of the HOMO within the diagonal, frequency-independent approximation.

[d] Variance of the binding energy of the HOMO within the frequency-independent approximation.