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Retarded van der Waals Potential between Pairs of Spinless Atoms^{*†}

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The retarded van der Waals potential between pairs of spinless atoms, H-H, H-He, He-He, Ne-Ne, Ne-Ar, and Ar-Ar, was computed with covariant formulas of Feinberg and Sucher. Electric and magnetic effects were treated on equal footing. For hydrogen, which possesses a large magnetic polarizability, magnetic effects dominate for large distance of separation, and for small distances, an additional contribution to the London constant for a pair of hydrogen atoms from the magnetic effects is found to be $0.0155\alpha a^3$, about 0.24% of the currently accepted value.

I. INTRODUCTION

Recently, using a model-independent approach, Feinberg and Sucher¹ have obtained a covariant formula (hereafter, the FS formula) for the retarded long-range electromagnetic interaction potential (the retarded van der Waals potential) between a pair of spinless and neutral particles, separated at a distance R on the assumption that the long-range force is due to two-photon exchange. This potential is written as

$$V_{2\gamma}^{A,B}(R) = \sum_{X,Y} V_{XY}(R), \quad (1)$$

where $X, Y = E$ or M corresponding to electric or magnetic effects, and

$$V_{X,Y} = \frac{-1}{(4\pi)^4 R} \int_0^\infty dt e^{-\sqrt{t}R} \times \int_{m_A^2}^\infty \int_{m_B^2}^\infty \frac{d\sigma'_A}{\pi} \frac{d\sigma'_B}{\pi} \rho_X^A(\sigma'_A, t) \rho_Y^B(\sigma'_B, t) \Phi_{XY}^0, \quad (2)$$

where Φ_{XY}^0 is a phase-space factor, the ρ 's the spectral functions of the corresponding form factors in the atomic Compton amplitude, and σ' and t denote, respectively, the invariant c. m. energy square and momentum transfer square of the Compton process. To a first approximation, we can put^{1,2}

$$\rho_X(\sigma, t) \text{ as } \rho_X(\sigma) \equiv \rho_X(\sigma, t=0). \quad (3)$$

Then V_{XY} in (2) simplifies to

$$V_{XY} = -C_{XY}(R)/R^6, \quad (4)$$

with

$$C_{XY} = \frac{1}{4\pi^5} \int_0^\infty dk_A \int_0^\infty dk_B k_A k_B \rho_X^A(k_A) \rho_Y^B(k_B) \times \int_0^\infty d\xi \frac{e^{-2\xi R} P_{XY}(\xi R)}{(k_A^2 + \xi^2)(k_B^2 + \xi^2)}, \quad (5)$$

where

$$P_{EE}(\eta) = P_{MM}(\eta) = \eta^4 + 2\eta^3 + 5\eta^2 + 6\eta + 3, \quad (6)$$

$$P_{EM}(\eta) = P_{ME}(\eta) = -(\eta^4 + 2\eta^3 + \eta^2). \quad (7)$$

The expression in (5) can be transformed to the familiar integral over imaginary frequency and to a one-dimensional integral over the real and imaginary parts of the Compton amplitude at real frequencies,¹ namely,

$$C_{XY} = (1/8\pi^4) P_{XY}^{\text{op}} \int_0^\infty d\omega f(z\omega R) \times [\text{Re} F_X^A(\omega) \text{Im} F_Y^B(\omega) + \text{Im} F_X^A(\omega) \text{Re} F_Y^B(\omega)], \quad (8)$$

where

$$f(x) = \cos x \text{ si} x - \sin x \text{ ci} x, \quad (9)$$

$$P_{EE}^{\text{op}} = P_{MM}^{\text{op}} = \frac{1}{16} R^4 \partial_R^4 - \frac{1}{4} R^3 \partial_R^3 + \frac{5}{4} R^2 \partial_R^2 - 3R \partial_R + 3, \quad (10)$$

$$P_{EM}^{\text{op}} = P_{ME}^{\text{op}} = -\frac{1}{16} R^4 \partial_R^4 + \frac{1}{4} R^3 \partial_R^3 - \frac{1}{4} R^2 \partial_R^2. \quad (11)$$

It has also been shown by Sucher and O'Car-

roll³ that there exists a simple interpolation formula $\tilde{C}_{EE}(R)$ for the function $C_{EE}(R)$,

$$\tilde{C}_{EE}(R) = C_{EE}(2/\pi) \tan^{-1}(d_{EE}/R), \quad (12)$$

where $C_{EE} = C_{EE}(R \rightarrow 0)$, and d_{EE} is a characteristic length defined by

$$d_{EE} = 23 \alpha_E^A \alpha_E^B / 8 C_{EE}, \quad (13)$$

where α_E^A is the static electric polarizability of the particle A . Feinberg and Sucher¹ give similar conjectured formulae to C_{MM} and C_{ME} . They conjecture

$$\tilde{C}_{MM}(R) = C_{MM}(2/\pi) \tan^{-1}(d_{EE}/R), \quad (14)$$

where $C_{MM} = C_{MM}(R \rightarrow 0)$,

$$d_{MM} = 23 \alpha_M^A \alpha_M^B / 8 C_{MM}, \quad (15)$$

and α_M^A is the magnetic counterpart of α_E^A ;

$$\tilde{C}_{ME}(R) = -R^2 C_{ME} \frac{2}{\pi} \left(\tan^{-1} \frac{d_{ME}}{R} - \frac{d_{ME}/R}{1 + d_{ME}/R} \right), \quad (16)$$

where

$$C_{ME} = -\lim_{R \rightarrow 0} C_{ME}(R)/R^2 \quad (17)$$

and

$$d_{ME} = (21 \alpha_M^A \alpha_E^B / 16 C_{ME})^{1/3}. \quad (18)$$

A similar expression for $\tilde{C}_{EM}(R)$ is just given by interchanging the subscripts E and M .

C_{XY} has been evaluated for H-H with both the one-dimensional formula in (8) and the triple-integral formula in (2). The results agree to within 0.5%. The discrepancy is due to an improvement of the computer program when we evaluate the triple integral. The results quoted in Table I are from the triple integral. We have also evaluated $C_{EM}^{\text{He-H}}$ and C_{EE} for pairs He-He, He-H, Ne-Ne, Ne-Ar, and Ar-Ar, with the triple-integral formula. In some cases, we have compared the interpolation formula. The results are given in Tables I to VI.

II. CONSTRUCTION OF E AND M FORM FACTORS

The interaction Hamiltonian for the process of emission and absorption of photons by atoms is taken to be, according to the Pauli theory of the electron spin,⁴

$$V = V_{\text{spatial}} + V_{\text{spin}}, \quad (19a)$$

$$V_{\text{spatial}} = (-e/m) \vec{p} \cdot \vec{A} + e^2 A^2 / 2m^2, \quad (19b)$$

$$V_{\text{spin}} = \mu_B \vec{\sigma} \cdot \vec{\nabla} \times \vec{A}, \quad (19c)$$

where $\mu_B = e/2m$ is the Bohr magneton and σ is the Pauli matrices.

In general the Compton amplitude is of the form

$$f(\omega, \theta) = A(\omega, \theta) \vec{\epsilon} \cdot \vec{\epsilon}' + B(\omega, \theta) \vec{\epsilon} \cdot \vec{k}' \vec{\epsilon}' \cdot \vec{k}, \quad (20)$$

where $(\omega, \vec{k}, \vec{\epsilon})$ and $(\omega', \vec{k}', \vec{\epsilon}')$ are the energies, momenta, and polarizations of the incident and outgoing photons.

The electric and magnetic form factors are related to A and B in the following way⁵:

$$F_M(\omega, \theta) = -4\pi B(\omega, \theta), \quad (21)$$

$$F_E(\omega, \theta) = 4\pi A(\omega, \theta) / \omega \omega' + 4\pi B(\omega, \theta) \cos \theta. \quad (22)$$

The V_{spin} part of the interaction Hamiltonian is unimportant for the atoms considered except hydrogen which exhibits a hyperfine transition due to V_{spin} . The state functions of the atom consist of a spatial part, a spin function of the electron, and a spin function of the proton, i. e.,

$$|n\rangle = |nlm\rangle \otimes S(e) \otimes S(p). \quad (23)$$

The ground state of hydrogen is

$$|0\rangle = |100\rangle \otimes |\alpha(s) \beta(I) - \beta(s) \alpha(I)\rangle, \quad (24)$$

namely, the $F=0$, $m_F=0$ state, $F=I+s$, where s , I denote electron and proton spins, and α and β indicating up and down spins. It can be shown⁶ that in the dipole approximation, V_{spin} contributes only to F_M and V_{spatial} contributes only to F_E . With the inclusion of retardation, both V_{spin} and V_{spatial} contribute to F_E and F_M . However, contributions from V_{spin} to F_E and F_M are smaller than the contribution from V_{spatial} by a factor of α^2 to the same order in t , the invariant momentum transfer square. Hence the dipole approximation is always retained for V_{spin} and we shall call the part of the magnetic form factor due to V_{spatial} to be $F_{M, \text{dia}}$, the diamagnetic part of the magnetic form factor. For systems considered here, other than those that involve hydrogen, the retarded van der Waals potential is accurately given by $-C_{EE}(R)/R^6$, since neglected terms are of order α^2 smaller.

III. H-H SYSTEM

For hydrogen, we have evaluated the real and imaginary parts of the form factors with the interaction in (19) and the identification from (20) to (22) using the dipole approximation, and, when photon energy is below the threshold, the Breit-Wigner formalism, i. e., by replacing the energy of the intermediate state E_n by $E_n - \frac{1}{2}i\Gamma_n$, where Γ_n is the total decay width. We obtain

$$\begin{aligned} \text{Re}F_E(\omega) = & -\frac{3\pi}{\omega^2} \sum_n' \frac{\Gamma_{n0}}{\omega_n} \left(\frac{\omega - \omega_n}{(\omega - \omega_n)^2 + \frac{1}{4}\Gamma_n} \right. \\ & \left. - \frac{1}{\omega + \omega_n} + \frac{2}{\omega_n} \right), \quad (25) \end{aligned}$$

$$\text{Im}F_E(\omega) = \frac{2\pi\alpha}{\omega^2 m} \sum_n' \omega_n f_{n0} \frac{\frac{1}{2}\Gamma_n}{(\omega - \omega_n)^2 + \frac{1}{4}\Gamma_n}$$

$$= \frac{2\pi^2}{\omega^2 m} \sum_n' \omega_n f_{n0} \delta(\omega - \omega_n), \quad (26)$$

$$\text{Re}F_M(\omega) = \frac{\pi\alpha}{m^2} \left(\frac{1}{\omega + \omega_H} - \frac{\omega - \omega_H}{(\omega - \omega_H)^2 + \frac{1}{4}\Gamma_H^2} \right), \quad (27)$$

$$\text{Im}F_M(\omega) = \frac{\pi\alpha}{m^2} \frac{\frac{1}{2}\Gamma_H}{(\omega - \omega_H)^2 + \frac{1}{4}\Gamma_H^2} = \frac{\pi^2\alpha}{m^2} \delta(\omega - \omega_H), \quad (28)$$

where we have made use of the smallness of the decay width Γ and replace the second factor in (19a) and (21a) by π times a δ function, and where

$$f_{n0} = 2m\omega_n |\langle 0|z|n \rangle|^2, \quad (29)$$

$$\Gamma_{n0} = \frac{4}{3} \omega_n^3 |\langle 0|z|n \rangle|^2 \quad (30)$$

are the familiar oscillator strength and partial decay widths;

$$\omega_H = 1420 \times 10^6 \text{ Hz} \quad (31)$$

is the hyperfine transition frequency and Γ_H is the width of the upper hyperfine state. \sum_n' indicates a sum over the discrete states and an integral over the continuum. The real and imaginary parts of the E and M form factors constructed in this fashion verify a dispersion relation numerically for hydrogen. Moreover, we shall approximate

$$\frac{\omega - \omega_n}{(\omega - \omega_n)^2 + \frac{1}{4}\Gamma_n^2} \frac{\frac{1}{2}\Gamma_n}{(\omega - \omega_n)^2 + \frac{1}{4}\Gamma_n^2} = -\frac{1}{2}\pi \delta'(\omega - \omega_n) \quad (32)$$

in the term that occurs in $\text{Re}F_E \text{Im}F_E$ and in $\text{Re}F_M \text{Im}F_M$. Then we arrive at

$$\begin{aligned} \text{Re}F_E(\omega) \text{Im}F_E(\omega) &= \frac{9\pi^3}{2\omega^4} \sum_n \frac{\Gamma_{n0}^2}{\omega_n^2} \delta'(\omega - \omega_n) - \frac{9\pi^3}{\omega^4} \sum_{n \neq m} \frac{\Gamma_{n0} \Gamma_{m0}}{\omega_n \omega_m} \frac{\delta(\omega - \omega_n)}{(\omega - \omega_n)} + \frac{9\pi^3}{\omega^4} \sum_{n,m} \left[\left(\frac{1}{\omega + \omega_n} - \frac{2}{\omega_n} \right) \right. \\ &\quad \left. \times \frac{\Gamma_{n0} \Gamma_{m0}}{\omega_n \omega_m} \delta(\omega - \omega_m) \right] + \sum_n \frac{3\pi^2}{\omega^2} \frac{\Gamma_{n0}}{\omega_n} \delta(\omega - \omega_n) C(\omega) + \text{Re}F_E(\omega) \text{Im}F_E(\omega) \theta(\omega - \omega_{th}), \quad (33) \end{aligned}$$

where ω_{th} is the threshold frequency, $C(\omega)$ is the contribution to the real part for $\omega < \omega_{th}$ from continuum states, and $\text{Re}F_E(\omega > \omega_{th})$ and $\text{Im}F_E(\omega > \omega_{th})$ are given by Gavrilu.⁷ Because of the δ function

present we only need to know $C(\omega)$ at the resonances. This has been evaluated for the first 100 resonances. We similarly introduce the derivative of the δ function in $\text{Re}F_M \text{Im}F_M$. Together with

$$P_{EE}^{\text{op}} f(2\omega R) = P_{MM}^{\text{op}} f(2\omega R) \equiv P(2\omega R) = (3 - 5\omega^2 R^2 + \omega^4 R^4) f(2\omega R) + (6\omega R - 2\omega^3 R^3) g(2\omega R) + \frac{1}{4}\omega R - \frac{1}{2}\omega^3 R^3, \quad (34)$$

$$P_{EM}^{\text{op}} f(2\omega R) = P_{ME}^{\text{op}} f(2\omega R) \equiv Q(2\omega R) = (\omega^2 R^2 - \omega^4 R^4) f(2\omega R) + 2\omega^3 R^3 g(2\omega R) - \frac{5}{4}\omega R + \frac{1}{2}\omega^3 R^3, \quad (35)$$

$$\begin{aligned} \frac{d}{d\omega} \frac{P_{EE}^{\text{op}} f(2\omega R)}{\omega^4} &= f(2\omega R) \left(\frac{-12}{\omega^5} + \frac{22R^2}{\omega^3} - \frac{4R^4}{\omega} \right) + (2\omega R) \left(-2R^5 + \frac{12R^3}{\omega^2} - \frac{24R}{\omega^4} \right) \\ &\quad + \frac{1}{2\omega R} \left(\frac{5R^4}{\omega} - \frac{63R^2}{2\omega^3} \right), \quad (36) \end{aligned}$$

$$\frac{d}{d\omega} P_{MM}^{\text{op}} f(2\omega R) = 2\omega R^2 f(2\omega R) + (4\omega^2 R^3 - 2\omega^4 R^5) g(2\omega R) - \frac{1}{4}R + \frac{1}{2}\omega^2 R^3, \quad (37)$$

where

$$g(z) = -\text{ciz} \cos z - \text{siz} \sin z, \quad (38)$$

we obtain

$$\begin{aligned} \frac{C_{EE}(\omega)}{2} &= \frac{9\pi}{16} \sum_n \frac{\Gamma_{n0}^2}{\omega_n} \left[f(2\omega_n R) \left(\frac{3}{\omega_n^5} - \frac{7R^2}{\omega_n^3} + \frac{R^4}{\omega_n} \right) + g(2\omega_n R) \left(\frac{6R}{\omega_n^4} - \frac{6R^3}{\omega_n^2} + 2R^2 \right) + \left(\frac{6R}{\omega_n^4} - \frac{R^3}{\omega_n} \right) \right] \\ &\quad - \frac{9}{4\pi} \sum_{n \neq m} \frac{\Gamma_{n0} \Gamma_{m0}}{\omega_n^2 \omega_m} \frac{\omega_n}{(\omega_n^2 - \omega_m^2)} \left[\left(\frac{3}{\omega_n^4} - \frac{5R^2}{\omega_n^2} + R^4 \right) f(2\omega_n R) + \left(\frac{6R}{\omega_n^2} - \frac{2R^3}{\omega_n} \right) g(2\omega_n R) + \left(\frac{13R}{4\omega_n^3} - \frac{R^3}{2\omega_n} \right) \right] \\ &\quad + \frac{3}{2\pi} \sum_n \frac{\Gamma_{n0}}{\omega_n^5} C(n) \left[(3 - 5\omega_n^2 R^2 + \omega_n^4 R^4) f(2\omega_n R) + (6\omega_n R - 2\omega_n^3 R^3) g(2\omega_n R) + \left(\frac{13\omega_n R}{4} - \frac{1}{2}\omega_n^3 R^3 \right) \right] \end{aligned}$$

$$+ \frac{2}{\pi^2} \int_{\text{th}}^{\infty} d\omega \operatorname{Re} f(\omega) \operatorname{Im} f(\omega) \frac{1}{\omega^4} P(2\omega R), \quad (39)$$

where contributions from continuum states are written explicitly; $c(n)$ is the contribution to the real part of the electric form factor from continuum states at the n th resonance, and $\operatorname{Re} f(\omega)$ and $\operatorname{Im} f(\omega)$ are the real and imaginary parts of the forward-elastic-scattering amplitudes as given by Gavrilá⁷

$$\frac{C_{\text{MM}}}{2}(R) = \frac{1}{\pi} \left(\frac{\alpha}{4m^2} \right)^2 \left[f(2\omega_{\text{H}}R) \left(\frac{3}{\omega_{\text{H}}} - 7\omega_{\text{H}}R^2 + \omega_{\text{H}}^3R^4 \right) + g(2\omega_{\text{H}}R)(6R - 6\omega_{\text{H}}^2R^3 + 2\omega_{\text{H}}^4R^5) + 16R - \omega_{\text{H}}^2R^3 \right], \quad (40)$$

$$C_{\text{EM}}(R) = \frac{2\alpha_{\text{E}}\alpha}{4m^2\pi} \left[f(2\omega_{\text{H}}R)(\omega_{\text{H}}^2R^2 - \omega_{\text{H}}^4R^4) + 2\omega_{\text{H}}^3R^3g(2\omega_{\text{H}}R) - \frac{5}{4}\omega_{\text{H}}R + \frac{1}{2}\omega_{\text{H}}^3R^3 - \frac{3}{4\pi}\alpha^3\omega_{\text{H}}\sum_n \frac{\Gamma_{n0}}{\omega_n^5} Q(2\omega_nR) \right], \quad (41)$$

where α_{E} is the electric dipole polarizability.

Next, we examine the asymptotic form with the triple-integral formula and use the δ -function approximations (26) and (28) in (5). For R much less than $1/\omega \sim a/\alpha$, we find

$$C_{\text{EE}} \xrightarrow{R \rightarrow 0} \sum_{n,m} \frac{3f_{n0}^A f_{m0}^B \alpha^4 a^2}{2\omega_n^A \omega_m^B (\omega_n^A + \omega_m^B)}, \quad (42)$$

which is the form of the London constant. For $R \rightarrow \infty$, we obtain

$$\lim_{R \rightarrow \infty} C_{\text{EE}}^{\text{H-H}}(R) = \frac{7}{4\pi R} \alpha_{\text{E}}^{\text{H}} \alpha_{\text{M}}^{\text{H}}, \quad (43)$$

$$\lim_{R \rightarrow \infty} C_{\text{HM}}^{\text{H-H}}(R) = \frac{23}{4\pi} \frac{\alpha_{\text{M}}^{\text{H}} \alpha_{\text{M}}^{\text{H}}}{R}, \quad (44)$$

where

TABLE I. van der Waals potential (E-E part) between a pair of H atoms. (ω) indicates a multiplicative factor 10^n (this applies to all tables henceforth). C_{EE} is in units of αa^5 .

R	FS formula		Arctan formula	
	$C_{\text{EE}}^{\text{H-H}}$	$C_{\text{EE},R}^{\text{H-H}}$	$C_{\text{EE}}^{\text{H-H}}$	$C_{\text{EE},R}^{\text{H-H}}$
1.0	6.5095	6.5095	6.5056	6.5056
10	6.5072	6.5072 (1)	6.4752	6.4752 (1)
25	6.4960	1.6240 (2)	6.4245	1.6061 (2)
50	6.4610	3.2305 (2)	6.3400	3.1700 (2)
75	6.4106	4.8079 (2)	6.2557	4.6918 (2)
100	6.3487	6.3487 (2)	6.1716	6.1716 (2)
250	5.8600	1.4650 (3)	5.6751	1.4188 (3)
500	4.9853	2.4927 (3)	4.9038	2.4519 (3)
750	4.2429	3.1822 (3)	4.2333	3.1750 (3)
1000	3.6506	3.6506 (3)	3.6730	3.6730 (3)
1200	3.2666	3.9199 (3)	3.2981	3.9578 (3)
1500	2.8057	4.2085 (3)	2.8386	4.2580 (3)
2000	2.2544	4.5088 (3)	2.2781	4.5561 (3)
3000	1.6098	4.8295 (3)	1.6071	4.8212 (3)
4000	1.2238	4.8951 (3)	1.2320	4.9279 (3)
5000	9.9215 (-1)	4.9607 (3)	9.9604 (-1)	4.9802 (3)
6000	8.3730 (-1)	5.0238 (3)	8.3491 (-1)	5.0095 (3)
10000	5.0556 (-1)	5.0556 (3)	5.0532 (-1)	5.0532 (3)
15000	3.3818 (-1)	5.0727 (3)	3.3781 (-1)	5.0671 (3)
20000	2.5394 (-1)	5.0788 (3)	2.5360 (-1)	5.0720 (3)
50000	1.0171 (-1)	5.0854 (3)	1.0155 (-1)	5.0774 (3)
100000	5.0864 (-2)	0.0864 (3)	5.0781 (-2)	5.0781 (3)

$$\alpha_{\text{M}}^{\text{H}} = \alpha/2m^2\omega_{\text{H}} \quad (45)$$

as predicted by Feinberg and Sucher. In addition we get

$$\lim_{R \rightarrow 0} C_{\text{EM}}^{\text{H-H}}(R) = -R^2 \left(\frac{1}{2} \alpha^4 a^4 \omega_{\text{H}} \right), \quad (46)$$

$$\lim_{R \rightarrow 0} C_{\text{MM}}^{\text{H-H}}(R) = 3\alpha^6 a^4 / 16\omega_{\text{H}}. \quad (47)$$

Equation (46) gives the magnetic analog of the London constant for a pair of H atoms. In magnitude it is $0.015496\alpha a^5$, which is about 0.24% of the currently accepted value of the London constant for a pair of H atoms.

It is also interesting to note that on inserting the δ -function approximation for $\operatorname{Im} F_{\text{E}}$ into the expression for C_{EE} in (5), we obtain the same integral as given by Casimir and Polder.⁸ This will be denoted as the Feinberg-Sucher-Casimir-Polder (FS-CP) integral formula. Analogous formulas are obtained for C_{EM} and C_{MM} when we use the δ -function approximation for $\operatorname{Im} F_{\text{M}}$ in (5). We have also calculated $C_{\text{M,dia-M,dia}}^{\text{H-H}}$ and $C_{\text{EM,dia}}^{\text{H-H}}$ by identify-

TABLE II. van der Waals potential (M-M part) between a pair of H atoms.

R in d_{MM}^a	FS formula		Arctan formula	
	C_{MM}^b	$C_{\text{MM},R}$	C_{MM}	$C_{\text{MM},R}$
1 (-4)	1.5480 (-2)	2.3675 (4)	1.5479 (-2)	2.3673 (4)
1 (-3)	1.5480 (-2)	2.3674 (5)	1.5470 (-2)	2.3659 (5)
1 (-2)	1.5473 (-2)	2.3644 (6)	1.5382 (-2)	2.3524 (6)
5 (-2)	1.5332 (-2)	1.1724 (7)	1.4988 (-2)	1.1461 (7)
0.1	1.4991 (-2)	2.2927 (7)	1.4498 (-2)	2.2172 (7)
0.5	1.1123 (-2)	8.5052 (7)	1.0911 (-2)	8.3433 (7)
1	7.7265 (-2)	1.1817 (8)	7.7400 (-3)	1.1837 (8)
1.5	5.7744 (-3)	1.3274 (8)	5.7947 (-3)	1.3293 (8)
2.0	4.5920 (-3)	1.4046 (8)	4.5692 (-3)	1.3976 (8)
3.0	3.1591 (-3)	1.4494 (8)	3.1708 (-3)	1.4548 (8)
5.0	1.9421 (-3)	1.4851 (8)	1.9453 (-3)	1.4875 (8)
10	9.8177 (-4)	1.5051 (8)	9.8223 (-4)	1.5022 (8)
20	4.9228 (-4)	1.5057 (8)	4.9237 (-4)	1.5059 (8)
40	2.4631 (-4)	1.5068 (8)	2.4632 (-4)	1.5069 (8)
100	9.8545 (-5)	1.5071 (8)	9.8546 (-5)	1.5071 (8)
500	1.9710 (-5)	1.5072 (8)	1.9710 (-5)	1.5072 (8)

^a $d_{\text{MM}} = 1.5293 \times 10^{10} \alpha$.

^b C_{MM} is in units of αa^5 .

TABLE III. van der Waals potential (E-M part) between a pair of H atoms.

R in d_{EM}^a	FS formula		Arctan formula	
	$-C_{EM}^b$	$-C_{EM}R$	$-C_{EM}$	$-C_{EM}R$
1 (-9)	2.6784 (-20)	6.2789 (-22)	2.6764 (-20)	6.2740 (-22)
1 (-8)	2.6764 (-18)	6.2743 (-19)	2.6764 (-18)	6.2740 (-19)
1 (-7)	2.6570 (-16)	6.2287 (-16)	2.6764 (-16)	6.2740 (-16)
1 (-6)	2.4804 (-14)	5.8146 (-13)	2.6764 (-14)	6.2740 (-13)
1 (-5)	1.5040 (-12)	3.5257 (-10)	2.6763 (-12)	6.2740 (-10)
1 (-4)	2.7321 (-11)	6.4046 (-8)	2.6760 (-10)	6.2732 (-7)
1 (-3)	2.8026 (-10)	6.5698 (-6)	2.6730 (-8)	6.3660 (-4)
1 (-2)	2.8031 (-9)	6.5712 (-4)	2.6423 (-6)	6.2942 (-1)
0.1	2.8013 (-8)	6.5669 (-2)	2.3379 (-4)	5.4805 (2)
1	2.7828 (-7)	6.5235	4.8267 (-3)	1.1399 (5)
3	8.2269 (-7)	5.7857 (1)	3.3353 (-3)	2.3456 (5)
10	2.6073 (-6)	6.1122 (2)	1.1224 (-3)	2.6312 (5)
20	4.8621 (-6)	2.2796 (3)	5.6624 (-4)	2.6548 (5)
40	8.5083 (-6)	7.9782 (3)	2.8376 (-4)	2.6608 (5)
100	1.4847 (-5)	3.4804 (4)	1.1258 (-4)	2.6624 (5)
500	1.5253 (-5)	1.7879 (5)	2.2718 (-5)	2.6628 (5)
1000	9.9204 (-6)	2.3256 (5)	1.1359 (-5)	2.6629 (5)
10000	1.1349 (-6)	2.6604 (5)	1.1359 (-6)	2.6629 (5)
100000	1.1367 (-7)	2.6648 (5)	1.1359 (-7)	2.6628 (5)
1000000	1.1368 (-8)	2.6648 (5)	1.1359 (-8)	2.6628 (5)

^a $d_{EM} = 2.3442 \times 10^7 a$.^b C_{EM} is in units of αa^5 .

ing the diamagnetic form factor from the expression for the elastic hydrogenic Compton amplitude given by Gavrilu and Costescu.⁹

IV. SYSTEMS INVOLVING He, Ne, AND Ar

For atoms other than hydrogen, the atomic wave functions are not so accurately known and it is not possible to construct the form factors in the way we have done for hydrogen. However, in the atoms

we are considering, i. e., helium, neon, and argon, the electric form factors are of order $1/\alpha^2$ larger than the magnetic counterpart for interesting range of energies and so although a measure of the total cross section gives $F_E + F_M$, we are justified to claim that the cross section measures F_E . Referring back to Eq. (26), we write

$$\rho_E(\omega) = \frac{2\pi^2\alpha}{m\omega^2} \left(\sum_j \omega_j f_{j0} \delta(\omega - \omega_j) + \sum_j (I_n + \nu) \frac{df}{d\nu} \Big|_{\nu=\omega-I_n} \right), \quad (48)$$

where I_n is the ionization threshold energy for the n th channel of excitation and ν is the energy of the photoelectron. For example, in He it would correspond to exciting the ground state to a $(ns, \nu p)^1P$ state.

For energies greater than the photoelectric threshold, we have constructed $\rho_E(\omega)$ for He, Ne, and Ar by analyzing the available data on the photoabsorption cross section of these gases.¹⁰ For the discrete oscillator strengths, experimental values¹¹ are adopted whenever available; for higher excited states, the oscillator strengths are estimated by extrapolation.⁴ Autoionization states are treated as discrete transitions superimposed on the continuum in the way prescribed by Madden *et al.*¹² The spectral function ρ_E so constructed is tested with the oscillator strength sum rules:

$$S(n) = \sum_j' f_{j0} (E_j - E_0)^n.$$

Similar analyses have been done by Delgarno and

TABLE IV. $RC_{M, dia-M, dia}^{H-H}$ and $RC_{E-M, dia}^{H-H}$ as calculated by the FS formula. The results, calculated by the arctangent interpolation formula, are in the 3rd and 5th columns.

R	$RC_{M, dia-M, dia}^{H-H}$	$\tilde{R}C_{M, dia-M, dia}^{H-H}$	$RC_{EM, dia}^{H-H}$	$\tilde{R}C_{EM, dia}^{H-H}$
0.100 (-02)	0.3809 (-12)	0.3809 (-12)	0.3473 (-18)	0.472 (-18)
0.100 (02)	0.3804 (-08)	0.3776 (-08)	0.3082 (-06)	0.3360 (-06)
0.200 (02)	0.7584 (-08)	0.7487 (-08)	0.2218 (-05)	0.2599 (-05)
0.300 (02)	0.1132 (-07)	0.1113 (-07)	0.6795 (-05)	0.8474 (-05)
0.400 (02)	0.1500 (-07)	0.1471 (-07)	0.1471 (-04)	0.1938 (-04)
0.500 (02)	0.1862 (-07)	0.1822 (-07)	0.2637 (-04)	0.3650 (-04)
0.750 (02)	0.2737 (-07)	0.2672 (-07)	0.7306 (-04)	0.1120 (-03)
0.100 (03)	0.3564 (-07)	0.3481 (-07)	0.1447 (-03)	0.2401 (-03)
0.250 (03)	0.7557 (-07)	0.7536 (-07)	0.9579 (-03)	0.1922 (-02)
0.500 (03)	0.1153 (-06)	0.1180 (-06)	0.2748 (-02)	0.5063 (-02)
0.750 (03)	0.1368 (-06)	0.1410 (-06)	0.4275 (-02)	0.6802 (-02)
0.100 (04)	0.1494 (-06)	0.1537 (-06)	0.5412 (-02)	0.7683 (-02)
0.125 (04)	0.1572 (-06)	0.1611 (-06)	0.6234 (-02)	0.8162 (-02)
0.150 (04)	0.1624 (-06)	0.1657 (-06)	0.6836 (-02)	0.8445 (-02)
0.200 (04)	0.1686 (-06)	0.1708 (-06)	0.7633 (-02)	0.8744 (-02)
0.400 (04)	0.1755 (-06)	0.1763 (-06)	0.8691 (-02)	0.9050 (-02)
0.100 (05)	0.1778 (-06)	0.1779 (-06)	0.9084 (-02)	0.9140 (-02)
0.500 (05)	0.1783 (-06)	0.1782 (-06)	0.9163 (-02)	0.9157 (-02)
0.100 (06)	0.1783 (-06)	0.1783 (-06)	0.9166 (-02)	0.9157 (-02)
0.100 (07)	0.1783 (-06)	0.1783 (-06)	0.9166 (-02)	0.9158 (-02)

TABLE V. van der Waals potential [E(He)-M(H) part] between a He atom and a H atom as calculated by the FS formula.

R	C_{EM}^{He-H}	$C_{EM}^{He-H} R$
0.1 (01)	0.3612 (-16)	0.3612 (-16)
0.1 (02)	0.3348 (-14)	0.3348 (-13)
0.5 (02)	0.6397 (-13)	0.3198 (-11)
0.1 (03)	0.1981 (-12)	0.1981 (-10)
0.5 (03)	0.1683 (-11)	0.8417 (-09)
0.1 (04)	0.3575 (-11)	0.3575 (-08)
0.5 (04)	0.1834 (-10)	0.9168 (-07)
0.1 (05)	0.3670 (-10)	0.3671 (-06)
0.5 (05)	0.1836 (-09)	0.9179 (-05)
0.1 (06)	0.3671 (-09)	0.3672 (-04)
0.5 (06)	0.1836 (-08)	0.9178 (-03)
0.1 (07)	0.3671 (-08)	0.3671 (-02)
0.5 (07)	0.1833 (-07)	0.9165 (-01)
0.1 (08)	0.3660 (-07)	0.3660 (00)
0.5 (08)	0.1807 (-06)	0.9036 (01)
0.1 (09)	0.3559 (-06)	0.3559 (02)
0.5 (09)	0.1577 (-05)	0.7888 (03)
0.1 (10)	0.2739 (-05)	0.2739 (04)
0.5 (10)	0.5550 (-05)	0.2775 (05)
0.1 (11)	0.4996 (-05)	0.4996 (05)
0.5 (11)	0.1578 (-05)	0.7889 (05)
0.1 (12)	0.8148 (-06)	0.8148 (05)
0.5 (12)	0.1636 (-06)	0.8179 (05)
0.1 (13)	0.8181 (-07)	0.8181 (05)
0.5 (13)	0.1636 (-07)	0.8182 (05)
0.1 (14)	0.8182 (-08)	0.8182 (05)
0.5 (14)	0.1636 (-08)	0.8182 (05)
0.1 (15)	0.8182 (-09)	0.8182 (05)
0.5 (15)	0.1636 (-09)	0.8182 (05)

Kingston¹³ and by Barker and Leonard¹⁴ in the calculation of the London constants. We obtain the values

$$S(0) = 9.667, \quad S(-1) = 1.819,$$

$$S(-2) = 0.632 \text{ for Ne;}$$

$$S(0) = 16.76, \quad S(-1) = 4.39,$$

$$S(-2) = 2.686 \text{ for Ar,}$$

compared with the values 9.95, 1.899, and 0.67 for Ne and 18, 4.437, and 2.769 for Ar of Barker and Leonard.¹⁴ For He, our values agree very well with those of Barker and Leonard. The spectral functions constructed this way are then used to compute the retarded van der Waals potential.

V. RESULTS AND COMMENTS

The retarded van der Waals potential between a pair of H atoms (including magnetic effects) has been calculated in great detail and the results are given in Tables I to IV. For the He-H and He-He system our results agree quite well (within 1%) to that of Karplus and Getzin.¹⁵ We have calculated in addition the retarded potentials C_{ME}^{H-He} and C_{EE}^{Ne-Ne} , and C_{EE}^{Ne-Ar} and C_{EE}^{Ar-Ar} , and the results are given in Tables V and VI. The arctangent extrapolation formulas conjectured by O'Carroll and Sucher, and by Feinberg and Sucher, are found to work very well for the potentials C_{EE}^{H-H} , C_{MM}^{H-H} , and C_{EE}^{H-He} . For the potentials C_{EE}^{Ne-Ne} , C_{EE}^{Ne-Ar} , and C_{EE}^{Ar-Ar} , the extrapolation formula has a maximum discrepancy of about $\pm 6\%$ with the results in Table VI. For the electromagnetic part of the retarded van der Waals potential the extrapolation formula is a rather poor approximation.

The London constants for the pairs considered, except for H-H where we discovered a large mag-

TABLE VI. van der Waals potential (EE part) between pair Ne-Ne, Ne-Ar, and Ar-Ar as calculated by the FS-CP formula.

R	C_{EE}^{Ne-Ne}	$C_{EE}^{Ne-Ne} R$	C_{EE}^{Ne-Ar}	$C_{EE}^{Ne-Ar} R$	C_{EE}^{Ar-Ar}	$C_{EE}^{Ar-Ar} R$
0.100 (02)	0.5908 (01)	0.5908 (02)	0.1880 (02)	0.1880 (03)	0.6428 (02)	0.6428 (03)
0.200 (02)	0.5852 (01)	0.1170 (03)	0.1869 (02)	0.3739 (03)	0.6409 (02)	0.1282 (04)
0.300 (02)	0.5777 (01)	0.1733 (03)	0.1855 (02)	0.5566 (03)	0.6380 (02)	0.1914 (04)
0.400 (02)	0.5690 (01)	0.2276 (03)	0.1839 (02)	0.7355 (03)	0.6345 (02)	0.2538 (04)
0.500 (02)	0.5598 (01)	0.2799 (03)	0.1820 (02)	0.9100 (03)	0.6304 (02)	0.3152 (04)
0.750 (02)	0.5349 (01)	0.4012 (03)	0.1768 (02)	0.1326 (04)	0.6185 (02)	0.4639 (04)
0.100 (03)	0.5097 (01)	0.5097 (03)	0.1712 (02)	0.1712 (04)	0.6050 (02)	0.6050 (04)
0.250 (03)	0.3828 (01)	0.9570 (03)	0.1387 (02)	0.3466 (04)	0.5164 (02)	0.1291 (05)
0.500 (03)	0.2593 (01)	0.1297 (04)	0.1007 (02)	0.5032 (04)	0.3953 (02)	0.1977 (05)
0.750 (03)	0.1925 (01)	0.1444 (04)	0.7737 (01)	0.5803 (04)	0.3129 (02)	0.2347 (05)
0.100 (04)	0.1518 (01)	0.1518 (04)	0.6226 (01)	0.6226 (04)	0.2561 (02)	0.2561 (05)
0.125 (04)	0.1249 (01)	0.1561 (04)	0.5185 (01)	0.6481 (04)	0.2156 (02)	0.2695 (05)
0.150 (04)	0.1058 (01)	0.1587 (04)	0.4430 (01)	0.6646 (04)	0.1856 (02)	0.2784 (05)
0.200 (04)	0.8060 (00)	0.1612 (04)	0.3413 (01)	0.6826 (04)	0.1444 (02)	0.2889 (05)
0.400 (04)	0.4111 (00)	0.1644 (04)	0.1757 (01)	0.7028 (04)	0.7510 (01)	0.3004 (05)
0.100 (05)	0.1654 (00)	0.1654 (04)	0.7094 (00)	0.7094 (04)	0.3043 (01)	0.3043 (05)
0.500 (05)	0.3310 (-01)	0.1655 (04)	0.1421 (00)	0.7106 (04)	0.6102 (00)	0.3050 (05)
0.100 (06)	0.1655 (-01)	0.1655 (04)	0.7107 (-01)	0.7107 (04)	0.3051 (00)	0.3051 (05)
0.100 (07)	0.1655 (-02)	0.1655 (04)	0.7107 (-02)	0.7107 (04)	0.3051 (-01)	0.3051 (05)

netic contribution, agree quite well with the values given by Dalgarno,¹⁶ who gives the following London constants: He-H, 2.83; He-He, 1.47; Ne-Ne, 6.3; Ne-Ar, 20; and Ar-Ar, 65. Our asymptotic forms also agree very well with the measured values of electric polarizabilities.¹⁷ In our case, the London constant is given by $\sum_{X,Y} C_{X,Y}(R \rightarrow 0)$, which is essentially $C_{EE}(R \rightarrow 0)$ except for the H-H system.

One-state approximations. As we have seen in the computation of the C_{MM}^{HH} potential where we have considered only the contribution from the hyperfine transition, the form of the potential comes out to be very easily calculable. It is well known that atomic oscillator strengths obey a series of sum

rules. In the case of sodium, we have a loose 3s electron outside a closed core $1s^2 2s^2 3p^6$. Essentially this makes the sodium atom behave much like an one-electron atom. Moreover, the 3s-3p transition gives an oscillator strength equal to 0.982. In this particular case, it is very legitimate to adopt the one-state approximation, and we just end up with a similar expression to $C_{MM}^{HH}(R)$. However, we have not carried out this computation numerically.

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$$\begin{aligned} \epsilon &= \frac{1}{2}\Gamma_n & \text{if } |\omega - \omega_n| < \delta_n & \text{ for some } n \\ &= 0 & \text{if } |\omega - \omega_n| > \delta_n & \text{ for all } n, \end{aligned}$$

where Γ_n is the width of the n th excited state and δ_n is a sequence of predetermined constants such that $\delta_n \sim \Gamma_n$. In this way, to lowest order in ϵ we obtain finite results for the imaginary part of the scattering amplitude expressible in the form of (19) and (21). In fact, to lowest order in ϵ , they agree with that calculated in the Breit-Wigner model.

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