

Factorization of static perturbation theory for weakly coupled systems using imaginary time

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Starting from the interaction picture in quantum mechanics it is shown that perturbation theory for a weak static coupling of two subsystems in a natural way can be reformulated through integrals over products of imaginary time cross correlation functions. This *inter alia* leads to an expression for the London dispersion energy contribution of intermolecular interactions offering new ways to its numerical computation. The frequency-dependent charge susceptibility functions at imaginary frequencies appearing in the Casimir-Polder expression for the dispersion energy and the imaginary time density fluctuation cross correlation functions occurring in the equivalent alternative formula turn out to be Fourier cosine transform pairs.

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Consider a quantum system composed of subsystems A and B , each of which may contain several indistinguishable particles within the subsystems which, however, are assumed to be distinguishable between A and B . In the following, the commuting Hamilton operators of both subsystems will be denoted as $\hat{H}^A$ and $\hat{H}^B$, respectively. Assume that the particles of A interact with those of B through some interaction operator $\hat{V}$ which, for simplicity, in the following will be taken as a two-body interaction potential

$$\hat{V} = \hat{\rho}_x^A T_{xx'} \hat{\rho}_{x'}^B, \quad (1)$$

where $\hat{\rho}_x^A$ and $\hat{\rho}_{x'}^B$ denote the one-particle density operators of A and B referring to spatial or grid positions x and x' , respectively. $T_{xx'}$ is the particle-particle interaction potential and integration or summation over repeated indices is meant to be implicit. Obviously, with the partitioning of the total Hamiltonian $\hat{H} = \hat{H}^0 + \hat{V}$ and $\hat{H}^0 = \hat{H}^A + \hat{H}^B$ Rayleigh-Schrödinger perturbation theory lends itself for treating the interacting subsystems, provided that the coupling potential is weak. This ansatz leads to an expansion of the total wavefunction into products $|a^A b^B\rangle = |a^A\rangle |b^B\rangle$ of the eigenfunctions of the subsystem Hamiltonians, e.g., $\hat{H}^A |a^A\rangle = E_a^A |a^A\rangle$, where E_a^A denotes the energy of the state a of subsystem A .

In the case of a description of interacting atoms or molecules in the clamped nuclei Born-Oppenheimer approximation this approach has been followed already in the early days of quantum mechanics [1]. Here the eigenfunctions of the subsystem Hamiltonians consist of properly antisymmetric many-electron wavefunctions and the interaction between the electrons is the Coulomb potential $T_{\mathbf{r}\mathbf{r}'} = \frac{1}{|\mathbf{r} - \mathbf{r}'|}$ (note that Coulomb interactions with and between the fixed nuclei are

also part of the interaction operator and that atomic units will be used throughout). While evidently in this case the assumption of distinguishability of the electrons of A and B is not justified (for an early discussion see Ref. [2]), application of perturbation theory to distant atoms or molecules leads to an understanding of important contributions to the long-range part of the interaction energy [3–6]. Among them are interactions between permanent averaged subsystem charge distributions (often represented as multipole moments) obtained in first order, usually named electrostatic interaction energy, and interactions between the permanent charge distributions and static susceptibilities obtained in second order which usually are called second-order induction energy. Another contribution appearing in second order is the famous London dispersion energy [1,7]

$$\mathcal{E}_{\text{disp}}^{(2)} = - \sum_{a>0} \sum_{b>0} \frac{\langle 0^A | \hat{\rho}_{\mathbf{r}}^A | a^A \rangle \langle 0^B | \hat{\rho}_{\mathbf{r}'}^B | b^B \rangle \langle a^A | \hat{\rho}_{\mathbf{r}''}^A | 0^A \rangle \langle b^B | \hat{\rho}_{\mathbf{r}'''}^B | 0^B \rangle}{|\mathbf{r} - \mathbf{r}'| (E_a^A - E_0^A + E_b^B - E_0^B) |\mathbf{r}'' - \mathbf{r}'''|}, \quad (2)$$

given here in a form which avoids the multipole expansion. This stabilizing contribution represents a genuine quantum correlation effect between fluctuations of the charge distributions of the subsystems. It explains the long-range attraction which exists between two atoms, molecules, or larger pieces of matter even in the absence of any permanent electric field emitted by them [8–10]. In passing note that while the above considerations employed a classical electromagnetic field the latter may also be quantized, allowing to account for retardation effects which seamlessly change the leading power of the London dispersion interactions from $1/R^6$ to $1/R^7$ for very long intermolecular distances R [11]. Furthermore, the antisymmetry requirement for the electronic wavefunction of the total system, ignored above, may at least be taken into account *a posteriori* through symmetry-adapted perturbation theory (SAPT) [12,13].

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An important goal of a perturbation theory for subsystem interactions is a “factorization” of the various contributions into properties of the individual subsystems. While this is straightforwardly obtained for the first order and the induction part of the second order contributions Eq. (2) at first sight does not factorize. However, it is well known that this may be achieved through the Casimir-Polder integral identity [11,14]:

$$\frac{1}{x+y} = \frac{2}{\pi} \int_0^\infty du \frac{x}{x^2+u^2} \frac{y}{y^2+u^2}, \quad x, y > 0. \quad (3)$$

Using Eq. (3) transforms Eq. (2) to

$$\mathcal{E}_{\text{disp}}^{(2)} = -\frac{1}{2\pi} \int_0^\infty d\omega \frac{\alpha_{\mathbf{r}\mathbf{r}''}^A(i\omega) \alpha_{\mathbf{r}\mathbf{r}'''}^B(i\omega)}{|\mathbf{r} - \mathbf{r}'| |\mathbf{r}'' - \mathbf{r}'''|}, \quad (4)$$

where

$$\alpha_{\mathbf{r}\mathbf{r}'}^A(i\omega) = \left(\sum_{a>0} \frac{2(E_a^A - E_0^A) \langle 0^A | \hat{\rho}_{\mathbf{r}}^A | a^A \rangle \langle a^A | \hat{\rho}_{\mathbf{r}'}^A | 0^A \rangle}{(E_a^A - E_0^A)^2 + \omega^2} \right) \quad (5)$$

is the frequency-dependent charge density susceptibility of molecule A at imaginary frequencies [15] (for simplicity assuming real-valued eigenstates $|a^A\rangle$), with an analogous definition of $\alpha_{\mathbf{r}\mathbf{r}'}^B(i\omega)$. The calculation of linear response functions is a standard task in electronic structure theory, and consequently the Casimir-Polder identity has been used numerous times for evaluating the dispersion energy.

Recently an approach resulting in a different way of factorization has been proposed for computation of multireference perturbation theory and SAPT contributions on a quantum computer [16]: here the reduced resolvent operator that allows for a convenient formulation of the perturbation series [6,10,12] is represented as a linear combination of real time-evolution unitary operators at a series of time steps. Their coefficients are obtained as the coefficients of the Fourier series of an appropriate function evaluating to $1/E$ in certain range of energies. If the Hamiltonian occurring in the real time-evolution operators consists of a sum of commuting operators, factorization is readily achieved.

However, the Laplace transform

$$\frac{1}{x+y} = \int_0^\infty d\tau e^{-x\tau} e^{-y\tau}, \quad x, y > 0, \quad (6)$$

introduced by Almlöf in the framework of Møller-Plesset perturbation theory [17] allows for a further straightforward factorization, which to the best of my knowledge hitherto remains unexploited. Below it will be shown that this kind of factorization naturally results from perturbation theory in the Dirac picture of quantum mechanics employing imaginary time.

In the interaction picture (aka Dirac picture) of quantum mechanics [18,19] a time-dependent Hamiltonian is partitioned as $\hat{H}(t) = \hat{H}^0 + \hat{V}(t)$ to transform the time-dependent Schrödinger picture wavefunction $|\psi(t)\rangle$ according to $|\psi_I(t)\rangle = e^{i\hat{H}^0 t} |\psi(t)\rangle$. In the following exclusively static perturbations will be considered, i.e. $\hat{V}(t) = \hat{V}$, and normal time will be replaced with imaginary time, $\tau = it$, which from now on will be denoted as i-time. Introducing the i-time dependent perturbation operator

$$\hat{V}_I(\tau) = e^{\hat{H}^0 \tau} \hat{V} e^{-\hat{H}^0 \tau} \quad (7)$$

and the i-time evolution operator $\hat{U}_I(\tau, \tau_0)$, obeying

$$\hat{U}_I(\tau, \tau_0) = \hat{1} - \int_{\tau_0}^{\tau} d\tau' \hat{V}_I(\tau') \hat{U}_I(\tau', \tau_0), \quad (8)$$

the wavefunction may be propagated from i-time τ_0 to τ ($\tau \geq \tau_0$) through

$$|\psi_I(\tau)\rangle = \hat{U}_I(\tau, \tau_0) |\psi_I(\tau_0)\rangle. \quad (9)$$

Setting $|\psi_I(\tau_0 = 0)\rangle = |0\rangle$, where $\hat{H}^0 |0\rangle = E_0 |0\rangle$, Hogervorst *et al.* have shown [20] that the energy shift due to the static perturbation may be obtained from

$$\Delta \mathcal{E}_0 = \mathcal{E}_0 - E_0 = -\lim_{\tau \rightarrow \infty} \left(\frac{1}{\tau} \ln \langle 0 | \hat{U}(\tau, 0) | 0 \rangle \right). \quad (10)$$

Expanding $\Delta \mathcal{E}_0 = \mathcal{E}_0^{(1)} + \mathcal{E}_0^{(2)} + \mathcal{E}_0^{(3)} + \dots$ in orders of the perturbation it is seen that

$$\mathcal{E}_0^{(1)} = \langle 0 | \hat{V} | 0 \rangle. \quad (11)$$

While this is the standard first-order energy expression the second-order contribution now takes the less familiar form

$$\mathcal{E}_0^{(2)} = -\int_0^\infty d\tau \langle 0 | \hat{V}_I(\tau) \hat{V}_I(0) | 0 \rangle_{\text{conn}}, \quad (12)$$

where

$$\langle 0 | \hat{V}_I(\tau) \hat{V}_I(0) | 0 \rangle_{\text{conn}} = \langle 0 | \hat{V}_I(\tau) \hat{V} | 0 \rangle - \langle 0 | \hat{V} | 0 \rangle^2 \quad (13)$$

is a connected i-time dependent autocorrelation function [20] (*cf.* the Appendix for elementary derivation). Noting that

$$\begin{aligned} \langle 0 | e^{\hat{H}^0 \tau} \hat{V} e^{-\hat{H}^0 \tau} \hat{V} | 0 \rangle - \langle 0 | \hat{V} | 0 \rangle^2 \\ = \langle 0 | \hat{V} (e^{(E_0 - \hat{H}^0) \tau} - \hat{P}_0) \hat{V} | 0 \rangle, \end{aligned} \quad (14)$$

where $\hat{P}_0 = |0\rangle \langle 0|$ projects on the (unperturbed) ground state, allows to define the operator

$$\hat{R}_0(\tau) = e^{(E_0 - \hat{H}^0) \tau} - \hat{P}_0, \quad (15)$$

leading to a reformulation of Eq. (12) as

$$\mathcal{E}_0^{(2)} = -\int_0^\infty d\tau \langle 0 | \hat{V} \hat{R}_0(\tau) \hat{V} | 0 \rangle. \quad (16)$$

The operator $\hat{R}_0(\tau)$ fulfills

$$\begin{aligned} \hat{R}_0(\tau) | 0 \rangle &= 0, \quad \hat{R}_0(0) = \hat{1} - \hat{P}_0, \\ \frac{d}{d\tau} \hat{R}_0(\tau) &= (E_0 - \hat{H}^0) \hat{R}_0(\tau) \end{aligned} \quad (17)$$

and has the explicit representation

$$\hat{R}_0(\tau) = \sum_{i>0} |i\rangle e^{(E_0 - E_i) \tau} \langle i|, \quad (18)$$

where $|i\rangle$ denotes the eigenfunction of $\hat{H}^0$ corresponding to the eigenvalue E_i . In the following it will be called reduced i-time evolution operator: $\hat{R}_0(\tau)$ fulfills the same differential equation as the i-time evolution operator belonging to $\hat{H}_0$, apart from an energy shift and elimination of ground state contributions, and additionally it relates to a (static) operator $\hat{R}_0$ which sometimes is denoted as the reduced resolvent [6,12] through

$$\hat{R}_0 = \sum_{i>0} \frac{|i\rangle \langle i|}{E_i - E_0} = \int_0^\infty d\tau \hat{R}_0(\tau). \quad (19)$$

It is also directly related to the Green's function of the unperturbed Hamiltonian $G_{E_0}(\mathbf{R}, \mathbf{R}', \tau) = \langle \mathbf{R} | e^{(E_0 - \hat{H}_0)\tau} | \mathbf{R}' \rangle$, where $\mathbf{R}$ denotes the positions of the particles, as $\langle \mathbf{R} | \hat{R}_0(\tau) | \mathbf{R}' \rangle = G_{E_0}(\mathbf{R}, \mathbf{R}', \tau) - \langle \mathbf{R} | 0 \rangle \langle 0 | \mathbf{R}' \rangle$ and thus it (or its action on wavefunctions) in principle is accessible through, *e.g.*, Green's function or diffusion quantum Monte Carlo [21], numerical split operator imaginary time propagation [22,23] now becoming available on quantum computers as well [24], or other numerical and analytical path integral methods. In some cases like that of the harmonic oscillator it is even known analytically [25].

Most relevant in the present context, however, is the property

$$\hat{R}_0(\tau) = (\hat{R}_0^A(\tau) + \hat{P}_0^A)(\hat{R}_0^B(\tau) + \hat{P}_0^B) - \hat{P}_0^A \hat{P}_0^B, \quad (20)$$

holding true if $[\hat{H}^A, \hat{H}^B] = \hat{0}$, where

$$\hat{R}_0^A(\tau) = e^{(E_0^A - \hat{H}^A)\tau} - \hat{P}_0^A, \quad \hat{P}_0^A = |0^A\rangle\langle 0^A| \quad (21)$$

is the reduced i-time evolution operator of subsystem A with analogous definitions for $\hat{R}_0^B(\tau)$ and $\hat{P}_0^B$. Eq. (20) is the key to factorization of interaction energy of coupled systems into monomer properties. It resembles a well-known property of the Green's function of non-interacting particles, *i.e.*, that the latter decomposes into products of one-particle Green's functions [19], yet here it refers to non-interacting subsystems allowing for interactions between the particles *within* the subsystems. Note that Eq. (20) is easily generalized to systems composed of more subsystems, yet here the focus will be on the two subsystem case.

Applying the above to the Hamiltonian $\hat{H} = \hat{H}^A + \hat{H}^B + \hat{V}$ with $\hat{V}$ given by Eq. (1), one may split the second-order interaction energy of the coupled systems into three contributions

$$\mathcal{E}_0^{(2)} = - \int_0^\infty d\tau \langle 0^A 0^B | \hat{V} \hat{R}_0(\tau) \hat{V} | 0^A 0^B \rangle = \mathcal{E}_{i,A}^{(2)} + \mathcal{E}_{i,B}^{(2)} + \mathcal{E}_d^{(2)}. \quad (22)$$

Here

$$\mathcal{E}_{i,A}^{(2)} = -\mathcal{V}_x^B \left(\int_0^\infty d\tau \mathcal{K}_{xx'}^A(\tau) \right) \mathcal{V}_{x'}^B, \quad (23)$$

where the definitions

$$\mathcal{V}_x^B = T_{xx'} \langle 0^B | \hat{\rho}_x^B | 0^B \rangle \quad (24)$$

$$\mathcal{K}_{xx'}^A(\tau) = \langle 0^A | \hat{\rho}_x^A \hat{R}_0^A(\tau) \hat{\rho}_{x'}^A | 0^A \rangle \quad (25)$$

were used along with analogous definitions of the corresponding quantities for the respective other subsystem. The quantity $\mathcal{K}_{xx'}^A$ may also be written as

$$\mathcal{K}_{xx'}^A = \langle 0^A | (\hat{\rho}_x^A(\tau) - \rho_x^A) (\hat{\rho}_{x'}^A(0) - \rho_{x'}^A) | 0^A \rangle, \quad (26)$$

where $\hat{\rho}_x^A(\tau) = e^{\hat{H}^A \tau} \hat{\rho}_x^A e^{-\hat{H}^A \tau}$ and $\rho_x^A = \langle 0^A | \hat{\rho}_x^A | 0^A \rangle$, showing that it represents a cross correlation function of i-time density fluctuations. The third contribution to the r.h.s. of Eq. (22) reads

$$\mathcal{E}_d^{(2)} = - \int_0^\infty d\tau \mathcal{K}_{xx''}^A(\tau) T_{xx'} T_{x''x'''} \mathcal{K}_{x''x'''}^B(\tau). \quad (27)$$

Since it is possible to express third and higher order contributions with the help of the reduced resolvent [10], it can be shown that similar factorizations can also be achieved in higher than second order, and this also holds for systems composed of more than two subsystems. Details will be given elsewhere.

If the subsystems consist of molecules coupled through Coulomb interactions $\mathcal{E}_{i,A}^{(2)}$ becomes the second-order induction energy $\mathcal{E}_{\text{ind},A}^{(2)} = -\frac{1}{2} V_{\mathbf{r}}^B \alpha_{\mathbf{r}\mathbf{r}'}^A V_{\mathbf{r}'}^B$ of molecule A. Here $V_{\mathbf{r}}^B = (Z_k \delta_{\mathbf{r}\mathbf{r}_k} - \langle 0^B | \hat{\rho}_{\mathbf{r}}^B | 0^B \rangle) / |\mathbf{r} - \mathbf{r}'|$ is the electric potential of molecule B, with Z_k as the proton number of atom k and $\mathbf{r}_k$ its position, while $\alpha_{\mathbf{r}\mathbf{r}'}^A = \alpha_{\mathbf{r}\mathbf{r}'}^A(0) = 2 \int_0^\infty d\tau \mathcal{K}_{\mathbf{r}\mathbf{r}'}^A(\tau)$ is the static charge density susceptibility of molecule A. The third contribution $\mathcal{E}_d^{(2)}$ to the r.h.s. of Eq. (22) then represents the dispersion contribution $\mathcal{E}_{\text{disp}}^{(2)}$, which now alternatively to Eqs. (2) or (4) can be determined from

$$\mathcal{E}_{\text{disp}}^{(2)} = - \int_0^\infty d\tau \frac{\mathcal{K}_{\mathbf{r}\mathbf{r}'}^A(\tau) \mathcal{K}_{\mathbf{r}'\mathbf{r}''}^B(\tau)}{|\mathbf{r} - \mathbf{r}'| |\mathbf{r}' - \mathbf{r}''|}. \quad (28)$$

The direct appearance of i-time density fluctuation cross correlation functions in this formula nicely underpins the interpretation of London dispersion forces as caused by Coulomb interactions between fluctuations of the charge densities of both molecules. Finally, note that

$$\int_{-\infty}^\infty d\tau e^{-x|\tau|} e^{-i u \tau} = \frac{2x}{x^2 + u^2}$$

also allows to calculate the frequency-dependent charge susceptibility at imaginary frequencies $\alpha_{\mathbf{r}\mathbf{r}'}(i\omega)$ from the i-time density fluctuation cross correlation function $\mathcal{K}_{\mathbf{r}\mathbf{r}'}(\tau)$, *i.e.*, essentially by a Fourier cosine transformation. This may be seen as a consequence of the fluctuation dissipation theorem in imaginary time [19], yet the latter usually is formulated for finite temperatures while the link between $\mathcal{K}(\tau)$ and $\alpha(i\omega)$ as a Fourier cosine transform pair holds at absolute zero.

In summary, employing a recently derived reformulation of Rayleigh-Schrödinger perturbation theory energy contributions in terms of integrals over imaginary time-dependent connected correlation functions [20] here it was shown that the second-order interaction energy of weakly coupled quantum systems in a natural way factorizes into integrals over products of correlation functions of the individual quantum systems. Key to this finding was the introduction of a reduced imaginary time evolution operator which also allows to factorize the higher-order interactions energies in a similar way, as will be detailed elsewhere. Application of the formalism to the second-order intermolecular interaction energy yields an alternative to the well-known Casimir-Polder factorization of the London dispersion energy contribution, offering hitherto unexploited routes to its numerical determination.

Data availability. No data were created or analyzed in this study.

Appendix: Derivation of Eqs. (11) and (12). Starting from Eq. (10) and plugging in the Dyson series

$$\begin{aligned} \hat{U}_I(\tau, 0) &= \hat{1} - \int_0^\tau d\tau_1 \hat{V}_I(\tau_1) \\ &\quad + \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \hat{V}_I(\tau_1) \hat{V}_I(\tau_2) - \dots \end{aligned}$$

for the i-time evolution operator one can expand the logarithm and separate the contributions of increasing order in the interaction potential as

$$\begin{aligned}\mathcal{E}_0^{(1)} &= \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau d\tau_1 \langle 0 | \hat{V}_1(\tau_1) | 0 \rangle, \\ \mathcal{E}_0^{(2)} &= - \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \left(\int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \langle 0 | \hat{V}_1(\tau_1) \hat{V}_1(\tau_2) | 0 \rangle \right. \\ &\quad \left. - \frac{1}{2} \int_0^\tau d\tau_1 \langle 0 | \hat{V}_1(\tau_1) | 0 \rangle \int_0^\tau d\tau_2 \langle 0 | \hat{V}_1(\tau_2) | 0 \rangle \right).\end{aligned}$$

Using

$$\langle 0 | \hat{V}_1(\tau_1) | 0 \rangle = \langle 0 | \hat{V}_1(0) | 0 \rangle = \langle 0 | \hat{V} | 0 \rangle$$

application of the rule of l'Hospital directly leads to

$$\mathcal{E}_0^{(1)} = \langle 0 | \hat{V} | 0 \rangle.$$

Furthermore

$$\begin{aligned}\langle 0 | \hat{V}_1(\tau_1) \hat{V}_1(\tau_2) | 0 \rangle &= \langle 0 | e^{E_0 \tau_1} \hat{V} e^{-\hat{H}_0(\tau_1 - \tau_2)} \hat{V} e^{E_0 \tau_2} | 0 \rangle \\ &= \langle 0 | \hat{V}_1(\tau_1 - \tau_2) \hat{V}_1(0) | 0 \rangle\end{aligned}$$

and the rule of l'Hospital allow to write

$$\mathcal{E}_0^{(2)} = - \int_0^\infty d\tau_2 (\langle 0 | \hat{V}_1(\tau - \tau_2) \hat{V}_1(0) | 0 \rangle - \langle 0 | \hat{V}_1(0) | 0 \rangle^2)$$

which, after first changing the integral variable to $\tau' = \tau - \tau_2$ and then reversing the resulting integration limits becomes

$$\mathcal{E}_0^{(2)} = - \int_0^\infty d\tau' (\langle 0 | \hat{V}_1(\tau') \hat{V} | 0 \rangle - \langle 0 | \hat{V} | 0 \rangle^2).$$

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