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Normalization corrections to perturbation theory for the time-independent nonlinear Schrödinger equation

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In higher orders of the Rayleigh-Schrödinger-type perturbation theory for nonlinear time-independent Hamiltonians care should be taken about the normalization in the wave-function-dependent perturbation operator. Low-order results, which have been presented earlier [P. R. Surján and J. Ángyán, Phys. Rev. A **28**, 45 (1983)], remain valid; nevertheless, small corrections appear for higher orders ($n \geq 3$). Explicit expressions are given for the energy correction in the generalized reaction-field theory in terms of nonlocal polarizabilities and reaction-field response functions.

I. INTRODUCTION

In a previous paper [1] a modification of the Rayleigh-Schrödinger (RS) perturbation theory has been proposed to solve the time-independent nonlinear Schrödinger equation,

$$[\hat{H}^0+\hat{V}(\psi)]|\psi\rangle = E|\psi\rangle , \tag{1}$$

which arises, e.g., in the average reaction field models of solvent effects [2–7]. The nonlinearity in these models appears as a consequence of the wave-function dependence of the potential. Explicit energy and wave-function corrections were given at the lowest orders and recursion formulas were derived at the general order for the following specific form of the nonlinear perturbation:

$$\hat{V}(\psi)=\hat{A}\langle\psi|\hat{B}|\psi\rangle . \tag{2}$$

The same equation has been treated with a different perturbation formalism by Cioslowski [8–10]. A related nonlinear problem concerning intermolecular interactions has also been discussed recently by one of us [11].

The form (2) of the nonlinear term in the solute-only reaction-field Hamiltonian is widespread in the literature [3,12]. Nevertheless, we should be aware of the fact that in Eq. (2) the wave function ψ is implicitly assumed to be normalized to 1.

While usual variational algorithms for the solution of the nonlinear Schrödinger equation (1) take normalization into account, this is not so in perturbation theory, when intermediate normalization is used. Normalization corrections are expected to appear from third order in the nonlinear perturbation operator. In our previous paper [1] such corrections have not been evaluated.

In the present paper normalization terms are considered explicitly, i.e., instead of Eq. (2) we write

$$\hat{V}(\psi)=\hat{A}\frac{\langle\psi|\hat{B}|\psi\rangle}{\langle\psi|\psi\rangle} . \tag{3}$$

Although the first- and second-order results of Ref. 1 remain valid, higher-order results must be revisited. In the following the RS-type perturbation theory (PT) will be developed first by *arbitrary* nonlinear perturbation. Low-order formulas, taking into consideration normalization effects, will be given explicitly. Specific results in the framework of the generalized reaction-field model will be given in Sec. IV.

II. NONLINEAR PERTURBATION THEORY

Any arbitrary nonlinear perturbation can be partitioned into contributions of a different order, such as

$$\hat{V}(\psi)=\hat{V}^{(1)}+\hat{V}^{(2)}+\hat{V}^{(3)}+\cdots . \tag{4}$$

We are looking for the solutions of the Schrödinger equation

$$[\hat{H}^0+\hat{V}(\psi_k)]|\psi_k\rangle = E_k|\psi_k\rangle . \tag{5}$$

Suppose that the solutions of the zeroth-order equation,

$$\hat{H}^0|\psi_k^{(0)}\rangle = E_k^{(0)}|\psi_k^{(0)}\rangle , \tag{6}$$

are known, and the exact solutions ψ_k satisfy the intermediate normalization condition:

$$\langle\psi_k^{(0)}|\psi_l\rangle=\delta_{kl} . \tag{7}$$

We introduce the reduced resolvent operator $\hat{R}_k$ which satisfies the following equation:

$$\hat{R}_k(\hat{H}^0-E_k^{(0)})=1-|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}| . \tag{8}$$

Let us define the perturbational energy correction ΔE_k as the difference of the exact and zeroth-order energies:

$$\Delta E_k = E_k - E_k^{(0)} . \tag{9}$$

Then the Schrödinger equation can be rewritten as

$$(\hat{H}^0 - E_k^{(0)})|\psi_k\rangle = (\Delta E_k - \hat{V}_k)|\psi_k\rangle , \tag{10}$$

where the subscript recalls the wave-function dependence of the perturbation. Apply the reduced resolvent operator from the left; use Eq. (8) and the intermediate normalization condition to get

$$\begin{aligned}\hat{R}_k(\hat{H}^0 - E_k^{(0)})|\psi_k\rangle &= (1 - |\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|)|\psi_k\rangle \\ &= |\psi_k\rangle - |\psi_k^{(0)}\rangle = \hat{R}_k(\Delta E_k - \hat{V}_k)|\psi_k\rangle .\end{aligned} \tag{11}$$

The following equation is obtained for the perturbed wave function:

$$|\psi_k\rangle = |\psi_k^{(0)}\rangle + \hat{R}_k(\Delta E_k - \hat{V}_k)|\psi_k\rangle , \tag{12}$$

while the energy correction can be obtained by multiplying the Schrödinger equation (10) with $\langle\psi_k^{(0)}|$ from the left:

$$\Delta E_k = \langle\psi_k^{(0)}|\hat{V}_k|\psi_k\rangle . \tag{13}$$

Explicit equations for corrections of a given order can be obtained by inserting the expansions of the wave function ψ_k, the perturbational energy correction, ΔE_k of Eq. (9) and the nonlinear perturbation operator $\hat{V}_k$ of Eq. (4):

$$|\psi_k\rangle = \sum_{\mu=0}^{\infty} |\psi_k^{(\mu)}\rangle , \tag{14}$$

$$\Delta E_k = \sum_{\mu=1}^{\infty} E_k^{(\mu)} , \tag{15}$$

$$\hat{V}_k = \sum_{\mu=1}^{\infty} \hat{V}_k^{(\mu)} , \tag{16}$$

The nth-order energy correction $E_k^{(n)}$ can be obtained by expanding Eq. (13):

$$E_k^{(n)} = \sum_{\mu=1}^{n} \langle\psi_k^{(0)}|\hat{V}_k^{(\mu)}|\psi_k^{(n-\mu)}\rangle , \tag{17}$$

while the nth-order wave-function correction is obtained immediately from Eq. (12):

$$|\psi_k^{(n)}\rangle = \hat{R}_k \sum_{\mu=1}^{n} (E_k^{(\mu)} - \hat{V}_k^{(\mu)})|\psi_k^{(n-\mu)}\rangle . \tag{18}$$

This result can be made more explicit by inserting the spectral resolution of the reduced resolvent operator and expanding the solution with respect to the unperturbed eigenvectors of $\hat{H}^0$:

$$|\psi_k^{(n)}\rangle = \sum_{l\neq k} c_{kl}^{(n)}|\psi_l^{(0)}\rangle . \tag{19}$$

The expansion coefficients $c_{kl}^{(n)}$ are obtained from Eq. (18) as

$$c_{kl}^{(n)} = \langle\psi_l^{(0)}|\psi_k^{(n)}\rangle = \sum_{\nu=1}^{n} \frac{\langle\psi_l^{(0)}|E_k^{(\nu)} - \hat{V}_k^{(\nu)}|\psi_k^{(n-\nu)}\rangle}{(E_l^{(0)} - E_k^{(0)})} \tag{20}$$

or

$$c_{kl}^{(n)} = \sum_{\nu=1}^{n} \frac{c_{kl}^{(n-\nu)}E_k^{(\nu)} - \sum_{m\neq k} c_{km}^{(n-\nu)}\langle\psi_l^{(0)}|\hat{V}_k^{(\nu)}|\psi_m^{(0)}\rangle}{(E_l^{(0)} - E_k^{(0)})} . \tag{21}$$

III. COMPARISON WITH PREVIOUS RESULTS

The above formulas are valid for arbitrary nonlinear perturbation, which can be expanded in a series, according to Eq. (4). The results, presented in our previous paper [1] can be obtained through an expansion of the operator $\hat{V} = \hat{A}\langle\psi|\hat{B}|\psi\rangle$, by inserting the series (14). In order to account for the normalization correction properly we are going to expand, however, the normalized operator (3). The energy corrections at the lowest orders remain unchanged:

$$E_k^{(1)} = \langle\psi_k^{(0)}|\hat{A}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{B}|\psi_k^{(0)}\rangle , \tag{22}$$

$$\begin{aligned}E_k^{(2)} = \sum_{i\neq k} \frac{\langle\psi_i^{(0)}|\hat{A}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{B}|\psi_k^{(0)}\rangle}{E_k^{(0)} - E_i^{(0)}} &\times (\langle\psi_k^{(0)}|\hat{A}|\psi_i^{(0)}\rangle\langle\psi_k^{(0)}|\hat{B}|\psi_k^{(0)}\rangle \\ &+ 2\langle\psi_k^{(0)}|\hat{A}|\psi_k^{(0)}\rangle\langle\psi_k^{(0)}|\hat{B}|\psi_i^{(0)}\rangle) .\end{aligned} \tag{23}$$

On the other hand the third-order energy correction has to be slightly modified with respect to Ref. [1]. Using the shorthand notation for the matrix elements of $\hat{A}$ and $\hat{B}$, we get

$$\begin{aligned}E_k^{(3)} = &\sum_{i\neq k} c_{ki}^{(2)}(2A_{kk}B_{ki} + A_{ki}B_{kk}) \\ &+ \sum_{i\neq k}\sum_{l\neq k} c_{ki}^{(1)}c_{kl}^{(1)}[2A_{ki}B_{kl} + A_{kk}(B_{il} - B_{kk}\delta_{il})] .\end{aligned} \tag{24}$$

The only difference from the formula (13) of Ref. [1], apart from a misprint, is that the B_{kk} matrix elements should be subtracted from the diagonal matrix elements of the $\hat{B}$ operator. This means that the normalization correction is

$$\delta = -A_{kk}B_{kk}\sum_{i\neq k}(c_{ki}^{(1)})^2 . \tag{25}$$

A similar correction holds for Eq. (21) of Ref. [1], too. Note that δ is always negative.

Higher-order energy corrections can be obtained in a similar manner. Perturbed wave functions, given in Ref. [1], are not repeated here because normalization corrections do not affect $c_{ki}^{(1)}$ and $c_{ki}^{(2)}$, which influence the energy up to third order.

It might be interesting to estimate the magnitude of energy corrections of various orders and the correction to the third-order energy δ. This can be done most easily in the framework of a simple dipolar model outlined in Sec. VI of Ref. 1. In this model we have $\hat{A} = \hat{\mu}$, $\hat{B} = -g\hat{\mu}$, where $\hat{\mu}$ is the dipole-moment operator and g is the reaction-field factor, which can be estimated to be around 0.01 in atomic units [13,14]. The formulas of low-order corrections and the normalization correction are collected in Table I. The corresponding values can be approximated by using a dipole moment $\mu = \langle \psi | \hat{\mu} | \psi \rangle = 0.73$ a.u., a dipole polarizability $\alpha = 8.3$ a.u., and a hyperpolarizabilty $\beta = 5.5$ a.u. These data, taken from Dykstra *et al.* [15], represent a typical polarizable polar species, the water molecule.

For the sake of completeness we report the definition of α and β:

$$\alpha = 2 \sum_{i \neq 0} \frac{\mu_{0i}\mu_{i0}}{E_i^{(0)} - E_0^{(0)}} , \tag{26}$$

$$\beta = 6 \sum_{i,j \neq 0} \frac{\mu_{0i}(\mu_{ij} - \delta_{ij}\mu_{00})\mu_{j0}}{(E_i^0 - E_0^0)(E_j^0 - E_0^0)} . \tag{27}$$

An upper bound to the normalization correction, δ, can be found by rewriting the definition (25) of δ for the ground state:

$$\begin{aligned} |\delta| &= A_{00} B_{00} \sum_{i \neq 0} B_{00}^2 \frac{|A_{0i}|^2}{[E_o^{(0)} - E_i(0)]^2} \\ &= g^3 \mu^4 \sum_{i \neq 0} \frac{|\mu_{0i}|^2}{[E_0^{(0)} - E_0(0)]^2} \\ &\leq \frac{1}{2\Delta E_{01}} \alpha g^3 \mu^4 , \end{aligned} \tag{28}$$

where ΔE_{01} is the lowest excitation energy, which has a typical value of 0.3 a.u. (8 eV) for the water molecule.

By taking a glance at the numerical estimates reported in Table I, one finds that the perturbational series converges reasonably well with the present parameters. The normalization correction is smaller by an order of magnitude than the total third-order contribution, although it is larger in absolute value than the hyperpolarizability contribution itself.

TABLE I. Low-order PT terms and their approximate values with an estimate of the normalization correction δ for a typical parameter set, given in the text.

Term	Formula	Value
$E^{(1)}$	$g\mu^2$	$+5.3\times10^{-3}$
$E^{(2)}$	$-\frac{3}{2}\alpha g^2\mu^2$	-6.6×10^{-4}
$E^{(3)}$	$2\alpha^2 g^3\mu^2$	$+7.4\times10^{-5}$
	$+\frac{2}{3}\beta g^3\mu^3$	$+1.4\times10^{-6}$
δ	$-(1/2\Delta E_{01})\alpha g^3\mu^4$	-3.9×10^{-6}

IV. GENERALIZED AVERAGE REACTION-FIELD OPERATOR

Recent developments of solvent effect theories put into evidence the general mathematical structure of the nonlinear term in the reaction-field model Hamiltonian. The simple Onsager model, discussed in [1], can be considered as a special case of this generalized reaction-field theory. Accordingly, the nonlinear model Hamiltonian operator is written in a more general form:

$$\hat{H} = \hat{H}^0 + \int \int d\mathbf{r}\, d\mathbf{s}\, \hat{\rho}(\mathbf{r}) G(\mathbf{r},\mathbf{s}) \frac{\langle \psi_k | \hat{\rho}(\mathbf{s}) | \psi_k \rangle}{\langle \psi_k | \psi_k \rangle} , \tag{29}$$

where $G(\mathbf{r},\mathbf{s})$ is the *reaction potential response function* of the solvent and $\hat{\rho}(\mathbf{r})$ is the total charge-density operator of the solute subsystem at the space point $\mathbf{r}$.

$\hat{H}^0$ can be considered as the zeroth-order operator and the rest of the Hamiltonian as perturbation. The normalized expectation value of the charge density, which appears in the nonlinear perturbation operator, can be developed in terms of the unperturbed charge density

$$\langle \hat{\rho}_r \rangle_k = \langle \psi_k^{(0)} | \hat{\rho}_k | \psi_k^{(0)} \rangle , \tag{30}$$

and charge-density response functions of the system. The subscripts of the charge-density operator may stand either for continuous or discrete arguments. At the lowest orders we need the generalized polarizability (linear charge-density response function), $\alpha_{rr'}$:

$$\alpha_{rr'} = \sum_{i \neq k} \left[\frac{\langle \psi_k^{(0)} | \hat{\rho}_r | \psi_i^{(0)} \rangle \langle \psi_i^{(0)} | \hat{\rho}_{r'} | \psi_k^{(0)} \rangle}{(E_i^{(0)} - E_k^{(0)})} + \frac{\langle \psi_k^{(0)} | \hat{\rho}_{r'} | \psi_i^{(0)} \rangle \langle \psi_i^{(0)} | \hat{\rho}_r | \psi_k^{(0)} \rangle}{(E_i^{(0)} - E_k^{(0)})} \right] \tag{31}$$

and hyperpolarizability (nonlinear charge-density response function):

$$\beta_{rr'r'} = \sum_{i \neq k} \sum_{l \neq k} S(r,r',r'') \frac{\langle \psi_k^{(0)} | \hat{\rho}_r | \psi_i^{(0)} \rangle \langle \psi_i^{(0)} | \hat{\rho}_{r'} - \langle \hat{\rho}_{r'} \rangle | \psi_l^{(0)} \rangle \langle \psi_l^{(0)} | \hat{\rho}_{r''} | \psi_k^{(0)} \rangle}{(E_i^{(0)} - E_k^{(0)})(E_l^{(0)} - E_k^{(0)})} , \tag{32}$$

where $S(r,r',r'')$ stand for all permutation of the $\hat{\rho}_r$, $\hat{\rho}_{r'}$, and $\hat{\rho}_{r''}$ operators. With the help for the above-mentioned quantities the charge density can be expanded to the lowest orders as

$$\begin{aligned} \frac{\langle \psi_k | \hat{\rho}_r | \psi_k \rangle}{\langle \psi_k | \psi_k \rangle} = {} & \langle \hat{\rho}_r \rangle_k - \alpha_{rs'} G_{s's} \langle \hat{\rho}_s \rangle_k \\ & + \alpha_{rs'} G_{s's''} \alpha_{s''s'''} G_{s'''s} \langle \hat{\rho}_s \rangle_k \\ & + \tfrac{1}{2} \beta_{rr'r''} G_{r's'} \langle \hat{\rho}_{s'} \rangle_k G_{r''s''} \langle \hat{\rho}_{s''} \rangle_k + \cdots , \end{aligned} \tag{33}$$

where repeated subscripts of the charge-density operators and response functions involve integration over continuous or summation over discrete variables.

The first-order eigenvalue and eigenvector corrections are analogous with the usual "linear PT" results:

$$E_k^{(1)} = \langle \hat{\rho}_r \rangle_k G_{rs} \langle \hat{\rho}_s \rangle_k , \tag{34}$$

$$c_{ki}^{(1)} = -\frac{\langle \psi_i^{(0)} | \hat{\rho}_r | \psi_k^{(0)} \rangle}{E_k^{(0)} - E_i^{(0)}} G_{rs} \langle \hat{\rho}_s \rangle_k , \tag{35}$$

where the $c_{ki}^{(1)}$ expansion coefficients are defined in Eq.

(19).

The second order eigenvalue correction is

$$E_k^{(2)} = -\tfrac{3}{2}\langle \hat{\rho}_r \rangle_k G_{rs}\alpha_{ss'}G_{r's'}\langle \hat{\rho}_s \rangle_k \ . \tag{36}$$

A linear Rayleigh-Schrödinger-type (RS) and a nonlinearity (non-RS) component can be easily identified in the second-order wave-function correction. The former is due to the first-order perturbation operator:

$$c_{ki}^{(2)}(\mathrm{RS}) = \sum_{j\neq k} \frac{\langle \psi_i^{(0)}|\hat{\rho}_r - \langle \hat{\rho}_r \rangle|\psi_k^{(0)}\rangle\langle \psi_j^{(0)}|\hat{\rho}_{r'}|\psi_k^{(0)}\rangle}{(E_i^{(0)}-E_k^{(0)})(E_j^{(0)}-E_k^{(0)})} \times G_{r's'}\langle \hat{\rho}_{s'} \rangle_k G_{rs}\langle \hat{\rho}_s \rangle_k \ , \tag{37}$$

while the $c_{ki}^{(2)}$ (non-RS) term is essentially a first-order wave-function correction, due to a higher-order reaction-field contribution:

$$c_{ki}^{(2)}(\text{non-RS}) = \frac{\langle \psi_i^{(0)}|\hat{\rho}_r|\psi_k^{(0)}\rangle}{E_i^{(0)}-E_k^{(0)}} G_{rs}\alpha_{ss'}G_{s'r'}\langle \hat{\rho}_s \rangle_k \ . \tag{38}$$

Third-order eigenvalue corrections can also be expressed in terms of polarizabilities and hyperpolarizabilities:

$$E_k^{(3)} = 2\langle \hat{\rho}_r \rangle_k G_{rs}\alpha_{ss''}G_{s''r''}\alpha_{r''s'}G_{s'r'}\langle \hat{\rho}_{r'} \rangle_k + \tfrac{1}{2}\beta_{rr'r''}G_{rs}\langle \hat{\rho}_s \rangle_k G_{r's'}\langle \rho_{s'} \rangle_k G_{r''s''}\langle \hat{\rho}_{s''} \rangle_k \ . \tag{39}$$

In the generalized reaction-field model the energy $\mathcal{E}_k$, associated with the total solute-solvent system is related to the eigenvalue of the nonlinear Schrödinger equation by

$$\mathcal{E}_k = E_k - \frac{1}{2}\frac{\langle \psi_k|\hat{V}(\psi_k)|\psi_k\rangle}{\langle \psi_k|\psi_k\rangle} \ , \tag{40}$$

where half of the expectation value of the nonlinear reaction-field operator is the polarization work, necessary to distort the solvent charge distribution, in the linear response approximation. Since in most of the physical applications this total energy is the meaningful one, we give the lowest-order corrections, as obtained by inserting the perturbational expansion of the wave function in Eq. (40):

$$\begin{aligned} \mathcal{E}_k^{(1)} &= \tfrac{1}{2}\langle \hat{\rho}_r \rangle_k G_{rs}\langle \hat{\rho}_s \rangle_k \ , \\ \mathcal{E}_k^{(2)} &= -\tfrac{1}{2}\langle \hat{\rho}_r \rangle_k G_{rs}\alpha_{ss'}G_{r's'}\langle \hat{\rho}_s \rangle_k \ . \end{aligned} \tag{41}$$

Note, that the appropriate factor in the total energy expression is $\frac{1}{2}$, which corrects the value of $\frac{3}{4}$ in Eq. (26) of Ref. [1].

The third-order correction reads

$$\mathcal{E}_k^{(3)} = \tfrac{1}{2}\langle \hat{\rho}_r \rangle G_{rs}\alpha_{ss''}G_{ss''r''}\alpha_{r''s'}G_{s'r'}\langle \hat{\rho}_{r'} \rangle + \tfrac{1}{2}\beta_{rr'r''}G_{rs}\langle \hat{\rho}_s \rangle G_{r's'}\langle \hat{\rho}_{s'} \rangle G_{r''s''}\langle \hat{\rho}_{s''} \rangle \ . \tag{42}$$

Two kinds of higher-order contributions can be distinguished in the third-order energy correction. One is due to the higher polarizabilities of the system, while the other term comes from the iteration of linear polarizabilities. Provided that the linear polarizability is much larger than the higher-order hyperpolarizabilities, these latter contributions might be neglected.

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