

Supplemental Material for "Exchange-correlation energy from Green's functions"

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Below we detail various results for the two-site Hubbard model (Hubbard dimer). Our results for the dimer include: the exact tight-binding and interacting dimer Green's functions, one-shot GW self-energy and Green's function beginning from Hartree-Fock. We report exact and approximate G_{xc} (with SP and MP decompositions) for several dimer parameters. Additionally, we detail our self-consistent GW method, and show how it compares with results reported in the literature. Lastly, we report G_{xc} for the Coulombically interacting Hooke's atom system.

1. TWO-SITE TIGHT-BINDING GF

For any two-site tight-binding model,

$$\hat{H}_S = -t \sum_{\sigma} (\hat{c}_{1\sigma}^{\dagger} \hat{c}_{2\sigma} + \text{h.c.}) + \sum_{j=1}^2 v_{s,j} \hat{n}_j, \quad (1)$$

with hopping t and on-site potential $v_{s,j}$, the ground-state time-ordered GF has an expression in terms of its site-occupations

$$G_S(\omega) = \frac{\rho_S(n_1, n_2)}{\omega - \epsilon_+ - i\delta} + \frac{\bar{\rho}_S(n_1, n_2)}{\omega - \epsilon_- + i\delta}. \quad (2)$$

Here the HOMO/LUMO eigenvalues ϵ_{\pm} are exactly

$$\epsilon_{\pm} = (\bar{v}_S - \mu_S) \mp t_S, \quad (3)$$

where μ_S is the KS chemical potential. We define the average on-site potential $\bar{v}_S = (v_{s,2} + v_{s,1})/2$, the rescaled hopping parameter $t_S = \sqrt{t^2 + (\Delta v_S/2)^2}$, and the on-site potential difference $\Delta v_S = v_{s,2} - v_{s,1}$. The amplitude matrices are function(al)s of the density, the first being the KS one-body reduced density (RDM)

$$\rho_S(n_1, n_2) = \frac{1}{2} \begin{pmatrix} n_1 & \sqrt{n_1 n_2} \\ \sqrt{n_1 n_2} & n_2 \end{pmatrix}, \quad (4)$$

and $\bar{\rho}_S(n_1, n_2) = \sigma_y \rho_S(n_1, n_2) \sigma_y$, using the Pauli σ_y matrix.

The KS kinetic energy is

$$T_S(n_1, n_2) = -2t\sqrt{n_1 n_2}, \quad (5)$$

and for $N = 2$ groundstate,

$$-2 \frac{dT_S(n_1, n_2)}{d(\Delta n)} = \Delta v_S = \frac{-2t\Delta n}{\sqrt{4 - \Delta n^2}}. \quad (6)$$

The ionization potential theorem (IPT) requires $\epsilon_+ = -I$, minus the ionization potential, so

$$\bar{v}_S = \bar{v} - I + t_S, \quad (7)$$

where we have absorbed the exact and KS chemical potentials into \bar{v} and \bar{v}_S , respectively. For both exact and approximate KS potentials, we fix the constant such that the IPT is satisfied.

2. EXACT GF OF HUBBARD DIMER

The groundstate for the dimer can be found by directly diagonalizing the Hamiltonian in the two-particle singlet subspace. Defining $\bar{v} = (v_1 + v_2)/2$:

$$H = \begin{pmatrix} U + 2\bar{v} - \Delta v & -t & -t & 0 \\ -t & 2\bar{v} & 0 & -t \\ -t & 0 & 2\bar{v} & -t \\ 0 & -t & -t & U + 2\bar{v} + \Delta v \end{pmatrix}, \quad (8)$$

where the two-electron groundstate is non-magnetic and has the generic form [1]

$$|\Psi_0\rangle = \alpha(t, U, \Delta v) |1 \uparrow 1 \downarrow\rangle + \bar{\alpha}(t, U, \Delta v) |2 \uparrow 2 \downarrow\rangle \\ + \beta(t, U, \Delta v) (|1 \uparrow 2 \downarrow\rangle + |2 \uparrow 1 \downarrow\rangle), \quad (9)$$

where the amplitudes depend on the system parameters and $\bar{\alpha}(t, U, \Delta v) = \alpha(t, U, -\Delta v)$ [1].

In the Lehmann representation,

$$\rho_{ij}^{\text{SP/MP}} = \langle \Psi_0 | \hat{c}_j^{\dagger} | \psi_{0,1}^{(1)} \rangle \langle \psi_{0,1}^{(1)} | \hat{c}_i | \Psi_0 \rangle, \quad (10)$$

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where $|\psi_{0,1}^{(1)}\rangle$ are the ground-state and only excited state of the one-electron space. The spectral weights are thus,

$$\rho^{\text{SP/MP}} = M_0 \mp (M_1 - M_2), \quad (11)$$

with matrices defined via the wave-function coefficients:

$$M_0 = \frac{1}{2} \begin{pmatrix} \alpha^2 + \beta^2 & \beta(\alpha + \bar{\alpha}) \\ \beta(\alpha + \bar{\alpha}) & \bar{\alpha}^2 + \beta^2 \end{pmatrix}, \quad (12)$$

$$M_1 = \frac{t}{2\bar{t}} \begin{pmatrix} (\beta^2 - \alpha^2) \frac{\Delta v}{2t} & \beta(\bar{\alpha} - \alpha) \frac{\Delta v}{2t} \\ \beta(\bar{\alpha} - \alpha) \frac{\Delta v}{2t} & (\bar{\alpha}^2 - \beta^2) \frac{\Delta v}{2t} \end{pmatrix}, \quad (13)$$

$$M_2 = \frac{t}{2\bar{t}} \begin{pmatrix} 2\alpha\beta & (\beta^2 + \alpha\bar{\alpha}) \\ (\beta^2 + \alpha\bar{\alpha}) & 2\bar{\alpha}\beta \end{pmatrix}, \quad (14)$$

where the rescaled hopping is $\bar{t} = \sqrt{t^2 + (\Delta v/2)^2}$.

The spectral weights sum to the interacting density matrix,

$$\rho = \rho^{\text{SP}} + \rho^{\text{MP}}, \quad (15)$$

and we define the separate contributions to the density,

$$n_i^{\text{SP/MP}} = \rho_{ii}^{\text{SP/MP}}, \quad (16)$$

where the subscripts 0, 1 in Eq. (10) denote SP or MP and i denotes the site. Using the non-interacting functional $\rho_s(n_1, n_2)$ we express the $\rho^{\text{SP/MP}}$ matrices as functionals of the single-particle and many-particle occupations,

$$\rho^{\text{SP}} = \rho_s(n_1^{\text{SP}}, n_2^{\text{SP}}), \quad \rho^{\text{MP}} = \bar{\rho}_s(n_2^{\text{MP}}, n_1^{\text{MP}}), \quad (17)$$

and by extension:

$$G(\omega) = \frac{\rho^{\text{SP}}}{\omega - \omega^{\text{SP}} - i\delta} + \frac{\rho^{\text{MP}}}{\omega - \omega^{\text{MP}} - i\delta} + \frac{\bar{\rho}^{\text{SP}}}{\omega + \omega^{\text{SP}} + i\delta} + \frac{\bar{\rho}^{\text{MP}}}{\omega + \omega^{\text{MP}} + i\delta}, \quad (18)$$

with SP and MP pole locations

$$\omega^{\text{SP/MP}} = E_0^{(2)} \pm \bar{t} - \frac{U}{2}, \quad (19)$$

where $E_0^{(2)}$ is the energy of the two-electron groundstate.

In this model, the only SP peak is identical to minus the ionization potential $\omega^{\text{SP}} = -I = E_0^{(2)} - E_0^{(1)}$, where $E_0^{(1)}$ is the one-electron ground-state energy. We omit all spin coordinates, as the exact GF is diagonal in spin for a non-magnetic groundstate. Summing over spins introduces a factor of 2, our results this far are not spin-summed.

Finally, we write SP contribution to the total two-electron ground-state energy,

$$E_0^{\text{SP}} = \frac{1}{2} \left(\omega^{\text{SP}} f^{\text{SP}} + T^{\text{SP}} + \frac{\Delta v \Delta n^{\text{SP}}}{2} \right), \quad (20)$$

where $f^{\text{SP}} = \text{tr}\{\rho^{\text{SP}}\}$ and $\Delta n^{\text{SP}} = n_2^{\text{SP}} - n_1^{\text{SP}}$. The MP contribution is defined analogously; together they sum to the total energy,

$$E_0^{(2)} = \frac{1}{2} \left(\omega^{\text{SP}} f^{\text{SP}} + \omega^{\text{MP}} f^{\text{MP}} + T + \frac{\Delta v \Delta n}{2} \right), \quad (21)$$

where the full interacting kinetic energy is the sum

$$T = T^{\text{SP}} + T^{\text{MP}}. \quad (22)$$

3. ONE-SHOT GW DIMER SELF-ENERGY

To produce the GW expressions we define the RPA polarization, of any G :

$$P_{ij\sigma}^{\text{RPA}}(\omega) = -i \int \frac{d\omega'}{2\pi} G_{ij}(\omega') G_{ij}(\omega + \omega'), \quad (23)$$

which has a form analogous to the symmetric case. Considering a generic two-site tight-binding GF, as in App. 1,

$$P_{s,ij\sigma}^{\text{RPA}}(\omega) = \frac{n_1 n_2}{4} \left\{ \frac{(-1)^{i+j}}{\omega - 2t_s + i\delta} - \frac{(-1)^{i+j}}{\omega + 2t_s - i\delta} \right\}, \quad (24)$$

with screened interaction,

$$W_{s,ij}(\omega) = U\delta_{ij} + \frac{(-1)^{i+j} 2Ut_s n_1 n_2}{(\omega - 2t_{\text{eff}} + i\delta)(\omega + 2t_{\text{eff}} - i\delta)}, \quad (25)$$

where $t_{\text{eff}} = 2\sqrt{t_s^2 + Ut_s n_1 n_2}$. Conveniently, the asymmetric screened interaction can be found from a simple rescaling of the inverse dielectric function $W_{ij}(\omega)/U$ computed by Romaniello and co-authors [2, 3] for the symmetric case: $t \rightarrow t_s$ and $U \rightarrow Un_1 n_2$.

Finally we compute the one-shot GW self-energy according to,

$$\Sigma_{ij}^{\text{GW}}(\omega) = v_{H,ij} + i \int \frac{d\omega'}{2\pi} G_{s,ij}(\omega) W_{s,ij}(\omega + \omega'), \quad (26)$$

which yields,

$$\Sigma_{ij}^{\text{GW}}(\omega) = \frac{Un_i \delta_{ij}}{2} + (-1)^{i+j} \frac{U^2 t_s n_1 n_2}{t_{\text{eff}}} \times \left\{ \frac{\rho_s(n_1, n_2)_{ij}}{\omega - (\bar{v}_s - t_1) - i\delta} + \frac{\bar{\rho}_s(n_1, n_2)_{ij}}{\omega - (\bar{v}_s + t_1) + i\delta} \right\}, \quad (27)$$

where $t_1 = t_s + t_{\text{eff}}$ and all quantities depend on $n_{1,2}$ explicitly or through Δv_s . If the exact site-occupations and KS potential is used, then the self-energy is the one-shot Kohn-Sham self-energy. It can be understood as the one-shot self-energy from the best possible DFT calculation for the dimer. For the case of a one-shot Hartree-Fock calculation we take $\bar{v}_s \rightarrow U/2$, $\Delta n \rightarrow \Delta n^{\text{HF}}$, $\Delta v_s \rightarrow \Delta v^{\text{HF}} = \Delta v + U\Delta n^{\text{HF}}/2$, the corresponding HF parameters [1].

4. ONE-SHOT GW DIMER GF

The amplitudes of the one-shot GW Green's function can be found directly from the Dyson equation,

$$G^{GW} = [G_0^{-1} - \Sigma^{GW}]^{-1}, \quad (28)$$

where G_0 is asymmetric tight-binding Green's function, which can be found by evaluating G_s at the non-interacting site-occupations, i.e. $G_0 = G_s(\Delta n = \Delta v/\bar{t}(\Delta v))$ and Σ^{GW} is given by Eq. (27). We choose $\bar{v} = 0$ for convenience.

Formally we express the Green's function as a sum of matrices,

$$G^{GW}(\omega) = \frac{X^{SP}}{\omega - \omega^{SP} - i\delta} + \frac{X^{MP}}{\omega - \omega^{MP} - i\delta} + \frac{\bar{X}^{SP}}{\omega + \omega^{SP} + i\delta} + \frac{\bar{X}^{MP}}{\omega + \omega^{MP} + i\delta}, \quad (29)$$

where $\bar{X}^{SP/MP} = \sigma_y X^{SP/MP} \sigma_y$, and $X^{SP/MP}$ has a cumbersome expression that can be computed in closed form. Here we only report G_{11}^{GW} and G_{12}^{GW} because entries of $X^{SP/MP}$ can be constructed explicitly from only these elements. For the moment we ignore the time-ordering in the pole structure,

$$G_{11}^{GW}(\omega) = \frac{(\omega - \frac{\Delta v^{HF}}{6})^3 - a(\omega - \frac{\Delta v^{HF}}{6}) + b}{(\omega^2 - (\omega^{SP})^2)(\omega^2 - (\omega^{MP})^2)}, \quad (30)$$

with

$$\Delta v^{HF} = \Delta v + \frac{U\Delta n^{HF}}{2}, \quad (31)$$

where the HF density is the solution of $\Delta v_s(\Delta n) = \Delta v + U\Delta n/2$, the HF problem. The associated coefficients

$$a = A + t_1^2 + \frac{1}{12}(\Delta v^{HF})^2, \quad (32)$$

$$b = \frac{At_1\Delta n^{HF}}{2} + \left(t_1^2 - \frac{A}{2}\right)\frac{\Delta v^{HF}}{3} - \frac{1}{4}\left(\frac{\Delta v^{HF}}{3}\right)^3, \quad (33)$$

are all functions of the HF density; either explicitly or implicitly through Δv^{HF} . Here $t_1 = t^{HF} + t_{\text{eff}}$, with $t^{HF} = t\sqrt{1 + (\Delta v^{HF}/2t)^2}$, $t_{\text{eff}} = 2\sqrt{(t^{HF})^2 + Ut^{HF}n_1^{HF}n_2^{HF}}$, and $A = U^2n_1^{HF}n_2^{HF}t^{HF}/t_{\text{eff}}$.

The exact pole locations can be expressed in terms of these parameters,

$$\begin{aligned} (\omega^{SP/MP})^2 &= A + \frac{1}{2} \left[t^2 + t_1^2 + \left(\frac{\Delta v^{HF}}{2} \right)^2 \right]^2 \\ &\mp \left[\left(\frac{t^2 - t_1^2}{2} + \frac{1}{2} \left(\frac{\Delta v^{HF}}{2} \right)^2 \right)^2 \right. \\ &\quad \left. + A \left((t^2 + t_1^2) + \left(\frac{\Delta v^{HF}}{2} \right)^2 \right) \right. \\ &\quad \left. - \frac{t_1}{2} \left(2t\sqrt{4 - (\Delta n^{HF})^2} + \Delta v^{HF} \Delta n \right) \right]^{1/2}, \quad (34) \end{aligned}$$

and thus, the poles are functions of the HF density. Since the poles are clearly identifiable, the associated SP and MP spectral weights can be determined via evaluation of the residues. For the SP matrix,

$$X_{11}^{SP} = \frac{(\omega^{SP} - \frac{\Delta v^{HF}}{6})^3 - a(\omega^{SP} - \frac{\Delta v^{HF}}{6}) + b}{2\omega^{SP}((\omega^{SP})^2 - (\omega^{MP})^2)}, \quad (35)$$

and the 22 element is found from simple substitution:

$$X_{22}^{SP} = \frac{(\omega^{SP} + \frac{\Delta v^{HF}}{6})^3 - a(\omega^{SP} + \frac{\Delta v^{HF}}{6}) - b}{2\omega^{SP}((\omega^{SP})^2 - (\omega^{MP})^2)}, \quad (36)$$

which is equivalent to $\Delta v^{HF} \rightarrow -\Delta v^{HF}$. Conveniently, the many-particle counterparts are analogous:

$$X_{11}^{MP} = \frac{(\omega^{MP} + \frac{\Delta v^{HF}}{6})^3 - a(\omega^{MP} + \frac{\Delta v^{HF}}{6}) - b}{2\omega^{MP}((\omega^{MP})^2 - (\omega^{SP})^2)}, \quad (37)$$

$$X_{22}^{MP} = \frac{(\omega^{MP} - \frac{\Delta v^{HF}}{6})^3 - a(\omega^{MP} - \frac{\Delta v^{HF}}{6}) + b}{2\omega^{MP}((\omega^{MP})^2 - (\omega^{SP})^2)}. \quad (38)$$

To produce the off-diagonal elements of X_{12}^{SP} we use

$$G_{12}^{GW}(\omega) = \frac{-(t\omega^2 - c^2)}{(\omega^2 - (\omega^{SP})^2)(\omega^2 - (\omega^{MP})^2)}, \quad (39)$$

where

$$c = \sqrt{\frac{t_1}{2} \left(2t_1t + A\sqrt{4 - (\Delta n^{HF})^2} \right)}, \quad (40)$$

and after computing the residue,

$$X_{12}^{SP} = X_{21}^{SP} = \frac{-(t(\omega^{SP})^2 - c^2)}{2\omega^{SP}((\omega^{SP})^2 - (\omega^{MP})^2)}, \quad (41)$$

where the MP contribution is exactly $\omega^{SP} \rightarrow \omega^{MP}$.

From $X^{SP/MP}$ we define the approximate SP and MP occupations $\tilde{n}_i^{SP/MP} = X_{ii}^{SP/MP}$. The KS expressions can be produced similarly, but they are slightly more complicated. Here we only report the one-shot GF beginning from a HF calculation. In the KS case, the constant \bar{v}_s is designed to guarantee that the IP theorem is satisfied; this constant alters the locations of the poles and the spectral weights in a more complicated way.

5. HUBBARD DIMER ONE-SHOT AND SELF-CONSISTENT GW TABLES

We report additional Hubbard dimer G_{xc} and associated spectral decompositions of the correlation energy. For the symmetric dimer ($\Delta v = 0$) each variant of GW recovers the correct site occupations ($\Delta n = 0$). For two electrons with spin-singlet ground-state, this results in exactly reproducing the Hartree and exchange energies. This is because $U = -E_x/2$ for this case. As a result, the errors between the

Exact				one-shot			self-consistent		
U	G_{XC}	G_{XC}^{SPI}	G_{XC}^{MPI}	G_{XC}	G_{XC}^{SPI}	G_{XC}^{MPI}	G_{XC}	G_{XC}^{SPI}	G_{XC}^{MPI}
0.25	0	1.93	-1.93	-1.14	2.54	-3.68	-15.4	2.58	-18.
0.5	0	7.46	-7.46	-6.01	7.25	-13.3	-27.4	7.65	-35.
1	0	26.4	-26.4	-25.4	17.3	-42.7	-46.9	19.8	-66.7
2	0	73.2	-73.2	-84.5	34.2	-119.	-106.	44.5	-151.
4	0	138.	-138.	-225.	56.4	-282.	-310.	89.2	-400.

Exact				one-shot			self-consistent		
U	E_C	E_C^{SPI}	E_C^{MPI}	E_C	E_C^{SPI}	E_C^{MPI}	E_C	E_C^{SPI}	E_C^{MPI}
0.25	-7.78	-5.82	-1.96	-12.6	-8.81	-3.74	-26.2	-8.17	-18.
0.5	-30.8	-22.9	-7.92	-42.1	-28.3	-13.8	-58.7	-23.1	-35.5
1	-118.	-85.4	-32.6	-127.	-81.	-46.3	-121.	-51.8	-69.7
2	-414.	-280.	-134.	-341.	-204.	-136.	-248.	-84.7	-163.
4	-1236.	-756.	-480	-807.	-460.	-347.	-512.	-76.6	-436.

TABLE I: Decompositions for G_{XC} (top) and E_C (bottom) for the exact and approximate symmetric dimer with $t = 1/2$ and $\Delta v = 0$. For the self-consistent result we report the sum of the MP contributions. All energies in milliHartrees (mH).

exact and approximate G_{XC} (and E_{XC}) are entirely due to correlation effects. In the asymmetric case, reported in the main text, the site-occupations are not correctly reproduced by the approximate methods, and thus they introduce errors to the Hartree and exchange energies.

In Table I we report G_{XC} and its decompositions with the IP contribution removed. We choose this partition because the magnitudes of the SP and MP contributions are reduced by a factor of 2.

The symmetric dimer has $E_{XC} = \langle v_{XC} \rangle / 2$ and so $G_{XC} = 0$, this implies,

$$T_C = (\omega^{SP} - \omega^{MP}) f^{MP}, \quad (42)$$

where $\omega^{SP} - \omega^{MP} = -2E_0(1)$ and f^{MP} is the MP occupations. One-shot and self-consistent GW will never be able to produce this result, as they both predict an interaction dependent energy for the one-electron space ($\omega^{SP} - \omega^{MP}$ changes with U), i.e., they have self-interaction error.

6. IMPLEMENTATION OF SELF-CONSISTENT GW

Self-consistent GW results for the symmetric Hubbard dimer have been reported in Refs [4] and [5]. Fully self-consistent results on a frequency and time grid, without a pole purging scheme, are computationally non-trivial. Even for a two-site model, to capture the emerging "satellite series" requires many points to accurately resolve the details of the spectrum [5].

We instead report a finite pole version of self-consistent GW . At each iteration we retain an explicit two-pole form

of the self-energy. This ensures a six-pole form of the GW Green's function. Purging the poles allows us to exploit the meromorphic representations of all quantities, avoiding the need for frequency grids. For increasing U values we find systematic deviations from the results of Mejuto-Zaera and Vlček, but we limit our analysis to small U values, where GW can be accurate and we find good agreement. In Fig. 1 we report the deviation of the single-particle and the first prominent many-particle pole position, we also include the relevant values from Ref[5], and the one-shot results for the symmetric dimer. The deviation between our results with Mejuto-Zaera and Vlček are much smaller in magnitude than the errors between the one-shot result and our respective flavors of GW . Thus, for small and moderate U , our dimer results should be consistent with GW results of Ref. [5]. For large values of U , GW is not expected to perform well, but we report the values from our finite pole scheme.

We have tested several pole truncation schemes and find that keeping a two-pole structure for W and Σ^{GW} produces converged total energies quickly for the full range of U values computed. To aid convergence, for cases with moderate to strong correlation we generated the n th GF according to: $G^{(n)} = \gamma G^{(n-1)} + (1 - \gamma)G^{(n-2)}$, with $\gamma = 0.67$. Our one-shot results are identical to Ref [2] in the symmetric limit $\Delta v \rightarrow 0$.

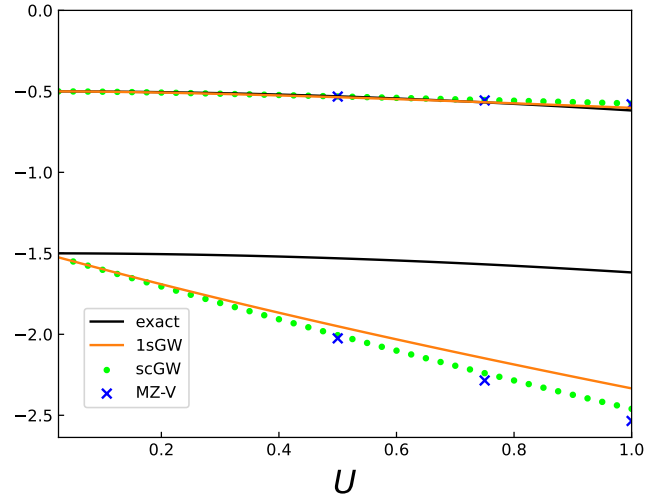


FIG. 1: Exact and approximate SP and MP energies as a function of interaction U . The upper lines are the SP energies while the lower are MP energies. We label the pole locations of [5] as "MZ-V" in blue.

7. G_{XC} FOR COULOMBICALLY INTERACTING SYSTEMS

Huang and Umrigar report exact and KS energies for two-electron ions with nuclear charge Z and the Hooke's atom system, which consists of two Coulombically interacting

electrons confined in a harmonic oscillator with strength ω [6]. Using these energies, we produce G_{XC} for a range of moderately and weakly correlated system parameters for Coulombically interacting electrons.

For the case of a two-electron spin-singlet groundstate, the exchange energy of the KS system is exactly minus half the Hartree energy. The multiplicative exchange potential v_{x} is a functional derivative of the exchange energy, and thus $v_{\text{x}} = -v_{\text{H}}/2$. While the full exchange self-energy evaluated with KS GF,

$$\Sigma_{\text{x}}[G_{\text{s}}](\mathbf{x}, \mathbf{x}') = -\frac{\rho_{\text{s}}(\mathbf{x}, \mathbf{x}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (43)$$

yields the KS exact exchange energy when it is traced with G_{s} ,

$$E_{\text{x}} = \frac{1}{2} \text{Tr}\{\Sigma_{\text{x}}[G_{\text{s}}]G_{\text{s}}\} = -U/2, \quad (44)$$

and thus

$$G_{\text{x}} = \text{Tr}\{(\Sigma_{\text{x}}[G_{\text{s}}] - v_{\text{x}}[n])G_{\text{s}}\} = 0. \quad (45)$$

Consequently, our tables contain only the correlation contribution G_{C} . Table II of the main text and Table II both show that $G_{\text{XC}}, G_{\text{C}}$ for this case, is generally smaller in magnitude than E_{XC} , its most analogous counter-part. We report the two-electron ion results in the main text.

ω	E_{XC}	$\langle v_{\text{XC}} \rangle / 2$	E_{C}	T_{C}	G_{XC}
0.1	-0.2402	-0.2311	-0.02924	0.01643	-0.009139
1	-0.7881	-0.7757	-0.04139	0.03393	-0.0124
4	-1.587	-1.574	-0.04529	0.04097	-0.01326
10	-2.515	-2.502	-0.04685	0.04397	-0.01357
100	-7.972	-7.958	-0.04878	0.04781	-0.01393
400	-15.95	-15.94	-0.04924	0.04875	-0.01402
1000	-25.22	-25.21	-0.04941	0.0491	-0.01404

TABLE II: Various X and C energies for the Hooke's atom system reported in Ref[6]. The weakly correlated limit is approached as well strength $\omega \rightarrow \infty$.

Table II shows the results for the Hooke's atom system. We find similar trends to the two-electron ion case, in the approach to the weakly-correlated limit ($\omega \rightarrow \infty$) G_{XC} converges to a finite value that is smaller in magnitude than $E_{\text{C}} \approx -T_{\text{C}}$ in this limit.

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