Brief Reports

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Estimation of the overlap between the approximate and exact wave function of the ground state from the connected-moments expansion

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A connected-moments expansion (CMX) is constructed for the overlap between the approximate and the exact (but unknown) wave function of the ground state. The CMX series provides approximations to the overlap that do not require the knowledge of the exact energy of either the ground or the first excited state. Moreover, the obtained approximate overlaps have a correct size extensivity. A numerical example is given, demonstrating the performance of the new method.

The quality of approximate description of the ground state can be judged from the magnitude of the overlap between the approximate and the exact wave function corresponding to this state.[1] Several upper and lower bounds to the overlap have been derived.[1–4] Upper bounds require usually the knowledge of the moments of Hamiltonian and the exact ground-state energy. Lower bounds, like Eckart's,[2] demand also the exact energy of the first excited state.

Despite the quite extensive information required, the performance of these bounds is often not very impressive, since their quality deteriorates for extended systems. The source of this shortcoming can be easily singled out: All the known bounds do not possess a proper size extensivity. The issue of size extensivity is most strikingly demonstrated in the example of Eckart's bound:

$$S^2=\langle\phi\mid Q\rangle^2\geq 1-[(E-E_0)/(E_1-E_0)]\ , \tag{1}$$

where

$$E=\langle\phi\mid\hat{H}\mid\phi\rangle,\quad E_0=\langle Q\mid\hat{H}\mid Q\rangle\ , \tag{2}$$

$\mid Q\rangle$ and $\mid\phi\rangle$ are the exact and approximate wave functions, respectively and E_1 is the exact energy of the first excited state possessing the same symmetry as the ground state. It is not difficult to find out that for the system of M independent particles (subsystems), the exact overlap is a product of the overlaps for the single-particle wave functions and therefore *the logarithm of the overlap is a size extensive quantity.* On the contrary, the Eckart's bound, Eq. (1), does not exhibit a proper size extensivity and for large values of M becomes negative, making the bound completely useless.

Quite recently, a new approach to the calculation of approximate eigenenergies of the Hamiltonian has been elaborated. The connected-moments expansions (CMX's) provide energies of the ground[5–7] and excited states[8] as well as the approximations to the expectation values of various operators.[8,9] In this paper we construct the CMX series for the overlap that bears a proper size extensivity and can be calculated *without* the knowledge of either the exact ground state or the first excited state energy.

As pointed out by several authors,[10,11] the ket

$$\mid\phi_t\rangle=\langle\phi\mid\exp(-t\hat{H})\mid\phi\rangle^{-1/2}\exp(-t\hat{H}/2)\mid\phi\rangle \tag{3}$$

is normalized and approaches the exact ground-state wave function, provided that

$$\langle\phi\mid Q\rangle\neq 0,\quad\langle\phi\mid\phi\rangle=1\ . \tag{4}$$

From this we immediately conclude that the function

$$\begin{aligned}U(t)&=\langle\phi\mid\phi_t\rangle^2\\&=\langle\phi\mid\exp(-t\hat{H}/2)\mid\phi\rangle^2/\langle\phi\mid\exp(-t\hat{H})\mid\phi\rangle\end{aligned} \tag{5}$$

has the limit

$$S^2=\lim_{t\to\infty}U(t)\ . \tag{6}$$

Furthermore,

$$[\ln U(t)]'=U'(t)/U(t)=F(t)-F(t/2)\ , \tag{7}$$

where $F(t)$ is the familiar Horn-Weinstein function[5,8,11]

$$F(t)=\langle \phi_t \mid \hat{H} \mid \phi_t \rangle = \langle \phi \mid \hat{H} \exp(-t\hat{H}) \mid \phi \rangle / \langle \phi \mid \exp(-t\hat{H}) \mid \phi \rangle \; . \tag{8}$$

In terms of the moments of the Hamiltonian,

$$\langle H^k \rangle = \langle \phi \mid \hat{H}^k \mid \phi \rangle \; , \tag{9}$$

$F(t)$ has the form

$$F(t)=\frac{\left[\sum_{k=0}^{\infty} (-t)^k \langle H^{k+1} \rangle / k!\right]}{\left[\sum_{k=0}^{\infty} (-t)^k \langle H^k \rangle / k!\right]} \tag{10}$$

and can be also expressed with the use of the connected moments, I_k, as

$$F(t)=\sum_{k=0}^{\infty} (-t)^k I_{k+1}/k! \; , \tag{11}$$

where

$$I_1=\langle H \rangle, \quad I_k=\langle H^k \rangle - \sum_{i=1}^{k-1} \binom{k-1}{i-1} I_i \langle H^{k-i} \rangle \; . \tag{12}$$

From the above discussion it is clear that

$$S^2=\exp\left[-\int_0^{\infty} [F(t)-F(\infty)]dt\right] \tag{13}$$

and therefore any size-extensive approximation to $F(t)$ will provide an estimate for S^2 that bears a proper size extensivity.

To derive the connected-moments expansion for the ground-state energy, the following Nth-order approximation to $F(t)$ has been proposed:[5]

$$F_N(t)=A_0+\sum_{i=1}^{N-1} A_i \exp(-b_i t), \quad b_i>0 \; . \tag{14}$$

The coefficients A_i and b_i are obtained from the condition that the first $2N-1$ terms in the Taylor expansion of $F_N(t)$ have to match those of $F(t)$, which gives rise to the equations

$$I_1=A_0+\sum_{i=1}^{N-1} A_i \; , \tag{15}$$

$$I_{k+1}=\sum_{i=1}^{N-1} A_i b_i^k, \quad k=1,2,\ldots,2N-1 \; . \tag{16}$$

Any quantity depending solely on A_i's and b_i's can be conveniently expressed in terms of the helper function[7]

$$f_N(t)=\sum_{i=1}^{N-1} A_i b_i (1-b_i t)^{-1} = \mathbf{V}_N(\underline{P}_N - t\underline{Q}_N)^{-1}\mathbf{V}_N^{\dagger} \; , \tag{17}$$

where

$$\mathbf{V}_N=(I_2,\ldots,I_N) \; , \tag{18}$$

$$\underline{P}_N=\begin{bmatrix} I_2 & \cdots & I_N \\ \cdots & \cdots & \cdots \\ I_N & \cdots & I_{2N-2} \end{bmatrix} \; , \tag{19}$$

and

$$\underline{Q}_N=\begin{bmatrix} I_3 & \cdots & I_{N+1} \\ \cdots & \cdots & \cdots \\ I_{N+1} & \cdots & I_{2N-1} \end{bmatrix} \; . \tag{20}$$

Taking into account Eqs. (13) and (17), we obtain for the Nth-order approximation to the overlap, S_N,

$$\ln S_N^2 = -\int_0^{\infty} [F_N(t)-F_N(\infty)]dt = \sum_{i=1}^{N-1} A_i/b_i = -\lim_{t\to\infty} [t^2 f_N(t)+t^3 f_N'(t)] \; , \tag{21}$$

or more explicitly

$$\ln S_N^2 = -\mathbf{V}_N \underline{\mathbf{Q}}_N^{-1} \underline{\mathbf{P}}_N \underline{\mathbf{Q}}_N^{-1} \mathbf{V}_N^{\dagger} \; . \tag{22}$$

As can be seen from Eq. (22), the Nth-order approximation to S^2, which we denote by CMX(N), requires the knowledge of only $2N-1$ connected moments. Various numerical tests indicate that the CMX series provides approximations to the exact overlap that, although not being rigorous bounds, have considerable accuracy.

Let us consider the following anharmonic oscillator Hamiltonian:

$$\hat{H}=-(\tfrac{1}{2})d^2/dx^2-(\tfrac{1}{2})d^2/dy^2+x^2/2+y^2/2+0.1x^2y^2 \; , \tag{23}$$

with the choice of the trial ket

$$|\phi\rangle=\pi^{-1/2}\exp[-(x^2+y^2)/2] \tag{24}$$

as an example. The exact overlap is 0.999 704 4, while Eckart's formula gives the value of 0.999 622 8 for the lower bound. On the other hand, we obtain the approximate overlaps of 0.999 809 7, 0.999 733 8, and 0.999 709 1 from CMX(2), CMX(3), and CMX(4), respectively.

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