

Resummation of the Holstein-Primakoff expansion and differential equation approach to operator square roots

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Operator square roots are ubiquitous in theoretical physics. They appear, for example, in the Holstein-Primakoff representation of spin operators and in the Klein-Gordon equation. Often the use of a perturbative expansion is the only recourse when dealing with them. In this paper, we show that under certain conditions, differential equations can be derived which can be used to find perturbatively inaccessible approximations to operator square roots. Specifically, for the number operator $\hat{n} = a^\dagger a$ we show that the square root $\sqrt{\hat{n}}$ near $\hat{n} = 0$ can be approximated by a polynomial in \hat{n} . This result is unexpected because a Taylor expansion fails. A polynomial expression in \hat{n} is possible because \hat{n} is an operator, and its constituents a and a^\dagger have a non trivial commutator $[a, a^\dagger] = 1$ and do not behave as scalars. We apply our approach to the zero-mass Klein-Gordon Hamiltonian in a constant magnetic field and, as a main application, the Holstein-Primakoff representation of spin operators, where we are able to find new expressions that are polynomial in bosonic operators. We prove that these new expressions exactly reproduce spin operators. Our expressions are manifestly Hermitian, which offers an advantage over other methods, such as the Dyson-Maleev representation.

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I. INTRODUCTION

Square roots of operators appear in a large number of contexts in theoretical physics and also play an important role in operator theory. In some cases, it is practical to calculate the operator square root (OSR) using explicit formulas or by diagonalizing the operator. Often, however, there is only a very limited set of analytical tools to treat them, typically in the form of perturbative expansions.

This is not because OSRs represent a niche problem. Indeed, one of the earliest appearances was near the beginning of quantum mechanics in the square root of the Klein-Gordon equation [1–7]. Even for such an old problem it may prove useful to have a larger analytical toolbox. Another prominent example of OSRs occurs in the Holstein-Primakoff spin representation [8,9], which is the usual starting point for spin-wave-theory calculations. A third important OSR shows up in the context of quantum information in the form of the fidelity function [10–23] and the Bures metric [12,17,20,23–25], both

used to quantify the closeness of two quantum states. The purpose of the current paper is, however, not to review all examples of OSRs, but to introduce a nonperturbative approximation of OSRs.

Our method is inspired by several flow equation approaches to many-body problems. For instance, the Wegner flow equation approach [26], which was applied to various problems [26–40], allows for a nonperturbative diagonalization of a Hamiltonian using flow equations for its couplings. In this approach, the problem of diagonalization is recast in terms of differential equations. Similar methods have recently been used by some of us to find effective Floquet Hamiltonians [41] and various approximations to the time evolution operator [42]. Differential equation approaches have also been used in the method of unitary integration for the Liouville-Bloch equation [43] and Lindblad equation [44]. We aim to use a similar approach to approximate an operator square root.

The application that may be of most current interest is the Holstein-Primakoff (HP) OSR. The HP representation is typically used in the context of spin (local moment) models to represent deviations around a well-defined spin order in terms of a single species of boson per lattice site. It allows for a perturbative expansion in the number operator of such bosons and ultimately leads to linear [45] and nonlinear [46] spin-wave descriptions of quantum magnets [9]. However, for many systems of interest a ground-state spin ordering may be unknown or fail to exist, such as in frustrated systems [47],

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spin liquids [48–51], and one-dimensional systems [52]. In such cases, the perturbative expansion often proves inaccurate or inconvenient.

Instead, more symmetric spin representations such as Schwinger bosons [9,53] and slave particle approaches [54,55] are commonly used, but require the introduction of auxiliary fields. Other fermionic approaches include the Jordan-Wigner representation of spin-1/2 operators [56] and its generally complicated-to-use generalizations to higher dimensions [57,58] and higher spin [59–61]. An important, equivalent alternative to the HP representation that also uses a single boson species, but avoids the square root, is the Dyson-Maleev representation [62–65]. However, it has the drawback of generically breaking Hermiticity. This is by no means an exhaustive list of spin representations—indeed, other representations can be found in Refs. [66–71]. Since each of the available approaches has its own unique advantages and drawbacks, we will in this paper derive expressions for spin operators that (i) involve only one boson species satisfying the canonical bosonic commutation relation, (ii) preserve Hermiticity, and (iii) do not include square roots of operators or other nonpolynomial functions of operators.

Some of the expressions we derive were previously found to finite order in Refs. [72,73] by a matching-matrix-elements (MME) method and have also been usefully applied in Ref. [74] to capture effects beyond the reach of a $1/S$ expansion (where S is spin length). Unlike the normal Taylor expansion of the HP OSR, the MME expansion and our result are able to correctly describe the symmetry in a Heisenberg model with easy-plane anisotropy as we will see later in the text. This is a long-standing problem and was discussed using a slightly different approach in Ref. [75]. Our expansion thus naturally captures the same physics. However, unlike previous works, we present results to all orders and show that the expressions are exact when truncated to an appropriate order that depends on the spin length S . This feature was missed in all previous discussions we are aware of, since they focused entirely on reproducing commutation relations of spin operators. We, however, use a slightly softer exactness criterion. Namely, we require only that the operators are block diagonal with physical and unphysical subspace blocks. In the commutator language we require that the commutators are reproduced up to a term that acts exclusively on the unphysical subspace, without coupling to the physical subspace. This is akin to allowing an inaccessible “dark sector” in the spin-operator algebra. A more detailed discussion of this rationale is given in a later section.

Our hope is that such a representation may prove useful in describing spectral features not readily captured by conventional spin-wave theory, as is the case in, e.g., the triangular-lattice antiferromagnet $\text{Ba}_3\text{CoSb}_2\text{O}_9$ [74,76] and quantum spin liquid candidates. Among the latter, the Kitaev spin liquid [77–96] is receiving particularly intense attention, since it hosts anyonic excitations of interest to topological quantum computing. While the ideal model is solvable [77], and its dynamics known [97], the description of realistic candidate materials [98–100] requires additional Hamiltonian terms, which generically breaks integrability. Some such candidates include $\alpha\text{-RuCl}_3$ [101–114], CrI_3 [115–119], and honeycomb iridium oxides [120–123].

This paper is structured as follows. In Sec. II we discuss how to compute square roots of operators by using a differential equation approach. In Sec. III we show how this formalism may be used to find a series expansion for $\sqrt{a^\dagger a}$ near $a^\dagger a \approx 0$ in terms of integer powers of $(a^\dagger a)$, which is an unexpected result because \sqrt{x} cannot be expanded in integer powers of x near $x = 0$. Of course, since $a^\dagger a$ is an operator, $a^\dagger a \approx 0$ is shorthand for “in the part of the Hilbert space where matrix elements are close to zero.” We will use similar kinds of shorthand throughout the text. This shows that a Taylor series may not always be ideal for finding power-series expansions of operator functions. In Sec. IV we then apply the method to the Klein-Gordon particle in a magnetic field with small or zero mass—such as in graphene. In Sec. V we present our main application to the Holstein-Primakoff representation of spin operators. We stress that the results we obtain are exact expressions for spin operators that are polynomial in bosonic operators. Lastly, we present our conclusion.

II. GENERAL FORMALISM

The goal of this section is to find an operator differential equation that can be used to calculate a square root of two operators, $\sqrt{O_1 + O_2}$, where O_1 and O_2 are both operators defined on the same complex Hilbert space \mathcal{H} . We will make two simplifying assumptions. First, we assume that a square root of one of the operators, O_1 , is known or easy to calculate. Second, we assume that the two operators commute, $[O_1, O_2] = 0$. Both these assumptions also have to be made in order for a Taylor expansion in O_2 to be viable (the more generic case is more involved; see Appendix A for details). For instance, one could have $O_1 = c\mathbb{1}$ with $c \in \mathbb{C}$, and O_2 could be any other operator. It should be noted that the OSR of an operator O_1 can have multiple branches, which may seem like an ambiguity. However, the choice of branch will be encoded in the initial conditions for the differential equations we derive and should be informed by the problem at hand. Different branch choices can lead to different physics; for example, a branch with complex eigenvalues could not be used to describe a Hermitian Hamiltonian. The way we will compute $\sqrt{O_1 + O_2}$ is by introducing the second operator O_2 in infinitesimal steps. To keep track of the steps, we introduce a dummy parameter s and define

$$O_{\sqrt{\cdot}}(s) := \sqrt{O_1 + sO_2}. \quad (1)$$

Using the assumption $[O_1, O_2] = 0$, we find that sending $s \rightarrow s + \delta s$ gives

$$O_{\sqrt{\cdot}}(s + \delta s) = O_{\sqrt{\cdot}}(s) + \frac{\delta s}{2O_{\sqrt{\cdot}}(s)} O_2 \quad (2)$$

if δs is infinitesimal, and we therefore did a Taylor expansion of the right-hand side.

A Taylor expansion of the left side gives us the differential equation

$$\frac{dO_{\sqrt{\cdot}}(s)}{ds} = \frac{1}{2O_{\sqrt{\cdot}}(s)} O_2 \quad (3)$$

that makes it possible to find $O_{\sqrt{\cdot}}(s)$ by introducing O_2 via infinitesimal steps. Note that this also means that $\sqrt{O_1}$ for the

branch used needs to be invertible, or at least the limit of an invertible operator as we will see in the upcoming section.

The issue with this equation is that calculating the inverse of an operator is difficult. That is, we cannot easily make an ansatz for $O_{\sqrt{\cdot}}(s) = \sum_n c_n(s) \hat{O}_n$ as a sum of operators with s -dependent coefficients and solve this equation because calculating the inverse of the ansatz is difficult.

This issue can be resolved with a little bit of extra work. We define

$$O_{\sqrt{\cdot}}^{-1}(s) := \frac{1}{O_{\sqrt{\cdot}}(s)}. \quad (4)$$

In this case, Eq. (3) becomes

$$\frac{dO_{\sqrt{\cdot}}(s)}{ds} = \frac{1}{2} O_{\sqrt{\cdot}}^{-1}(s) O_2, \quad (5)$$

and we now need to find a differential equation for $O_{\sqrt{\cdot}}^{-1}(s)$, which can be obtained by Taylor expanding $O_{\sqrt{\cdot}}^{-1}(s + \delta s)$ in a similar way to above,

$$\frac{dO_{\sqrt{\cdot}}^{-1}(s)}{ds} = -\frac{1}{2} [O_{\sqrt{\cdot}}^{-1}(s)]^3 O_2. \quad (6)$$

$$C'_0 = 0,$$

$$\frac{C'_1(s)}{2} = -C'_1(s)^3,$$

$$\frac{C'_2(s)}{2} = -6C'_1(s)C'_2(s)[C'_1(s) + C'_2(s)] - C'_1(s)^3 - 2C'_2(s)^3, \quad (9)$$

$$\begin{aligned} \frac{C'_3(s)}{4} = & -36C'_2(s)C'_3(s)[C'_1(s) + C'_2(s) + C'_3(s)] - 3C'_1(s)C'_2(s)[C'_1(s) + 4C'_2(s)] \\ & - 9C'_1(s)C'_3(s)[C'_1(s) + 2C'_3(s)] - 10C'_2(s)^3 - 12C'_3(s)^3 \end{aligned}$$

and initial conditions

$$C_{0,1,2,3}(0) = 0, \quad C'_1(0) = \frac{1}{2\sqrt{0^+}}, \quad C'_{2,3}(0) = 0. \quad (10)$$

The initial conditions were found by comparison to the infinitesimal case that is accurately described by a first-order Taylor series. Note that the term with $\frac{1}{2\sqrt{0^+}}$ represents a directional limit that has to be taken at the end but 0^+ can first be replaced by a dummy variable.

If we solve the equations, set $s = 1$, and take the limit for 0^+ , we find that

$$\sqrt{a^\dagger a} \approx a^\dagger a + \frac{\sqrt{2}-2}{2} a^{\dagger 2} a^2 + \frac{3-3\sqrt{2}+\sqrt{3}}{6} a^{\dagger 3} a^3. \quad (11)$$

One should note that this expression can be put in terms of powers of $\hat{n} = a^\dagger a$ and is valid near $a^\dagger a = 0$. More precisely, in what sense does this expansion converge to the correct operator? The answer is that by including terms up to $(a^\dagger)^n a^n$ the $n+1$ lowest eigenvalues are exactly reproduced; higher eigenvalues are approximated more accurately as well.

It is important to stress that the square root \sqrt{x} is nonanalytic near $x = 0$. Yet we were able to find an expansion in terms of powers of x that is valid near $x = 0$.

One may insert Eq. (5) into Eq. (6), and we find after rearranging that

$$\frac{1}{2} O_2 \frac{d^2 O_{\sqrt{\cdot}}(s)}{ds^2} = -\left(\frac{dO_{\sqrt{\cdot}}(s)}{ds}\right)^3. \quad (7)$$

The equation in this form is now useful to find coefficients C_i for an ansatz $O_{\sqrt{\cdot}}(s) = \sum_n c_n(s) \hat{O}_n$ because powers of this operator are trivial to compute.

III. EXPANDING THE SQUARE ROOT OF THE NUMBER OPERATOR

We may now use Eq. (7) to find an expansion of $\sqrt{a^\dagger a}$. In the language of the previous section, for this case, $O_2 = a^\dagger a$ and $O_1 = 0^+ \mathbb{1}$, where 0^+ signifies a dummy variable that eventually will take a directed limit to zero. One can make the ansatz

$$\sqrt{sa^\dagger a} \approx \sum_n C_n(s) (a^\dagger)^n a^n \quad (8)$$

and compare coefficients of $(a^\dagger)^n a^n$ to find a set of differential equations for C_n . If we truncate at third order, we find

IV. APPLICATION TO THE KLEIN-GORDON SQUARE ROOT

The method for finding a nonperturbative expansion of an operator square root can of course also be used for the Klein-Gordon square-root Hamiltonian for relativistic particles. Let us for instance consider the two-dimensional (2D) Hamiltonian

$$H = \sqrt{m^2 + p^2} + V(x, y). \quad (12)$$

If this system is subjected to a constant magnetic field given by $\mathbf{A} = \frac{B}{2}(-y, x)$, one may introduce the magnetic field by minimal substitution $p_i \rightarrow \Pi_i = p_i - A_i$, and one can introduce creation and annihilation operators, $a = \sqrt{\frac{1}{2B}}(\Pi_x + i\Pi_y)$, to find the Hamiltonian

$$H = \sqrt{4|B|S} \sqrt{1 + \frac{a^\dagger a}{2S}} + V(x, y), \quad (13)$$

where we introduced a shorthand $S = \frac{m^2 + |B|}{4|B|}$. The operator now bears a striking resemblance to the square root that appears in the Holstein-Primakoff spin representation, which we will discuss later. A straightforward Taylor expansion of the

square root in terms of $1/S$ already yields corrections

$$H \approx \sqrt{4|B|S} - \frac{1}{4}\sqrt{\frac{|B|}{S}} + \frac{1}{4}\sqrt{\frac{1}{|B|S}}\Pi^2 + V(x, y) \quad (14)$$

to what one would expect from the nonrelativistic limit of large mass

$$\sqrt{m^2 + \Pi^2} \approx m + \frac{\Pi^2}{2m} + V(x, y). \quad (15)$$

This approximation lifts the restrictions to large masses from the nonrelativistic limit as long as one considers strong magnetic fields.

However, we can do better without the introduction of further complications. That is, we can make the ansatz $\sqrt{1 + sa^\dagger a} = \sum_n C_n(s)(a^\dagger)^n a^n$, which means that we can employ the first two differential equations from (10) to approximate the square root. For this we have to choose slightly different initial conditions from those chosen previously, $C_0(0) = 1$, $C_1(0) = 0$, $C_1'(0) = 1/2$, and let s run up to $s = 1/(2S)$. The initial conditions are again found by comparison to a first-order Taylor expansion. The result we find is

$$H \approx \sqrt{4|B|S} \left[1 + \left(\sqrt{1 + \frac{1}{2S}} - 1 \right) \frac{S}{2|B|} \Pi^2 \right] + V(x, y). \quad (16)$$

This new approximation is now more reliable for small $|B|$, m , and level number n . This is seen most easily in the case of $V(x, y) = 0$, where it is easy to check that it reproduces the lowest two energy levels $n = 0, 1$ exactly [recall that $\hat{n} = a^\dagger a = S\Pi^2/(2|B|)$].

The advantage of this approximation over an exact solution is that a quadratic $V(x, y)$ can be added and an analytic solution of this approximate problem is still possible because this is still a harmonic oscillator. Note that in this case we would be able to find an approximation that is nonperturbative in $1/S$.

V. RESUMMED HOLSTEIN-PRIMAKOFF EXPANSION

We will now turn to our most interesting application—an expansion for the square root in the Holstein-Primakoff representation of a spin operator.

A. Review of the method

The Holstein-Primakoff representation [8] of spin- S operators is given as

$$\begin{aligned} S^+ &= \hbar\sqrt{2S}\sqrt{1 - \frac{a^\dagger a}{2S}} a, \\ S^- &= \hbar\sqrt{2S}a^\dagger \sqrt{1 - \frac{a^\dagger a}{2S}}, \\ S^z &= \hbar(S - a^\dagger a). \end{aligned} \quad (17)$$

A few notes are due. For finite S only finitely many bosonic excitations correspond to physical states. That is, bosonic excitations correspond to spin projections, i.e., S^z can only take eigenvalues in $\{-S, -S+1, \dots, S\}$. Hence, for spin S , we have the restriction $a^\dagger a \leq 2S$, which is also signaled by the fact that the square root becomes imaginary for higher

occupation numbers. This means that the Hilbert space is a Fock space, $F(\mathcal{H}) = \bigoplus_{n=0}^{\infty} S\mathcal{H}^{\otimes n}$, where S is the symmetrization operator and $\mathcal{H}^{\otimes n}$ denotes n tensor products of the single-particle Hilbert space \mathcal{H} . For spin S the physical part of the Hilbert space is restricted such that it has the basis $\{|0\rangle, \dots, |2S\rangle\}$.

B. Exactness of the Holstein-Primakoff approximation

To see that the Holstein-Primakoff representation is an exact description of spin operators, it is enough to check that it fulfills the correct spin algebra. For instance, $[S^+, S^-] = 2S^z$.

This reasoning is slightly restrictive, so let us soften it a bit. The key feature of the Holstein-Primakoff representation is that the spin operators $S^{+, -, z}$ reproduce the exact spin operators on the physical part of the Hilbert space and at the same time have no elements that couple to the unphysical part of the Hilbert space. That is, in the occupation basis they have the form

$$S^{+, -, z} = \begin{pmatrix} S_{\text{phys}}^{+, -, z} & 0 \\ 0 & S_{\text{unphys}}^{+, -, z} \end{pmatrix}. \quad (18)$$

In particular, for $S = \frac{1}{2}$ the explicit form of S^+ in the occupation basis is

$$S^+ = \left(\begin{array}{cc|cccc} 0 & 1 & & & & \\ 0 & 0 & & & & \\ \hline & & 0 & i\sqrt{3} & 0 & \cdots & 0 \\ & & \vdots & & \ddots & & \vdots \\ & & 0 & \cdots & & & 0 \end{array} \right). \quad (19)$$

One sees that it splits into the physical (upper left quadrant of matrix) and unphysical (lower right quadrant) Hilbert spaces, as in Eq. (18). The physical block is just the conventional S^+ matrix for spin $1/2$. Importantly, there is no coupling between physical and unphysical parts of the Hilbert space. This is what makes the method exact.

Note that because of this block structure, a spin Hamiltonian exactly written in the bosonic language will also separate into physical and unphysical blocks because the product of block-diagonal matrices stays block diagonal. That is, the Hamiltonian is block diagonal of the form

$$H = \begin{pmatrix} H_{\text{phys}} & 0 \\ 0 & H_{\text{unphys}} \end{pmatrix}. \quad (20)$$

One now can see that diagonalizing the Hamiltonian, one will find the exact physical eigenvalues and spurious unphysical ones.

C. Usual approach: Taylor expansion

While the expressions in Eq. (17) provide an exact way to represent the spin operators, this is not too useful by itself because the square roots are impractical to work with. One usually does a Taylor expansion around large S , using $1/S$ as the expansion parameter.

$$\begin{aligned} S^+ &\approx \hbar\sqrt{2S} \left(1 - \frac{1}{4S}a^\dagger a - \frac{1}{32S^2}(a^\dagger a + a^{\dagger 2} a^2) \right. \\ &\quad \left. - \frac{1}{128S^3}(a^\dagger a + 3a^{\dagger 2} a^2 + a^{\dagger 3} a^3) \right) a. \end{aligned} \quad (21)$$

up to the addition of a term that acts solely in the unphysical part of the Hilbert space and does not couple to the physical part of the Hilbert space.

In some cases, more stringent exactness criteria have been applied, such as requiring that all nonphysical matrix elements vanish [71]. This type of criteria can simplify formal quantum statistical treatments, since one does not have to be careful about excluding nonphysical states in sums over states. However, in practice these approaches are cumbersome because the associated expansions are infinite and more complicated. Therefore this is only an advantage at the purely formal level.

F. Additional properties of the expansion and comparison with other expansions

One may wonder how this expansion compares with a more conventional Dyson-Maleev expansion with $S^+ = \hbar a$ and $S^- = \hbar a^\dagger(2S - a^\dagger a)$. Our method has the advantage that S^+ and S^- are treated on the same footing and therefore are related by conventional Hermitian conjugation. This guarantees that the approach will not break Hermiticity in the conventional sense, unlike the Dyson-Maleev expansion.

Next one may wonder if an additional perturbative expansion around classical spin configurations may be stacked on top of the expansion as is done for the more conventional $1/S$ expansion in nonlinear spin-wave theory [46]. One may therefore be tempted to identify $\delta = (\sqrt{1 - \frac{1}{2S}} - 1)$ in Eq. (26) as an expansion parameter since it corresponds to fluctuation corrections around a classical ground state. That is, one would write $S^+ \approx \hbar\sqrt{2S}[1 + \delta a^\dagger a]$. This, however, is not possible and becomes clear if one considers that $S^z = 1/2[S^+, S^-]$. Then, one can write

$$S^z = \frac{1}{2}[S^+, S^-] \approx \underbrace{S + 2S(2\delta + \delta^2)a^\dagger a}_{S^z} + 3\delta^2 S(a^\dagger)^2 a^2. \quad (30)$$

We find that the physical part of S^z has contributions from different orders of δ . This of course means that any expansion in δ will treat S^z and $S^{x,y}$ on unequal footing, even at low orders in such an expansion. This, for instance, will result in an unphysical breaking of symmetries in a Heisenberg model or similar even at the lowest-order expansion. Therefore δ cannot be used as an expansion parameter. Additionally, there is no other obvious choice of expansion parameter, and *ad hoc* expansions in powers of a also lead to unphysical results in nonlinear spin-wave theories. Therefore it seems that the expansion does not allow for an additional perturbative expansion in terms of fluctuations around a classical spin configuration. A mean-field-theory treatment must include all the terms that are needed to accurately describe spin S for each operator S^+ and S^- .

G. Symmetries and exact properties in the improved expansion

To study symmetries in the new expansion, we consider the Hamiltonian for the Heisenberg model with easy-plane single-ion anisotropy,

$$H = \sum_i [J\mathbf{S}_i \cdot \mathbf{S}_{i+1} + D(S_i^x)^2]. \quad (31)$$

Let us first recognize that for $S = \frac{1}{2}$ the single-ion anisotropy $(S_i^x)^2$ should result in a trivial number $(S_i^x)^2 = \frac{1}{4}$ that does not affect the spin-wave excitation spectrum. However, in the usual Taylor expansion with $S^+ \approx a - \frac{1}{2}a^\dagger a^2$ one finds that

$$(S^x)^2 = \frac{1}{4} + \frac{1}{16}(2a^\dagger{}^2 + 2a^\dagger a - 2a^\dagger a^3 - 3a^\dagger{}^2 a^2 + a^\dagger{}^2 a^4 - 2a^\dagger{}^3 a + 2a^\dagger{}^3 a^3 + a^\dagger{}^4 a^2 + 2a^2), \quad (32)$$

which has unphysical contributions in the physical part of the Hilbert space, e.g., $a^\dagger a$. In other words, the Taylor expansion introduces unphysical artifacts.

In the new expansion for $S = \frac{1}{2}$, however, we have $S^+ = a - a^\dagger a^2$ and find that

$$(S^x)^2 = \frac{1}{4} + \frac{1}{4}(a^\dagger{}^2 a^2 + a^\dagger{}^2 a^4 + 2a^\dagger{}^3 a^3 + a^\dagger{}^4 a^2). \quad (33)$$

The additional nonconstant terms we find have nonzero contributions only in the nonphysical part of the Hilbert space and do not couple to the physical part of the Hilbert space. This can easily be verified explicitly by computing the operator in the occupation-number basis using Eq. (27). The nonphysical terms are therefore of no consequence for physical states and could just as well be dropped. This means that the new expansion properly reproduces the fact that $(S_i^x)^2$ contributes only a trivial scalar for spin $1/2$.

Next we recall that the Hamiltonian is symmetric with respect to the symmetry generated by the generator $g = \sum_i S_i^x$, i.e., $C = [H, g] = 0$. Again we will only check spin $1/2$ for simplicity, but similar results will hold for higher spins. Let us first see what happens if we use the usual Taylor expansion approach to compute the commutator. We find that

$$C = \sum_i \frac{1}{16} a_{i+1}^\dagger a_{i+1} (2a_i^\dagger + a_i^\dagger a_i^2 - a_i^\dagger{}^2 a_i - 2a_i) + \frac{3}{32} a_{i+1}^\dagger{}^2 a_{i+1}^2 (2a_i^\dagger + a_i^\dagger a_i^2 - a_i^\dagger{}^2 a_i - 2a_i) + (i \leftrightarrow (i+1)), \quad (34)$$

where $(i \leftrightarrow (i+1))$ is shorthand for the same terms with i and $i+1$ switched. Here, we can see that the operators in the first line couple the physical two-site states in $A_p = \{|0\rangle_i |0\rangle_{i+1}, |1\rangle_i |0\rangle_{i+1}, |0\rangle_i |1\rangle_{i+1}, |1\rangle_i |1\rangle_{i+1}\}$ to nonphysical two-site states in $A_{np} = \{|n\rangle_i |m\rangle_{i+1} | (n > 1) \vee (m > 1)\}$, which are the states where at least one of the two sites is more-than-single occupied. The symbol \vee denotes the inclusive ‘‘or’’ (disjunction) operator.

For the new expansion, on the other hand, we find that

$$C = \frac{3}{4} \sum_i (a_{i+1}^\dagger{}^2 a_{i+1}^2 [a_i^\dagger - a_i + a_i^\dagger a_i^2 - a_i^\dagger{}^2 a_i] + a_i^\dagger{}^2 a_i^2 [a_{i+1}^\dagger - a_{i+1} + a_{i+1}^\dagger a_{i+1}^2 - a_{i+1}^\dagger{}^2 a_{i+1}]). \quad (35)$$

From here one may observe the term $a_j^\dagger{}^2 a_j^2$ to see that only matrix elements for the unphysical states A_{np} will be nonzero. The operator also does not couple to the physical states in A_p . We can hence conclude that unlike the Taylor expansion, the bosonic expressions for the spin operators in the new expansion do not break symmetries present in the original spin-operator language.

VI. CONCLUSION

We were able to demonstrate the surprising result that the square root of an operator $\sqrt{\hat{O}}$ may be expanded in an integer power series around $\hat{O} = 0$. We believe that the approach can be usefully applied to other operator square roots in theoretical physics and that the observation is useful for finding better expansions of other operator functions where a Taylor expansion fails.

The methods described in this paper allowed us to find a significant nonperturbative improvement on the Taylor expansion for the Holstein-Primakoff realization of spin operators. We expect these results to be useful to better treat spin models in different mean-field approaches if there is no clear classical spin configuration around which one could expand. We therefore hope that the approach will prove useful for the study of spin liquid phases.

Note added. Recently, expressions equivalent to those in (25) in closed form were also found by elegant alternative means via a Newton series expansion [124].

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APPENDIX A: MORE GENERIC CASE FOR OPERATOR SQUARE ROOT

An operator square root

$$S = \sqrt{O_1 + \delta O_2} \quad (\text{A1})$$

with small $\delta \ll 1$ can generically be treated as follows. One may write

$$S^2 = O_1 + \delta O_2 \quad (\text{A2})$$

and make the ansatz $S = \sqrt{O_1} + \delta S_1$ to find

$$S_0 S_1 + S_1 S_0 = O_2. \quad (\text{A3})$$

This equation is a Lyapunov equation, which for S_0 Hermitian with positive spectrum can be solved for S_1 as

$$S_1 = \int_0^\infty dt e^{-S_0 t} O_2 e^{-S_0 t}, \quad (\text{A4})$$

which can be seen if it is inserted in the equation above and a chain rule for differentiation is used. Therefore to linear order one finds

$$\sqrt{O_1 + \delta O_2} \approx \sqrt{O_1} + \delta \int_0^\infty dt e^{-\sqrt{O_1} t} O_2 e^{-\sqrt{O_1} t}. \quad (\text{A5})$$

It is easy to see that this, with the assumption $[O_1, O_2] = 0$ we made earlier in the text, reduces to a Taylor-series result. This result, however, is much more cumbersome, and we will therefore not work on it further.

If we set $O_1 = O(s)$, $O_2 = \frac{dO_1}{ds}$, and $\delta = ds$, we find that a derivative of the square-root map is

$$\frac{d}{ds} \sqrt{O(s)} = \int_0^\infty dt e^{-\sqrt{O(s)} t} \frac{dO(s)}{ds} e^{-\sqrt{O(s)} t}. \quad (\text{A6})$$

APPENDIX B: REPRODUCING SPIN-S OPERATORS EXACTLY

Let us first prove that truncating (25) at $n_{\max} = 2S$ produces terms that do not couple to the nonphysical parts of the Hilbert space. In the number basis we find that

$$\langle m | S^+ | n \rangle = \hbar \sqrt{2S} \delta_{m,n-1} \sqrt{n} \sum_{l=0}^{2S} Q_l \frac{m!}{(m-l)!}. \quad (\text{B1})$$

The only *a priori* nonzero matrix element that could couple physical and unphysical parts of the Hilbert space is $n = 2S + 1$ and $m = 2S$. It is zero if

$$\sum_{l=0}^{2S} Q_l \frac{2S!}{(2S-l)!} = 0, \quad (\text{B2})$$

which we checked explicitly for spins $S = \frac{1}{2}, \dots, 16$ using MATHEMATICA and expect to be true in general.

Furthermore, we also checked explicitly that the other nonzero matrix elements for the physical couplings, i.e., $n < 2S + 1$ and $m = n - 1$, agree with the ones given by the exact Holstein-Primakoff expansion.

$$\langle m | S^+ | n \rangle = \hbar \sqrt{2S} \delta_{m,n-1} \sqrt{1 - \frac{m}{2S}} \sqrt{n}. \quad (\text{B3})$$

That is, we just needed to show that

$$\sum_{l=0}^{2S} Q_l \frac{m!}{(m-l)!} = \sqrt{1 - \frac{m}{2S}} \quad (\text{B4})$$

for all $m \in \mathbb{N}^+ / 2$ and $m < 2S$. Again using MATHEMATICA, we found this to hold at the minimum up to spin $S = 16$ and expect it to be true generally.

APPENDIX C: EXPLICIT EXPRESSIONS FOR HIGHER SPIN S

In this Appendix we give exact expressions for spin operators of spins up to $S = 3$. For this, one first has to solve (25) for the different Q_n given below.

$$\begin{aligned}
 Q_0 &= 1, \\
 Q_1 &= \sqrt{1 - \frac{1}{2S}} - 1, \\
 Q_2 &= \frac{1}{2} \left(-\sqrt{4 - \frac{2}{S}} + \sqrt{\frac{S-1}{S}} + 1 \right), \\
 Q_3 &= \frac{1}{12} \left(3\sqrt{4 - \frac{2}{S}} + \sqrt{4 - \frac{6}{S}} - 6\sqrt{\frac{S-1}{S}} - 2 \right), \\
 Q_4 &= \frac{\sqrt{S-2} + 6\sqrt{S-1} + \sqrt{S} - 2\sqrt{4S-6} - 2\sqrt{4S-2}}{24\sqrt{S}}, \\
 Q_5 &= \frac{-10\sqrt{S-2} - 20\sqrt{S-1} - 2\sqrt{S} + \sqrt{4S-10} + 10\sqrt{4S-6} + 5\sqrt{4S-2}}{240\sqrt{S}}, \\
 Q_6 &= \frac{\sqrt{S-3} + 15\sqrt{S-2} + 15\sqrt{S-1} + \sqrt{S} - 3\sqrt{4S-10} - 10\sqrt{4S-6} - 3\sqrt{4S-2}}{720\sqrt{S}}. \tag{C1}
 \end{aligned}$$

This result may now be inserted into $S_+ = \hbar\sqrt{2S}[\sum_{n=0}^{2S} Q_n a^{\dagger n} a^n]a$, and we set the appropriate values for S to find the exact expressions for spin operators up to spin $S = 3$, given below.

$$\begin{aligned}
 S = \frac{1}{2}: \quad \frac{S^+}{\hbar} &= a - a^\dagger a^2, \\
 S = 1: \quad \frac{S^+}{\hbar} &= \sqrt{2}a + (1 - \sqrt{2})a^\dagger a^2 + \left(\frac{1}{\sqrt{2}} - 1\right)a^{\dagger 2} a^3, \\
 S = \frac{3}{2}: \quad \frac{S^+}{\hbar} &= \sqrt{3}a + (\sqrt{2} - \sqrt{3})a^\dagger a^2 + \frac{1}{2}(1 - 2\sqrt{2} + \sqrt{3})a^{\dagger 2} a^3 + \frac{1}{6}(\sqrt{21} - 6\sqrt{6} - 3)a^{\dagger 3} a^4, \\
 S = 2: \quad \frac{S^+}{\hbar} &= 2a + (\sqrt{3} - 2)a^\dagger a^2 + \left(1 - \sqrt{3} + \frac{1}{\sqrt{2}}\right)a^{\dagger 2} a^3 + \frac{1}{6}(3\sqrt{3} - 3\sqrt{2} - 1)a^{\dagger 3} a^4 + \frac{1}{12}(3\sqrt{2} - 2\sqrt{3} - 1)a^{\dagger 4} a^5, \\
 S = \frac{5}{2}: \quad \frac{S^+}{\hbar} &= \sqrt{5}a + (2 - \sqrt{5})a^\dagger a^2 + \frac{1}{2}(\sqrt{3} + \sqrt{5} - 4)a^{\dagger 2} a^3 + \frac{1}{6}(\sqrt{2} - 3\sqrt{3} - \sqrt{5} + 6)a^{\dagger 3} a^4 \\
 &\quad + \frac{1}{24}(\sqrt{5} - 4\sqrt{2} + 6\sqrt{3} - 7)a^{\dagger 4} a^5 + \frac{1}{120}(10\sqrt{2} - 10\sqrt{3} - \sqrt{5} + 5)a^{\dagger 5} a^6, \\
 S = 3: \quad \frac{S^+}{\hbar} &= \sqrt{6}a + (\sqrt{5} - \sqrt{6})a^\dagger a^2 + (1 - \sqrt{5} + \sqrt{\frac{3}{2}})a^{\dagger 2} a^3 + \frac{1}{6}(\sqrt{3} + 3\sqrt{5} - \sqrt{6} - 6)a^{\dagger 3} a^4 \\
 &\quad + \frac{1}{24}(\sqrt{2} - 4\sqrt{3} - 4\sqrt{5} + \sqrt{6} + 12)a^{\dagger 4} a^5 + \frac{1}{120}(10\sqrt{3} - 5\sqrt{2} + 5\sqrt{5} - \sqrt{6} - 19)a^{\dagger 5} a^6 \\
 &\quad + \frac{1}{720}(15\sqrt{2} - 20\sqrt{3} - 6\sqrt{5} + \sqrt{6} + 24)a^{\dagger 6} a^7. \tag{C2}
 \end{aligned}$$

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