Generalized moments expansion applied to the two-dimensional $S=\frac{1}{2}$ Heisenberg model

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In this work we derive a generalized moments expansion (GMX), to third order, of which the well-established connected moments expansion and the alternate moments expansion are shown to be special cases. We discuss the benefits of the GMX with respect to the avoidance of singularities which are known to plague such moments methods. We then apply the GMX estimates for the ground-state energy for the two-dimensional $S=1/2$ Heisenberg square lattice and compare these results to those of both spin-wave theory and the linked-cluster expansion.

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I. INTRODUCTION

Since its development nearly 20 years ago, the connected moments expansion (CMX) of Cioslowski[1] has found great use as a calculational tool for both the quantum chemist as well as the many-body physicist. This scheme is based on the "t expansion" of Horn and Weinstein[2] wherein the ground-state expectation values of any Hamiltonian system may be evaluated. The value of any analytic methodology for calculating the energy spectrum for (strongly) interacting many-body systems is immense. Of particular interest is the accurate estimation of the ground-state energy of such systems and the settling of questions involving the nature of the ground state or, in the case of Horn and Weinstein, of the vacuum state. A number of calculational tools remain available to the theorist from standard perturbation and variational schemes to the more demanding and computationally more time consuming and detail-laden exact diagonalizations. Also Monte Carlo studies have, at zero temperature and finite cluster size and extrapolated to the bulk limit, proven to be a useful tool. In this paper we wish to briefly review the work of Horn and Weinstein in order to reconsider those arguments that led to Cioslowski's development of the CMX. We also shall review the paper of Mancini, Zhou, and Meier[3] in which they were able to derive a calculational cousin of the CMX, the alternate moments expansion (AMX). We will then derive a generalized moments expansion (GMX) of which both the CMX and AMX are special cases. Finally, as a straightforward application of the GMX we then apply it to the $S=\frac{1}{2}$ Heisenberg antiferromagnet on a square lattice (at zero temperature).

II. THEORY

As a first step in deriving the GMX it is both useful and instructional to review the original derivation of the CMX equations of Cioslowski. We then reconstruct the motivation of Mancini *et al.* in their derivation of the AMX. Once this methodology has been presented and after we have introduced the idea of a "helper function," the derivation (and motivation) of the GMX will become, we hope, clear. In the t expansion, Horn and Weinstein pointed out that for any Hamiltonian $\hat{H}$ one may construct the operator $\exp(-t\hat{H})$ which has the property of contracting any trial state $|\phi_0\rangle$ onto to the ground state $|\psi_0\rangle$ provided that there is a nonzero overlap between these states. It is then straightforward to show that all ground-state operator expectation values in these (contracted) states may be expressed as a power series in the parameter t. As noted by Stubbins,[4] the $t\to\infty$ limit of this series must be handled carefully. Among the extrapolation methods considered by Stubbins are the Padé approximant, the D-Padé analysis, Laplace or resolvent analysis, inversion analysis, and the "E of F" or partition function method.[4,5]

Of particular interest is a theorem relating the ratio

$$\frac{\langle\phi_0|\hat{H}\exp(-\hat{H}t)|\phi_0\rangle}{\langle\phi_0|\exp(-\hat{H}t)|\phi_0\rangle}$$

to a series expansion in the parameter t wherein the coefficients in the expansion are connected moments of expectation values of the Hamiltonian. This then was the initiation point for Cioslowski who considered the t expansion

$$E(t)=E_0+\sum_k(-t)^k\frac{I_{k+1}}{k!}. \tag{1}$$

Here the I_k are the connected moments of the Hamiltonian defined recursively by

$$I_k=\langle\hat{H}^k\rangle-\sum_{p=0}^{k-2}\begin{bmatrix}k-1\\ p\end{bmatrix}I_{p+1}\langle\hat{H}^{k-p-1}\rangle \tag{2}$$

where we have introduced the notation $\langle\hat{H}^k\rangle=\langle\phi_0|\hat{H}^k|\phi_0\rangle$. Cioslowski then recast the expansion in Eq. (1) by comparing it to the series

$$E(t) = E_0 + \sum_j A_j e^{-b_j t}. \tag{3}$$

Then expanding Eq. (3) in a Taylor series

$$E(t) = \sum_n a_n t^n \tag{4}$$

with

$$a_n = \frac{1}{n!} \left. \frac{d^n}{dt^n} E(t) \right|_{t=0}$$

yields explicit expressions for the coefficients a_n,

$$a_0 = E_0 + \sum_j A_j,$$

$$a_1 = -\sum_j A_j b_j,$$

$$a_2 = \frac{1}{2!} \sum_j A_j b_j^2,$$

$$\vdots$$

$$a_n = \frac{(-1)^n}{n!} \sum_j A_j b_j^n. \tag{5}$$

That is,

$$E(t) = E_0 + \sum_j A_j + \left(-\sum_j A_j b_j \right) t + \left(\frac{1}{2!} \sum_j A_j b_j^2 \right) t^2 + \cdots. \tag{6}$$

Now comparing Eq. (1) with Eq. (6), we make the identification

$$I_1 = E_0 + \sum_j A_j,$$

$$I_2 = \sum_j A_j b_j,$$

$$\vdots$$

$$I_n = \sum_j A_j b_j^{n-1}. \tag{7}$$

At this point Cioslowski introduces the functions

$$P_1 = I_1 - E_0 = \sum_j A_j,$$

$$P_k = I_k = \sum_j A_j b_j^{n-1}, \tag{8}$$

where the P_k's are related through

$$P_1 = \sum_k W_k(P_2, P_3, P_4, \ldots). \tag{9}$$

The problem has now been recast into one in which we must determine the functions W_k. Consider the helper function

$$S_k = P_k P_{k+2} - P_{k+1}^2. \tag{10}$$

This was the critical insight of Cioslowski. He noted that substitution of Eq. (8) into Eq. (10) leads to a functional relationship of the S_k's similar to that of the P_k's through the coefficients A_j and b_j. Thus we may write $S_1 = \Sigma_k W_k(S_2, S_3, S_4, \ldots)$, with $S_1 = P_1 P_3 - P_2^2$. Solving for P_1

$$P_1 = \frac{P_2^2}{P_3} + \frac{1}{P_3} \sum_k W_k(S_2, S_3, S_4, \ldots). \tag{11}$$

Comparison of Eq. (11) and Eq. (9) yields

$$W_1 = \frac{P_2^2}{P_3},$$

$$W_{k+1} = \frac{1}{P_3} W_k. \tag{12}$$

Then the CMX expression for the ground-state energy E_0 (to third order) is given by

$$E_0^{(\mathrm{CMX})} = I_1 - \frac{I_2^2}{I_3} - \left(\frac{1}{I_3} \right) \frac{(I_4 I_2 - I_3^2)^2}{(I_5 I_3 - I_4^2)}. \tag{13}$$

With a bit of clever mathematical maneuvering, Stubbins was able to rewrite the expansion Eq. (13) in matrix form which permitted him to make the following two important observations: (i) a disadvantage of methods that approximate the series as exponentials is that if one has an odd power series then the last order is not included in the approximation and (ii) the matrix inverse may not exist and thus answers in this region should be discarded. This second point, the existence of singularities in certain regions of parameter space is a major object of concern in each of these moments systems. It should be noted that the success of this expression in estimating the ground-state energy has been mixed.[6–9] Following the approach of Cioslowski, Mancini *et al.*[3] hit upon the idea of using a different helper function than Eq. (10). Instead they chose

$$S_k = P_k P_{k+3} - P_{k+1} P_{k+2}, \tag{14}$$

which, systematically, leads to the alternate moments expansion for the ground-state energy (to third order)

$$E_0^{(\mathrm{AMX})} = I_1 - \frac{I_3 I_2}{I_4} - \frac{1}{I_4} \frac{(I_2 I_5 - I_3 I_4)(I_3 I_6 - I_4 I_5)}{(I_4 I_7 - I_5 I_6)}. \tag{15}$$

Most recently both the CMX and the AMX have been applied to the Rabi Hamiltonian.[10]

At this point there are no *a priori* means of determining which expansion (if either) converges more rapidly.[11] Indeed, singularities in parameter space are known to plague these moments methods.[3,12–14] One reason for these singularities may be that a symmetric differential operator acting on a given functional space is not automatically a self-adjoint operator and may have many self-adjoint extensions.[15]

We now wish to generalize the arguments, and hence the helper functions used to derive both the CMX and AMX. If we look at the helper functions for these expansions,

TABLE I. Ground-state energy to second order calculated using GMX(1,1) to (1,13).

λ	GMX(1,1)	GMX(1,2)	GMX(1,3)	GMX(1,4)	GMX(1,5)	GMX(1,6)	GMX(1,7)	GMX(1,8)	GMX(1,9)	GMX(1,10)	GMX(1,11)	GMX(1,12)	GMX(1,13)
0.20	−0.50666667	−0.50674157	−0.50701893	−0.50794596	−0.51313410	−0.49457117	−0.50140053	−0.50275591	−0.50377271	−0.50697705	−0.49704178	−0.50085098	−0.50173876
0.50	−0.54166667	−0.54477612	−0.56250000	−0.41497462	−0.50510760	−0.51642240	−0.53085695	−0.46812126	−0.50368489	−0.51070242	−0.52229349	−0.48528970	−0.50320386
0.80	−0.60666667	−0.62972973	−3.61578947	−0.49865941	−0.53605709	−0.58600538	−0.46649864	−0.51312991	−0.53345704	0.02289639	−0.50092738	−0.51673982	−0.54768367
0.90	−0.63500000	−0.67419355	−0.04510870	−0.51019437	−0.55176660	−0.69326168	−0.48703861	−0.52290390	−0.55877719	−0.46042145	−0.50983722	−0.52935352	−0.17067123
0.95	−0.65041667	−0.70074143	−0.19576434	−0.51603636	−0.56123868	−0.89849526	−0.49384489	−0.52857582	−0.58281414	−0.47686613	−0.51429208	−0.53923138	−0.43909399
0.98	−0.66006667	−0.71830580	−0.24396110	−0.51961846	−0.56756060	−1.47480410	−0.49749816	−0.53232224	−0.60625162	−0.48322923	−0.51711119	−0.54742698	−0.46177868
0.99	−0.66335000	−0.72445895	−0.25654728	−0.52082848	−0.56978708	−2.33084502	−0.49866946	−0.53363728	−0.61678455	−0.48503797	−0.51808511	−0.55073370	−0.46655290
1.00	−0.66666667	−0.73076923	−0.26785714	−0.52204724	−0.57207719	−14.22274143	−0.49982264	−0.53498825	−0.62935277	−0.48673012	−0.51907888	−0.55441625	−0.47055658

TABLE II. Ground-state energy to second order calculated using GMX(2,2) to (2,12).

λ	GMX(2,2)	GMX(2,3)	GMX(2,4)	GMX(2,5)	GMX(2,6)	GMX(2,7)	GMX(2,8)	GMX(2,9)	GMX(2,10)	GMX(2,11)	GMX(2,12)
0.20	−0.50709779	−0.50836581	−0.51565445	−0.48930458	−0.49885951	−0.50057896	−0.50155959	−0.50394836	−0.49690405	−0.49962239	−0.50022195
0.50	−0.56716418	−0.37246193	−0.48957739	−0.50201310	−0.51216188	−0.47639166	−0.49718073	−0.50094649	−0.50572626	−0.49212934	−0.49886888
0.80	−4.28947368	−0.46084069	−0.49954683	−0.52907285	−0.47298784	−0.49587622	−0.50411832	−0.33598847	−0.49545383	−0.50014554	−0.50748327
0.90	0.08695652	−0.46564942	−0.50390909	−0.57410742	−0.48144489	−0.49780099	−0.50997205	−0.48276803	−0.49711598	−0.50213894	−0.42839289
0.95	−0.09397651	−0.46756454	−0.50652884	−0.66223816	−0.48369340	−0.49883067	−0.51573284	−0.48726330	−0.49780190	−0.50372763	−0.48411461
0.98	−0.15080314	−0.46861876	−0.50828052	−0.91144326	−0.48476381	−0.49949480	−0.52145537	−0.48886763	−0.49820720	−0.50506996	−0.48867521
0.99	−0.16547205	−0.46895776	−0.50889843	−1.28218141	−0.48508721	−0.49972601	−0.52404845	−0.48930313	−0.49834350	−0.50561692	−0.48961191
1.00	−0.17857143	−0.46929134	−0.50953462	−6.43457944	−0.48539650	−0.49996277	−0.52715496	−0.48970103	−0.49848095	−0.50622921	−0.49038680

TABLE III. Ground-state energy to second order calculated using GMX(3,3) to (3,11).

λ	GMX(3,3)	GMX(3,4)	GMX(3,5)	GMX(3,6)	GMX(3,7)	GMX(3,8)	GMX(3,9)	GMX(3,10)	GMX(3,11)
0.20	−0.51629849	−0.48739384	−0.49777807	−0.49953378	−0.50032400	−0.50161406	−0.49826745	−0.49960920	−0.49990261
0.50	−0.48545178	−0.49617733	−0.50138730	−0.49134125	−0.49805713	−0.49932614	−0.50047125	−0.49811875	−0.49943683
0.80	−0.48911606	−0.49969957	−0.49249224	−0.49726611	−0.49893649	−0.48340044	−0.49882755	−0.49941338	−0.50005349
0.90	−0.48979174	−0.50433700	−0.49448582	−0.49756027	−0.49925800	−0.49773425	−0.49902686	−0.49951401	−0.49595614
0.95	−0.49010516	−0.51296051	−0.49502547	−0.49767873	−0.49951760	−0.49818691	−0.49909319	−0.49957042	−0.49886902
0.98	−0.49028823	−0.53697513	−0.49528475	−0.49774414	−0.49975412	−0.49835175	−0.49912743	−0.49961051	−0.49911234
0.99	−0.49034858	−0.57258186	−0.49536343	−0.49776518	−0.49985745	−0.49839697	−0.49913813	−0.49962559	−0.49916301
1.00	−0.49040863	−1.06697819	−0.49543882	−0.49778588	−0.49997913	−0.49843851	−0.49914853	−0.49964180	−0.49920523

$$S_k^{(\mathrm{CMX})} = P_k P_{k+2} - P_{k+1} P_{k+1},$$

$$S_k^{(\mathrm{AMX})} = P_k P_{k+3} - P_{k+1} P_{k+2},$$

we note that there is a sum rule for the subscripts. The sum rule states that the subscript sum in any S_k expression must be equal, even though the subscripts of each term in the products can be different. For example, consider

$$S_k = P_k P_{k+4} - P_{k+3} P_{k+1} \tag{16}$$

and

$$S_k = P_k P_{k+5} - P_{k+3} P_{k+2},$$

$$S_k = P_k P_{k+5} - P_{k+4} P_{k+1}, \tag{17}$$

we see in Eq. (17) that there are actually two sum rules for the combination $P_k P_{k+5}$. Inspired by this symmetry we write the following helper function:

$$S_k^{(m,n)} = P_k P_{k+(m+n)} - P_{k+m} P_{k+n} \tag{18}$$

and observe that $S_k^{(1,1)} = S_k^{(\mathrm{CMX})}$ and $S_k^{(1,2)} = S_k^{(\mathrm{AMX})}$. Now using the ansatz of Eq. (18) and the recursive argument of Cioslowski we arrive at a generalized moments expansion to third order,

$$E_0^{\mathrm{GMX}(m,n)} = I_1 - \frac{I_{n+1} I_{m+1}}{I_{n+m+1}} - \frac{1}{I_{n+m+1}} \left(\frac{(I_{m+1} I_{n+2m+1} - I_{m+n+1} I_{2m+1})(I_{n+1} I_{2n+m+1} - I_{2n+1} I_{n+m+1})}{(I_{n+m+1} I_{2(n+m)+1} - I_{2n+m+1} I_{n+2m+1})} \right). \tag{19}$$

Equation (19) represents our main result. Once again the condition of size extensiveness is preserved since the moments I_k are related to cumulants.[19] Here it should be noted that one obvious advantage of the GMX expression is in the avoidance of singularities. That is, it is well established that both the CMX and the AMX are plagued by poles appearing in the denominators of each respective expansion. However, the GMX allows for one to avoid a particular pole by choosing a different value for (m,n). Hence, in theory at least, all regions of parameter space may now be examined. This is an exciting result and thus adds to the versatility afforded by such moments methods.

Before we apply Eq. (19) to the $S=\frac{1}{2}$ Heisenberg square lattice, we should mention a word on scaling. As has been shown previously[16] each of the connected moments of the

TABLE IV. Ground-state energy to second order calculated using GMX(4,4) to (4,10).

λ	GMX(4,4)	GMX(4,5)	GMX(4,6)	GMX(4,7)	GMX(4,8)	GMX(4,9)	GMX(4,10)
0.20	−0.49748461	−0.49912758	−0.49974940	−0.50032206	−0.49931973	−0.49978994	−0.49990319
0.50	−0.49811271	−0.49929239	−0.49948950	−0.49966731	−0.49975964	−0.49988908	−0.49990356
0.80	−0.50000323	−0.49996836	−0.49997064	−0.50017848	−0.49999506	−0.49999370	−0.49999102
0.90	−0.50012358	−0.50027764	−0.50031524	−0.49993544	−0.50004900	−0.50006280	−0.49964816
0.95	−0.50026221	−0.50046724	−0.50063186	−0.49996332	−0.50008517	−0.50011693	−0.49991400
0.98	−0.50036130	−0.50059525	−0.50093614	−0.49998389	−0.50011015	−0.50016163	−0.49994186
0.99	−0.50039668	−0.50064062	−0.50107205	−0.49999124	−0.50011908	−0.50017961	−0.49994856
1.00	−0.50043319	−0.50068745	−0.50123373	−0.49999881	−0.50012833	−0.50019959	−0.49995457

TABLE V. Ground-state energy to third order calculated using GMX(1,1) to (1,6).

λ	GMX(1,1)	GMX(1,2)	GMX(1,3)	GMX(1,4)	GMX(1,5)	GMX(1,6)
0.20	−0.50664537	−0.50660489	−0.50650783	−0.50591683	−0.52650975	−0.52007212
0.50	−0.54084839	−0.53900032	−0.52519335	−0.29419611	−0.51797880	−0.51735817
0.80	−0.60146341	−0.58643916	−0.42004626	−0.37539936	−0.53723727	−0.53254509
0.90	−0.62677201	−0.60097607	−0.38051451	−0.57589170	−0.54965238	−0.50625670
0.95	−0.64027274	−0.60719414	−0.36989634	−0.54457181	−0.55606226	−0.48248887
0.98	−0.64862891	−0.61047112	−0.36610920	−0.53978018	−0.55989123	−0.46696204
0.99	−0.65145564	−0.61147791	−0.36521698	−0.53905920	−0.56115608	−0.46188642
1.00	−0.65430267	−0.61243920	−0.36449223	−0.53863427	−0.56241245	−0.45694710

Hamiltonian $I_k \sim \langle \hat{H}^k \rangle$ to leading order. Thus for example (to third order) CMX $\sim I_5$ while AMX $\sim I_7$. For the generalized expansion Eq. (19), we have that $E_0^{(m,n)} \sim I_{2(m+n)+1}$ to third order.

We are now poised to study the ground-state energy of the $S=\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice. Here we shall use the already calculated connected moments of Zheng, Oitma, and Hamer[17] who extended the work of Lee and Lo.[18] We shall also compare our results to those of Mancini, Massano, and Murawski.[8]

The anisotropic $S=\frac{1}{2}$ Heisenberg antiferromagnet may be described by the well-known Hamiltonian

$$H = \sum_{\langle lm \rangle} S_l^z S_m^z + \lambda (S_l^x S_m^x + S_l^y S_m^y) \tag{20}$$

where $\langle lm \rangle$ denotes nearest-neighbor pairs and S^x, S^y, S^z are spin operators and λ is the coupling parameter. A spin rotation on the odd sublattice m yields the following transformed Hamiltonian:

$$H = \sum_{\langle lm \rangle} S_l^z S_m^z - \frac{\lambda}{2} (S_l^+ S_m^+ + S_l^- S_m^-) \tag{21}$$

which has a ground state at $\lambda=0$ of all spins "up." Here $S^{\pm}$ are the usual spin raising and lowering operators. A listing of the connected moments for this system may be found in the Appendix of Ref. 17.

In Tables I–VII we have summarized our results for the two-dimensional $S=1/2$ Heisenberg model using the GMX(m,n) expansion for the ground-state energy. Once again we reiterate that the particular cases GMX$(1,1)$ and GMX$(1,2)$ are just the well-known CMX and AMX expansions, respectively. First some general comments regarding the nature of this particular Hamiltonian. The physically most interesting point is the isotropic point $\lambda=1$, where standard perturbation theory has given more accurate results than the best current Monte Carlo estimates for the ground-state energy, while coupled-cluster methods are 3–5 times less accurate and t-expansion methods are an order of magnitude worse.[17] As Zheng *et al.* have noted, this may not be a fair comparison of these different schemes as the value $\lambda=1$ is a singular point corresponding to a Goldstone-type first-order transition in which physical observables display square-root singularities (from spin-wave theory). Hence it is a bit surprising that overall, all orders of GMX(m,n) are relatively well behaved and consistent with extrapolations of the ground-state energy from the small-coupling regime. Once again this result is encouraging.

In second order, we notice a number of interesting features. For example GMX$(1,8)$ appears to have a local minimum (signaling perhaps a pole) near the value $\lambda=0.5$ while GMX$(1,3)$ is well behaved only for values of $\lambda \leqslant 0.5$. GMX$(1,7)$ also is fine only at small values of λ. On the other hand GMX$(2,5)$ grossly undershoots the CMX $=$GMX$(1,1)$ results for small λ while at $\lambda=1$ there is large discrepancy. So how do we interpret such data? Well, by its very nature for (m,n) "large," GMX(m,n) contains only higher-order moments of the Hamiltonian. Physically this means that the very low-energy excitations are not being included in the expansions for E_0. Hence one would expect,

TABLE VI. Ground-state energy to third order calculated using GMX(2,2) to (2,5) and GMX(3,3) to (3,4).

λ	GMX(2,2)	GMX(2,3)	GMX(2,4)	GMX(2,5)	GMX(3,3)	GMX(3,4)
0.20	−0.50639731	−0.50533305	−0.48975331	−0.48496548	−0.49270540	−0.49061509
0.50	−0.51889962	−0.45152196	−0.48403716	−0.50176056	−0.48557484	−0.49506369
0.80	−0.43441975	−0.45885139	−0.49861516	−0.50737448	−0.48453357	−0.49899526
0.90	−0.40434037	−0.46288339	−0.50282857	−0.49497429	−0.48586896	−0.49683825
0.95	−0.39331392	−0.46514041	−0.50515244	−0.48524702	−0.48638879	−0.48845469
0.98	−0.38790044	−0.46668398	−0.50660019	−0.47953783	−0.48667752	−0.48490639
0.99	−0.38627869	−0.46724984	−0.50708968	−0.47776911	−0.48677088	−0.48448904
1.00	−0.38474284	−0.46785045	−0.50758192	−0.47609014	−0.48686301	−0.48437658

TABLE VII. For comparison reasons we list ground-state energy calculated using different methods (Ref. 17).

λ	CMX-LT seventh order	Spin-wave theory third order	Laplace method seventh order
0.20	−0.50666529	−0.50657179	−0.5066653
0.50	−0.54163641	−0.5413803	−0.5416359
0.80	−0.60677223	−0.607376	−0.6067604
0.90	−0.63537633	−0.636654	−0.6353801
0.95	−0.65101764	−0.652718	−0.6510589
0.98	−0.66083842	−0.66287	−0.6609227
0.99	−0.66418527	−0.66637	−0.6642888
1.00	−0.66756890	−0.6699993	−0.6676946

for example, GMX(1,8) to yield poor results for the ground-state energy, especially at small values of the coupling constant λ. The appearance of local minima may indicate for these particular expansions the existence of singularities in parameter space. For the third order results, it is apparent that the GMX(1,1)=CMX(3) values are best throughout the entire range of λ. Once again there seems to be a bit of anomalous behavior in most of the GMX expressions, most of which exhibit a (local) minimum at $\lambda=0.2$ followed by oscillatory behavior before settling down (i.e., converging). Again we attribute this to the onset of singularities. An earlier calculation by Mancini *et al.*[8] using a Lanczos tridiagonal scheme as well as the AMX and CMX up to CMX(8) was also severely plagued by the appearance of singularities. In particular, they made the following observations: (i) all orders of the AMX have poles and (ii) all orders of the CMX(N) (for $N\geqslant 4$) have poles. One then is encouraged that GMX(m,n) may avoid such singularities for any particular choice of (m,n) and thus investigate the entire range of parameter space.

At this point there is no way to determine *a priori* which values of (m,n) will yield the lowest estimate for E_0 at any particular order. A general observation may be made, however, that the best overall results for the two-dimensional $S=1/2$ Heisenberg model, for all regions of parameter space, seem to be the well-established CMX and AMX expansions. It is certainly the case that, overall, at small values of the parameter λ, the GMX(m,n) results appear to have lower estimates for E_0 than the CMX and AMX. However, at the singular point $\lambda=1.0$ the CMX gives the best (most negative) results. The ultimate accuracy depends both on the particular Hamiltonian under investigation and most importantly on the quality of the reference function, chosen to have maximal overlap with the true ground-state wave function. Clearly more results are needed for a variety of Hamiltonian systems in order to determine whether or not there does indeed exist a systematic way of predicting which values of (m,n) will be best. In the meantime, through the derivation of the GMX we have at least uncovered a way to avoid unwanted poles without resorting to any particular approximation scheme or continuity trickery.[12] This then allows for a study of E_0 throughout all regions of parameter space.

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[1] J. Cioslowski, Phys. Rev. Lett. **58**, 83 (1987); Phys. Rev. A **36**, 374 (1987); **36**, 3441 (1987); Chem. Phys. Lett. **134**, 507 (1987).
[2] D. Horn and M. Weinstein, Phys. Rev. D **30**, 1256 (1984).
[3] J. D. Mancini, Y. Zhou, and P. F. Meier, Int. J. Quantum Chem. **50**, 101 (1994).
[4] C. Stubbins, Phys. Rev. D **38**, 1942 (1988).
[5] For a list of original references see N. S. Witte, Int. J. Mod. Phys. B **11**, 1503 (1997).
[6] W. J. Massano, S. P. Bowen, and J. D. Mancini, Phys. Rev. A **39**, 4301 (1989).
[7] J. D. Mancini and W. J. Massano, Phys. Lett. A **160**, 457 (1991).
[8] J. D. Mancini, W. J. Massano, and R. Murawski, Solid State Commun. **104**, 517 (1997).
[9] J. D. Mancini, J. D. Prie, W. J. Massano, and Y. Zhou, Phys. Lett. A **236**, 232 (1997).
[10] V. Fessatidis, J. D. Mancini, and S. P. Bowen, Phys. Lett. A **297**, 170 (2002).
[11] V. Fessatidis, J. D. Mancini, and S. P. Bowen, and W. J. Massano, Int. J. Quantum Chem. **103**, 792 (2005).
[12] N. Ullah, Phys. Rev. A **51**, 1808 (1995).
[13] J. D. Mancini, W. J. Massano, J. D. Prie, and Y. Zhou, Phys. Lett. A **209**, 107 (1995).
[14] J. D. Mancini, Y. Zhou, P. F. Meier, W. J. Massano, and J. D. Prie, Phys. Lett. A **185**, 435 (1994).
[15] G. Bonneau, J. Faraut, and G. Valent, Am. J. Phys. **69**, 322 (2001).
[16] J. D. Mancini, J. D. Prie, D. Schwall, and D. Kraus, Nuovo Cimento Soc. Ital. Fis., D **16**, 433 (1994).
[17] W. Zheng, J. Oitmaa, and C. J. Hamer, Phys. Rev. B **52**, 10278 (1995).
[18] K. C. Lee and F. C. Lo, J. Phys.: Condens. Matter **6**, 7075 (1994).
[19] R. Kubo, J. Phys. Soc. Jpn. **17**, 1100 (1962).