

C₆ dispersion coefficients from reduced dipole pseudospectra

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Abstract A recently proposed interpolation technique for FDPs is extended to cover static pseudospectra of monomers as well. Reduced 4-term dipole pseudospectra are obtained for the ground states of H, He, H₂⁺, H₂, LiH, BeH₂, BH, giving dispersion constants from which highly accurate C₆ dispersion coefficients for all homo- and hetero-dimers are obtained by use of the generalized London formula.

1 Introduction

The uniform tabulation of conveniently reduced dipole pseudospectra is of great interest for the accurate evaluation of the leading term of the long-range dispersion interaction between atoms and molecules [1].

Dispersion coefficients can be evaluated either in terms of pseudospectral decomposition of static polarizabilities (SPs) using second-order Rayleigh–Schrodinger (RS) perturbation theory or in terms of the frequency spectrum of dynamic polarizabilities (FDPs) at imaginary frequencies using time-dependent variation-perturbation methods [1–3]. In the first case, the dispersion constants C_{ab}, the basic quantum-mechanical ingredient entering the calculation of dispersion coefficients, are then given directly in terms of a suitable generalization of the London formula [1], while in the second case some numerical quadrature of frequency-dependent integrals of the Casimir–Polder type [4] is

required. In both cases, a typical *two-body* quantity is expressed exactly in terms of *one-body* second-order properties related to the electric polarizabilities of the monomers. Recently, alternative variational CI techniques for the accurate two-body computation of dispersion constants have been proposed [5].

Accurate static dipole pseudospectra obtained by us previously for H [6], He [7], H₂⁺ [8], H₂ [9,10], and, more recently, Full-CI FDPs for LiH [11], BeH₂ [12], BH [13] from a joint work with the Physical Chemistry Department of the University of Bologna, allowed to obtain the C₆ dispersion coefficients for the homodimers. In this paper, in the context of the one-body approach, a recently proposed interpolation technique for FDPs [14] is extended to cover static pseudospectra of monomers as well. A reduced 4-term interpolation is found to be adequate in the accurate reproduction of sensibly more extended pseudospectra, giving dipole dispersion constants from which C₆ dispersion coefficients for homo- and heterodimers of all above atomic and molecular systems were obtained to a high level of accuracy in a uniform way.

2 Method

C₆ dispersion coefficients can be evaluated in terms of the symmetry combinations of elementary dipole dispersion constants C_{ab} [1,9,15]. All the dispersion constants whose values are reported in this paper were obtained through application of the one-centre technique suggested by Casimir and Polder [4], which requires an integration over the product of the two dynamic (i.e. frequency-dependent) multipole polarizabilities at imaginary frequency, $\alpha_a^A(iu)$ and $\alpha_b^B(iu)$, of

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the individual interacting systems. The integration path covers the whole range of the frequency u :

$$C_{ab} = \frac{1}{2\pi} \int_0^{\infty} du \alpha_a^A(iu) \alpha_b^B(iu). \quad (1)$$

The FDPs needed to get the dispersion constants were represented through our recently proposed interpolating expression [14]:

$$\alpha(iu) = \sum_{i=1}^n \frac{\sigma_i}{\tau_i + u^2} \quad (n = 1, 2, \dots) \quad (2)$$

Once the number n of terms to be included in the interpolation procedure has been fixed, the involved $2n$ parameters τ_i and σ_i are univocally obtained by imposing the exact intercept of $2n$ values $\{\alpha(iu_1), \alpha(iu_2), \dots, \alpha(iu_{2n})\}$ available for the interpolated polarizability $\alpha(iu)$ at $2n$ known frequencies u_1, u_2, \dots, u_{2n} .

A small set of interpolating parameters ($n \leq 4$) is usually sufficient to yield high accuracy in the interpolation, especially when the $2n$ frequencies implying evaluations performed on the multipole polarizability are selected using the following efficient formula:

$$u_p = \frac{p-1}{2n+1-p} \quad (p = 1, 2, \dots, 2n) \quad (3)$$

This formula gives values which are expressed in atomic units (like all the other numerical quantities presented in this work) and whose mutual interspacing progressively increases.

When n -term interpolative representations are built for the FDPs of the interacting atoms or molecules, the related dispersion constants can be obtained in a very simple way by treating analytically the Casimir–Polder's integral:

$$\begin{aligned} C_{ab} &= \frac{1}{2\pi} \int_0^{\infty} du \alpha_a^A(iu) \alpha_b^B(iu) \\ &= \frac{1}{4} \sum_{i=1}^n \sum_{j=1}^n \frac{\sigma_i^a \sigma_j^b}{\sqrt{\tau_i^a \tau_j^b} (\sqrt{\tau_i^a} + \sqrt{\tau_j^b})}. \end{aligned} \quad (4)$$

It is now possible to extend the interpolation technique to cover the case of *static* polarizabilities as well, simply by taking into account the full equivalence between generalized London formula and Casimir–Polder formula for the dispersion constants C_{ab} [1].

In fact, use of the well-known integral transform:

$$\begin{aligned} \frac{1}{\varepsilon_i + \varepsilon_j} &= \frac{2}{\pi} \int_0^{\infty} du \frac{\varepsilon_i}{\varepsilon_i^2 + u^2} \frac{\varepsilon_j}{\varepsilon_j^2 + u^2} \\ \frac{\varepsilon_i \varepsilon_j}{\varepsilon_i + \varepsilon_j} &= \frac{2}{\pi} \int_0^{\infty} du \frac{\varepsilon_i^2}{\varepsilon_i^2 + u^2} \frac{\varepsilon_j^2}{\varepsilon_j^2 + u^2} \end{aligned} \quad (5)$$

allows to write for the N -term generalized London formula:

$$\begin{aligned} C_{ab} &= \frac{1}{4} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j \frac{\varepsilon_i \varepsilon_j}{\varepsilon_i + \varepsilon_j} \\ &= \frac{1}{4} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j \frac{2}{\pi} \int_0^{\infty} du \frac{\varepsilon_i^2}{\varepsilon_i^2 + u^2} \frac{\varepsilon_j^2}{\varepsilon_j^2 + u^2}. \end{aligned} \quad (6)$$

Now, if:

$$\alpha_a^A(iu) = \sum_{i=1}^N \frac{\alpha_i \varepsilon_i^2}{\varepsilon_i^2 + u^2}, \quad \alpha_b^B(iu) = \sum_{j=1}^N \frac{\alpha_j \varepsilon_j^2}{\varepsilon_j^2 + u^2} \quad (7)$$

are the frequency-dependent polarizabilities of A and B, giving the pseudospectral decomposition of the polarizabilities in the static limit ($u = 0$):

$$\alpha_a^A(0) = \sum_{i=1}^N \alpha_i, \quad \alpha_b^B(0) = \sum_{j=1}^N \alpha_j \quad (8)$$

we immediately obtain from Eq. (6) upon substitution:

$$\begin{aligned} C_{ab} &= \frac{1}{2\pi} \int_0^{\infty} du \left(\sum_{i=1}^N \frac{\alpha_i \varepsilon_i^2}{\varepsilon_i^2 + u^2} \right) \left(\sum_{j=1}^N \frac{\alpha_j \varepsilon_j^2}{\varepsilon_j^2 + u^2} \right) \\ &= \frac{1}{2\pi} \int_0^{\infty} du \alpha_a^A(iu) \alpha_b^B(iu) \end{aligned} \quad (9)$$

which is the Casimir–Polder formula for the dispersion constant specified by the labels a, b .

It is possible (i) to transform to FDPs all previously existing static pseudospectral data on polarizabilities [6–8, 10], and (ii) use next the interpolation procedure [14] to get the appropriately reduced pseudospectra.

All the 4-term interpolations supported by initial static data necessarily implied preliminary static/dynamic conversions. The latter were accomplished through the evaluation of the dipole FDPs whose static expansions were available, performed at the eight frequencies that arise from putting $n = 4$ in the auxiliary formula (3), by using Eqs. (7). In such a way, all static pseudospectra were *reduced* from N - to n -term.

The resulting sets of n -term interpolation parameters can, in fact, be transformed back to n -term reduced static pseudospectra using the equivalence:

$$\begin{aligned}\alpha_i &= \sigma_i/\tau_i \\ \varepsilon_i &= \sqrt{\tau_i}.\end{aligned}\quad (10)$$

Eight interpolation parameters (4 linear coefficients σ_i + 4 non-linear coefficients τ_i) were found to replace efficiently sensibly more extended static sets, whose size was 10 for H (5 pseudospectral contributions α_i + 5 excitation energies ε_i), 54 (27 + 27) for H_2^+ , 68 for H_2 (34 + 34) and 80 for He (40 + 40). Transforming N -term extended pseudospectra into reduced n -term ones by means of evaluations involving the FDPs may apparently seem a redundant step, since the dispersion constants could already be obtained from the extended spectra. The reduction was performed in order to achieve uniformity along the whole sequence of pseudospectral data, since only reduced sets could be made available for LiH, BeH_2 and BH.

3 Results and discussion

The results of the calculations are given in Tables 1, 2, 3, and 4 below. For the diatomic molecules, dipole polarizabilities were evaluated at the minimum of the potential energy curve ($R = 2a_0$ for H_2^+ , $R = 1.4a_0$ for H_2 , $R = 3.015a_0$ for LiH, $R = 2.506a_0$ for BeH_2 , $R = 2.329a_0$ for BH).

Table 1 collects the 4-term reduced dipole pseudo-spectra $\{\alpha_i, \varepsilon_i\}$ $i = 1, 2, 3, 4$ obtained from the interpolation parameters arising from the evaluation of dipole FDPs of the monomers at the eight frequencies provided by formula (3), except for LiH. For this molecule, 8 appropriate frequencies were selected out of the 32 available for the Gauss–Legendre quadrature used in that work [11].

The static dipole polarizabilities (atomic units) calculated from Table 1 according to Eq. (8) with $n = 4$ are:

$$\begin{aligned}\text{H} &= 4.500000, & \text{He} &= 1.382910, \\ \text{H}_2^+|| &= 5.077649, & \text{H}_2^+\perp &= 1.757648, \\ \text{H}_2|| &= 6.382679, & \text{H}_2\perp &= 4.577531, \\ \text{LiH}|| &= 26.13287, & \text{LiH}\perp &= 29.69388, \\ \text{BeH}_2|| &= 19.94072, & \text{BeH}_2\perp &= 19.67005, \\ \text{BH}|| &= 23.01637, & \text{BH}\perp &= 20.63713.\end{aligned}$$

To facilitate comparison, we give below the accurate polarizabilities from our previous calculations:

$$\begin{aligned}\text{H} &= 4.5 [6], & \text{He} &= 1.382910 [7], \\ \text{H}_2^+|| &= 5.077649, & \text{H}_2^+\perp &= 1.757649 [8], \\ \text{H}_2|| &= 6.3827, & \text{H}_2\perp &= 4.5775 [10], \\ \text{LiH}|| &= 26.15, & \text{LiH}\perp &= 29.70 [11], \\ \text{BeH}_2|| &= 19.94072, & \text{BeH}_2\perp &= 19.67005 [12].\end{aligned}$$

Table 1 4-term reduced dipole pseudospectra (atomic units) for a few simple atoms and linear molecules

	α_i	ε_i		α_i	ε_i
H	3.366482×10^0	3.794676×10^{-1}	LiH	1.695591×10^1	1.449226×10^{-1}
	1.000023×10^0	5.683764×10^{-1}		8.409862×10^0	3.735047×10^{-1}
	1.306093×10^{-1}	1.106618×10^0		6.437668×10^{-1}	1.009690×10^0
	2.885753×10^{-3}	3.322886×10^0		1.233306×10^{-1}	3.611446×10^0
He	7.071107×10^{-1}	8.022210×10^{-1}	LiH \perp	2.446670×10^1	1.751053×10^{-1}
	4.977223×10^{-1}	1.118638×10^0		4.648334×10^0	4.023576×10^{-1}
	1.613181×10^{-1}	1.910251×10^0		4.505748×10^{-1}	1.184342×10^0
	1.675926×10^{-2}	4.259569×10^0		1.282684×10^{-1}	3.595837×10^0
$\text{H}_2^+ $	5.067316×10^0	4.351008×10^{-1}	$\text{BeH}_2 $	1.471246×10^1	3.631637×10^{-1}
	4.944614×10^{-3}	9.118537×10^{-1}		4.474225×10^0	5.374278×10^{-1}
	4.323572×10^{-3}	1.913057×10^0		7.431079×10^{-1}	9.990290×10^{-1}
	1.064524×10^{-3}	4.252045×10^0		1.092569×10^{-2}	3.499773×10^0
$\text{H}_2^+\perp$	1.529475×10^0	6.742115×10^{-1}	$\text{BeH}_2\perp$	1.425507×10^1	3.232516×10^{-1}
	1.841430×10^{-1}	9.750040×10^{-1}		4.566497×10^0	5.348032×10^{-1}
	4.184725×10^{-2}	1.552454×10^0		8.188295×10^{-1}	1.065332×10^0
	2.182900×10^{-3}	3.522694×10^0		2.965019×10^{-2}	2.958492×10^0
$\text{H}_2 $	4.656280×10^0	4.737530×10^{-1}	BH	1.248248×10^1	2.627887×10^{-1}
	1.501906×10^0	6.657903×10^{-1}		9.384623×10^0	4.506600×10^{-1}
	2.224207×10^{-1}	1.083145×10^0		1.113820×10^0	9.923927×10^{-1}
	2.073253×10^{-3}	3.394450×10^0		3.544974×10^{-2}	6.061755×10^0
$\text{H}_2\perp$	2.909189×10^0	4.954656×10^{-1}	BH \perp	6.787413×10^0	1.170582×10^{-1}
	1.368299×10^0	7.171300×10^{-1}		1.247128×10^1	4.147770×10^{-1}
	2.866886×10^{-1}	1.269471×10^0		1.334336×10^0	1.016659×10^0
	1.335458×10^{-2}	2.948926×10^0		4.410018×10^{-2}	5.605912×10^0

Table 2 4-term dipole dispersion constants $C_{ab}(E_h a_0^6)$ from static data

	H	He	H ₂ ⁺	H ₂ ⁺ ⊥	H ₂	H ₂ ⊥
H	1.083171	0.470118	1.233561	0.531062	1.698301	1.276434
He		0.243377	0.533156	0.254797	0.766654	0.591346
H ₂ ⁺			1.405205	0.603805	1.933319	1.452229
H ₂ ⁺ ⊥				0.276250	0.852705	0.650309
H ₂					2.688818	2.032396
H ₂ ⊥						1.542009

Table 3 4-term dipole dispersion constants $C_{ab}(E_h a_0^6)$ from frequency-dependent data

	LiH	LiH ⊥	BeH ₂	BeH ₂ ⊥	BH	BH⊥
LiH	17.796024	20.087540	18.410391	17.624247	19.886597	16.530281
LiH⊥		22.715786	20.582003	19.727793	22.291400	18.521913
BeH ₂			20.450775	19.424881	21.720389	17.965761
BeH ₂ ⊥				18.466908	20.670081	17.102142
BH					23.163330	19.172040
BH ⊥						15.904700

Table 4 4-term dipole dispersion constants $C_{ab}(E_h a_0^6)$ from mixed static and frequency-dependent data

	LiH	LiH ⊥	BeH ₂	BeH ₂ ⊥	BH	BH⊥
H	4.217389	4.710958	4.705749	4.467410	4.992332	4.129621
He	1.678026	1.840304	2.027524	1.908264	2.108798	1.757041
H ₂ ⁺	4.798431	5.360264	5.359374	5.087358	5.684732	4.699945
H ₂ ⁺ ⊥	1.953410	2.157846	2.296937	2.167783	2.405035	1.995519
H ₂	6.450907	7.173425	7.364669	6.973398	7.768514	6.430837
H ₂ ⊥	4.789075	5.311858	5.529469	5.229178	5.816129	4.819571

As expected, since $u = 0$ is one of the knots of the interpolation, complete coincidence was observed for H, He, H₂⁺, H₂, BeH₂ and BH, so confirming that our interpolation procedure was correct, while the 3-digit accuracy for LiH¹ gives a rough estimate of the overall precision of the 4-term interpolation procedure at frequencies falling outside the reference set.

As far as Tables 2, 3, and 4 are concerned, wherever comparison is possible, agreement with the results of the more extended pseudospectra [6–10] is excellent for either the homodimers or the heterodimers, except for LiH. It must be remarked that for LiH our previous calculations involve a Gauss-Legendre quadrature truncated at the finite frequency $u = 20$ a.u. Therefore, all our previous dispersion constants underestimate the complete integration results. For LiH and BeH₂, whose dipole dispersion constants were evaluated by us for the first time [11, 12], comparison data for the heterodimers are lacking, and we must content ourselves with the excellent reproduction observed for the homodi-

mers (the diagonal terms). As far as the BH results are concerned, our present dispersion constants are in good agreement with the corresponding calculations performed by Bendazzoli and Monari [13] using their technique of Ref. [5]. Of course, the ultimate accuracy of the calculated dispersion constants depends on the accuracy with which the corresponding static or dynamic polarizabilities are calculated. Eventually improved results for the latter would imply the corresponding revision of the dispersion constants.

It seems important to notice at this point that the 1-term approximation to the FDPs yields a simple way of determining the off-diagonal dispersion constants C_{ab} for heterodimers, resulting in the formula (see Appendix):

$$C_{ab} = \frac{2 \alpha_a^A(0) \alpha_b^B(0) C_{aa} C_{bb}}{C_{aa} \alpha_b^B(0)^2 + C_{bb} \alpha_a^A(0)^2} \quad (11)$$

which is seen to coincide with an earlier result by Tang [16] based on the [1,0] Padé approximant [17] to the polarizabilities. Results using Eq. (11), which require knowledge of the static polarizabilities of the molecules

¹ Accurate results would imply new calculations of the FDPs at the prescribed frequencies.

Table 5 Isotropic C_6 dispersion coefficients ($E_h a_0^6$) from 4-term reduced dipole pseudospectra

	H	He	H ₂ ⁺	H ₂	LiH	BeH ₂	BH
H	6.499026	2.820708	4.591370	8.502338	27.27861	27.28114	26.50315
He		1.460262	2.085500	3.898692	10.71727	11.68810	11.24576
H ₂ ⁺			3.283617	6.096282	18.70477	19.19940	18.58451
H ₂				11.32429	34.41556	35.52474	34.36049
LiH					126.0062	115.8227	114.4117
BeH ₂						114.6786	111.6004
BH							108.9802

and of the dispersion constants of the homodimers, are found to reproduce the accurate values to within 1% or better, but cannot be used in high quality calculations.

Lastly, from the dipole dispersion constants of Tables 2, 3 and 4, only *isotropic* C_6 dispersion coefficients were calculated for short in this paper, while the corresponding anisotropy coefficients γ_6 can be immediately obtained from the formulae given in Ref. [15]. In the $L_A L_B M$ -scheme of coupling the angular momenta, the symmetry relations connecting $C_6 = C_6^{000}$ to the elementary dispersion constants are given by [1, 9, 15]:

$$C_6 = \frac{2}{3} (A + 2B + 2C + 4D) \quad (12)$$

for the linear molecule-linear molecule interaction;

$$C_6 = 2A + 4B \quad (13)$$

for the atom-linear molecule;

$$C_6 = 6A \quad (14)$$

for the atom-atom interaction. Here, A, B, C, D are the elementary dispersion constants, which in Casimir-Polder form are given by:

$$\begin{aligned} A &= \frac{1}{2\pi} \int_0^\infty du \alpha_{\parallel}^A(iu) \alpha_{\parallel}^B(iu) \\ B &= \frac{1}{2\pi} \int_0^\infty du \alpha_{\parallel}^A(iu) \alpha_{\perp}^B(iu) \\ C &= \frac{1}{2\pi} \int_0^\infty du \alpha_{\perp}^A(iu) \alpha_{\parallel}^B(iu) \\ D &= \frac{1}{2\pi} \int_0^\infty du \alpha_{\perp}^A(iu) \alpha_{\perp}^B(iu). \end{aligned} \quad (15)$$

The results are collected with seven significant figures in Table 5.

It is seen that our 4-term reduced pseudospectra results agree to all figures given with the accurate values reported by us elsewhere [6–10, 12], except for LiH [11] for the reasons explained above. This means that the

interpolation procedure is highly performant even for the static sets.

4 Conclusions

In conclusion, we have shown in this paper that the determination of the interpolation parameters $\{\tau_i, \sigma_i\}_{i=1, 2, \dots, n}$ by the procedure described in Ref. [14] for the FDPs is *fully equivalent* to the determination of n -term reduced pseudospectra $\{\alpha_i, \varepsilon_i\}_{i=1, 2, \dots, n}$ for either dynamic or static polarizabilities. In this way, it is possible to answer to the question posed in Ref. [1], on how to get *optimized* n -term reduced pseudospectra allowing for a uniform tabulation of atomic or molecular polarizability data for the subsequent calculation of accurate dispersion coefficients for the interacting dimers. The present results show that the 4-term approximation is an excellent compromise between accuracy and simplicity.

It should also be evident that, for reasons of computational time, *one-body* techniques such as those reported in this paper seem to be the most appropriate tool for the evaluation of the dispersion constants for *heterodimers*. This is certainly true for static data, as we have shown in Table 2, while for frequency-dependent data accuracy is limited to some extent by the need of performing some kind of integration of the Casimir-Polder formula (1).

Appendix: The 1-term approximation for C_{ab}

From Eqs. (7) and (6), the 1-term approximation for FDPs and dispersion constants for heterodimers are:

$$\alpha_a(iu) = \frac{\alpha_a \varepsilon_a^2}{\varepsilon_a^2 + u^2}, \quad \alpha_b(iu) = \frac{\alpha_b \varepsilon_b^2}{\varepsilon_b^2 + u^2} \quad (16)$$

$$C_{ab} = \frac{1}{4} \alpha_a \alpha_b \frac{\varepsilon_a \varepsilon_b}{\varepsilon_a + \varepsilon_b} \quad (17)$$

with $\alpha_a = \alpha_a(0)$, $\alpha_b = \alpha_b(0)$ the single pseudostate contributions to the static polarizabilities of A and B, and the superscripts A and B dropped for short. Then it follows for the homodimers:

$$C_{aa} = \frac{1}{8} \alpha_a^2 \varepsilon_a \Rightarrow \varepsilon_a = 8 \frac{C_{aa}}{\alpha_a^2} \quad (18)$$

$$C_{bb} = \frac{1}{8} \alpha_b^2 \varepsilon_b \Rightarrow \varepsilon_b = 8 \frac{C_{bb}}{\alpha_b^2} \quad (19)$$

so that:

$$\frac{1}{\varepsilon_a + \varepsilon_b} = \frac{\alpha_a^2 \alpha_b^2}{8 (C_{aa} \alpha_b^2 + C_{bb} \alpha_a^2)}. \quad (20)$$

Upon substitution of (18) and (20) into (17) we immediately obtain Eq. (11) of the main text.

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