

## Method to identify parent Hamiltonians for trial states

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We describe a general method to identify exact, local parent Hamiltonians for trial states such as quantum Hall or spin-liquid states, which we have used extensively during the past decade. It can be used to identify exact parent Hamiltonians, either directly or via the construction of simpler annihilation operators from which a parent Hamiltonian respecting all the required symmetries can be constructed. Most remarkably, however, the method provides approximate parent Hamiltonians whenever an exact solution is not available within the space of presumed interaction terms.

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*Introduction.* In the study of condensed matter systems with conceptually or even topologically nontrivial properties including superconductors [1], fractionally quantized Hall fluids [2–4], or spin liquids in one [5–8] or two dimensions [9–13] (1D or 2D), it has often been extremely helpful to resort to trial wave functions which serve as paradigms for the universality classes at hand. These trial wave functions are usually amenable to analytic formulations, and instruct us on the properties, and in particular the quantum numbers, of the excitations above the ground state. Well-known examples of such trial states are the BCS wave function [1], which supports Bogoliubov quasiparticles, the Laughlin [2], Moore-Read [14], and Read-Rezayi [15] states in the quantum Hall effect, which support fractionally charged quasiparticles with Abelian [16] or non-Abelian statistics [14,17], and the Gutzwiller ground state [18–20] of the Haldane-Shastry (HS) model [5–7], which supports spinon excitations with half-Fermi statistics.

In some cases, it is only possible to study these paradigms using approximate parent Hamiltonians. Whenever available, however, it is highly desirable to construct exact parent Hamiltonians, and thus elevate the paradigm from a wave function to an exact model. This has been accomplished for all the examples mentioned above [3,5,6,15,21–24], and has been particularly rewarding in the case of the Gutzwiller ground states of 1D spin chains, where the model turned out to be an exact lattice realization of the  $SU(2)_1$  Wess-Zumino-Witten (WZW) model [25–28]. This model was subsequently generalized from  $SU(2)$  to  $SU(M, N)$  supersymmetry [29,30], and also to higher spin representations of  $SU(2)$  [8,31,32], where the low-energy sector is described by the  $SU(2)_{k=2S}$  WZW model. All these developments have been inspired not by the Gutzwiller states directly, but by its parent Hamiltonian, which was independently discovered by Haldane and Shastry [5,6].

In this Rapid Communication, we describe a general, numerical method to obtain exact parent Hamiltonians for given trial wave functions, which almost trivially yields parent Hamiltonians for the Laughlin and for the Gutzwiller wave functions discussed above. The approach is in part similar to recent proposals by Xi and Renard [33] as well as by Chertkov and Clark [34]. Over the years, we have obtained results using this method for the hierarchical quantum Hall states [35] (with

wave functions obtained either through a composite fermion construction or through an explicit condensation of quasiparticles in the hierarchy), for the non-Abelian chiral spin liquid (NACSL) [12,13,36], and most recently, for a universality class of fractional topological insulators [37] we propose. In the latter two examples, the method not only revealed that there do not exist exact parent Hamiltonians containing only the interaction terms we considered, but provided us with meaningful approximate parent Hamiltonians, which were instrumental to our studies.

*General method.* With these introductory remarks, we now turn to the method itself. Let  $|\psi_0\rangle$  be a known trial ground state for a finite system, of a system size amenable to exact diagonalization studies. We now wish to ask whether  $|\psi_0\rangle$  is the exact ground state of a (local) model Hamiltonian specified by a finite number  $L$  of terms  $H_i$  with unknown coefficients  $a_i$ ,

$$H = \sum_{i=1}^L a_i H_i, \quad (1)$$

and determine the coefficients. To begin with, this requires that  $|\psi_0\rangle$  is an exact eigenstate,

$$H|\psi_0\rangle = E_0|\psi_0\rangle, \quad (2)$$

which we write as

$$(H + a_0)|\psi_0\rangle = 0. \quad (3)$$

Clearly, the additional variational parameter  $a_0$  is to be interpreted as  $-E_0$ . Defining  $H_0 \equiv 1$ , we may write this compactly as

$$\sum_{i=0}^L a_i H_i |\psi_0\rangle = 0. \quad (4)$$

Since we are interested in identifying parent Hamiltonians for highly correlated many-body states, and the number of translationally invariant  $m$ -body terms  $H_i$  for a system with  $N$  sites scales roughly as  $N^{m-1}$ , the dimension of the Hilbert space for system sizes with more than about four particles will in general be larger than the number of terms  $L$ . This means that some special principle must be at work for each solution of

(4). In most applications, there are one or several solutions due to conserved quantities (e.g., total spin in a spin system, total angular momentum for quantized Hall fluids on the sphere), and an additional one if an exact parent Hamiltonian exists.

To find these solutions, we define the state vectors  $|\psi_i\rangle \equiv H_i|\psi_0\rangle$ , and multiply (4) from the left with the corresponding dual  $\langle\psi_j|$ . With  $M_{ji} \equiv \langle\psi_j|\psi_i\rangle$ , this yields

$$\sum_{i=0}^L M_{ji} a_i = 0 \quad \text{for } j = 0, 1, \dots, L. \quad (5)$$

Obviously, there is one solution of (5) for each zero eigenvalue of the  $L + 1$  dimensional, Hermitian matrix  $M_{ji}$ . Substitution of the corresponding eigenvectors  $a_i$  into (4) yields operators annihilating the ground state, which enable us to extract the desired parent Hamiltonian (1). If  $\det M_{ji} \neq 0$ , (5) has only the trivial solution  $a_i = 0$ , and no exact parent Hamiltonian or parent operator exists within the space spanned by the operators  $H_i$ . Even though this may come across as a trivial observation, the models one can obtain with this method are in general highly nontrivial.

Possibly the most outstanding feature is that, according to our long-standing experience, the method usually yields a highly nontrivial approximate parent Hamiltonian if no exact one exists within the operator space spanned by the  $H_i$ 's. In these cases, there are likewise one or several zero eigenvalues due to conserved quantities, and one small or very small nonzero eigenvalue. The eigenstate corresponding to this eigenvalue defines the approximate Hamiltonian.

An obvious drawback is that the method guarantees that  $|\psi_0\rangle$  is an exact or approximate eigenstate of  $H$ , but not that it is the ground state. This has hence to be verified *a posteriori* by exact numerical diagonalization of  $H$ . Our experience here is that whenever an exact parent Hamiltonian exists, it will have  $|\psi_0\rangle$  as its unique ground state. In the case of approximate solutions, we have sometimes encountered situations where the method suggested operators for which  $|\psi_0\rangle$  has only been an approximate eigenstate, not the ground state. In the cases we have studied, however, it was always possible to find a suitable set of operators  $H_i$  such that the method converged on an approximate parent Hamiltonian for the ground state.

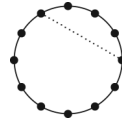
*Example: The Haldane-Shastry Hamiltonian.* The ground state of the model can be obtained by Gutzwiller projection from a completely filled one-dimensional band, which in total contains as many spin- $\frac{1}{2}$  fermions as there are lattice sites [18–20],

$$|\psi_0^{\text{HS}}\rangle = P_{\text{GW}}|\psi_{\text{SD}}^N\rangle, \quad |\psi_{\text{SD}}^N\rangle \equiv \prod_{q \in \mathcal{I}} c_{q\uparrow}^\dagger c_{q\downarrow}^\dagger |0\rangle, \quad (6)$$

where the interval  $\mathcal{I}$  contains  $M = \frac{N}{2}$  adjacent momenta, and the Gutzwiller projector  $P_{\text{GW}}$  eliminates doubly occupied sites.

While it is irrelevant to the applicability of the numerically executed method proposed above, a different formulation of the Gutzwiller ground state is convenient for the discussion below. Consider a spin- $\frac{1}{2}$  chain with periodic boundary conditions and an even number of sites  $N$  on a unit circle embedded in the

complex plane:



$N$  sites with spin- $\frac{1}{2}$  on unit circle:

$$\eta_\alpha = e^{i\frac{2\pi}{N}\alpha} \quad \text{with } \alpha = 1, \dots, N.$$

The ground state (6) can be written as

$$|\psi_0^{\text{HS}}\rangle = \sum_{\{z_1, \dots, z_M\}} \psi_0^{\text{HS}}(z_1, \dots, z_M) S_{z_1}^+ \dots S_{z_M}^+ |\underbrace{\downarrow\downarrow \dots \downarrow}_{N \text{ spins } \downarrow}\rangle, \quad (7)$$

where the sum extends over all possible ways to distribute the  $M = \frac{N}{2}$   $\uparrow$ -spin coordinates  $z_i$  on the unit circle and

$$\psi_0^{\text{HS}}(z_1, \dots, z_M) = \prod_{i < j} (z_i - z_j)^2 \prod_{i=1}^M z_i. \quad (8)$$

We now search numerically for an exact parent Hamiltonian which is invariant under all the symmetries of the ground state, i.e., translations, SU(2) spin rotations, time reversal ( $T$ ), and parity ( $P$ ). It is further reasonable to first try an ansatz with two-body interactions only. [In fact, the only SU(2) invariant three-spin interaction term for spin- $\frac{1}{2}$  is  $i S_\alpha (\mathbf{S}_\beta \times \mathbf{S}_\gamma)$ , which violates  $T$ .] Following the notation in (1), we write

$$H = \sum_{i=1}^{N/2} a_i H_i, \quad H_i = \sum_{\alpha=1}^N S_\alpha S_{\alpha+i}. \quad (9)$$

Numerical execution of the steps described above for a chain with  $N \geq 8$  sites yields two zero eigenvalues of the matrix  $M_{ji}$  of (5). The corresponding eigenvectors yield, upon rewriting in a more convenient form, the ground-state annihilation operators

$$H^a = S_{\text{tot}}^2, \quad S_{\text{tot}} \equiv \sum_{\alpha=1}^N S_\alpha, \quad (10)$$

and

$$H^b = -E_0 + \left(\frac{2\pi}{N}\right)^2 \sum_{\alpha < \beta} \frac{S_\alpha S_\beta}{|\eta_\alpha - \eta_\beta|^2}, \quad (11)$$

where  $|\eta_\alpha - \eta_\beta|$  is the chord distance between the sites  $\alpha$  and  $\beta$ , and  $E_0 = -\frac{\pi^2}{24}(N + \frac{5}{N})$ . While  $H^a$  just confirms that the ground state is a spin singlet,  $H^b$  is the model Hamiltonian discovered by Haldane and Shastry [5,6].

*First generalization: Ground-state annihilation operators.* While the method in its most direct form works extremely well for 1D models (such as spin chains or 2D electrons confined to a Landau level) with two-body interactions, and is still feasible for 1D models with three-body interactions, it is less so for higher dimensions. In some instances it can be extremely helpful to employ the method to identify not the coefficients in a model Hamiltonian directly, but in an annihilation operator for the ground state. Such an operator can be much simpler than the Hamiltonian, is not required to share any of the symmetries of the ground state, and does not need to be Hermitian. Once the operator is known, it is usually possible to construct a local and positive semidefinite parent Hamiltonian from it. Returning to

our example of the HS model, an operator of this kind is

$$\Omega_\alpha = \sum_{i=1}^{N-1} a_{\alpha,i} H_{\alpha,i}, \quad H_{\alpha,i} = S_\alpha^- S_{\alpha+i}^- \quad (12)$$

Note that even though the operators  $H_{\alpha,i}$  are no longer Hermitian, the matrices  $M_{\alpha,j_i}$  of (5) still are. We now find three zero eigenvalues for each  $\alpha$ , which yield the ground-state annihilation operators

$$\Omega_\alpha^a = S_\alpha^- S_{\text{tot}}^- \quad (13)$$

where we have used  $(S_\alpha^-)^2 = 0$ ,

$$\Omega_\alpha^b = \sum_{\substack{\beta=1 \\ \beta \neq \alpha}}^N \frac{1}{\eta_\alpha - \eta_\beta} S_\alpha^- S_\beta^-, \quad \text{and} \quad \Omega_\alpha^c = (\Omega_\alpha^b)^* \quad (14)$$

It is then an elementary exercise [8] to show that the  $T$  and  $P$  invariant scalar component [scalar with regard to  $SU(2)$  spin rotations] of the translationally invariant, Hermitian, and semidefinite positive operator

$$H_{\text{intermediate}} = \sum_{\alpha=1}^N \Omega_\alpha^{b\dagger} \Omega_\alpha^b \quad (15)$$

is, up to an overall normalization, equal to (11). Since  $\Omega_\alpha^c$  is just the  $T$  or  $P$  conjugate of  $\Omega_\alpha^b$ , it yields the same parent Hamiltonian.

The advantages of an approach via an annihilation operator of the kind (12) over the direct approach (9) become apparent as we consider models which are not as readily obtained as the HS model (11). Consider the higher spin  $S$  generalizations [38] of the Gutzwiller state,

$$|\psi_0^S\rangle = (\Psi_0^{\text{HS}}[a^\dagger, b^\dagger])^{2S} |0\rangle, \quad (16)$$

where  $\Psi_0^{\text{HS}}[a^\dagger, b^\dagger]$  is the operator generating the HS ground state in terms of Schwinger bosons, such that

$$|\psi_0^{\text{HS}}\rangle = \Psi_0^{\text{HS}}[a^\dagger, b^\dagger] |0\rangle. \quad (17)$$

If we view the HS ground state (8) as a bosonic Laughlin state for spin-flip operators, we would view (16) as a bosonic Read-Rezayi state for renormalized spin flips. For (16), we can numerically determine the coefficients  $a_i$  in (12) with  $H_{\alpha,i} = (S_\alpha^-)^{2S} S_{\alpha+i}^-$ , which then turn out to be equivalent to those found in (13) and (14) for spin- $\frac{1}{2}$ . Following the same steps as above, this yields the parent Hamiltonian [8]

$$H^S = \frac{2\pi^2}{N^2} \left[ \sum_{\alpha \neq \beta}^N \frac{S_\alpha S_\beta}{|\eta_\alpha - \eta_\beta|^2} - \frac{1}{2(S+1)(2S+3)} \right. \\ \left. \times \sum_{\substack{\alpha, \beta, \gamma \\ \alpha \neq \beta, \gamma}}^N \frac{(S_\alpha S_\beta)(S_\alpha S_\gamma) + (S_\alpha S_\gamma)(S_\alpha S_\beta)}{(\bar{\eta}_\alpha - \bar{\eta}_\beta)(\eta_\alpha - \eta_\gamma)} \right], \quad (18)$$

with ground-state energy

$$E_0^S = -\frac{2\pi^2}{N^2} \frac{S(S+1)^2}{2S+3} \frac{N(N^2+5)}{12}. \quad (19)$$

Obviously, it would be much more difficult to obtain the coefficients in (18) directly with our numerical method than it is with annihilation operators. The direct method, however, does convey the information that an exact parent Hamiltonian with three-body terms of the form in (18) does exist for the higher spin states.

*Second generalization: Approximate parent Hamiltonians.* Possibly the most important feature of our method is that it delivers approximate parent Hamiltonians whenever an exact parent Hamiltonian for the trial ground state is not available in the space spanned by the terms  $H_i$  one considers. More often than not, this situation arises because no simple, local, analytically amenable parent Hamiltonian exists for the state in question. Examples for such a situation are provided by the hierarchy wave functions of the quantized Hall effect, which is also the instance where one of us applied this method first [35], or for the NACSL [12].

As explained in the context of the general method above, in situations where no exact, but an approximate, parent Hamiltonian can be constructed with the terms  $H_i$  included in (1), the eigenvector associated with the smallest nonzero eigenvalue of  $M_{j_i}$  usually provides such an approximate Hamiltonian  $H$ . The result, however, will slightly depend on the relative normalizations  $w_i$  of the operators  $H_i$  used in the numerical procedure. In this context, however, the optimal solution will depend on what one desires to optimize. This could be the relative variance of the ground-state energy

$$\frac{\langle \psi_0 | H^2 | \psi_0 \rangle - \langle \psi_0 | H | \psi_0 \rangle^2}{\langle \psi_0 | H | \psi_0 \rangle^2}, \quad (20)$$

the overlap  $\langle \psi | \psi_0 \rangle$  between the exact ground state  $|\psi\rangle$  of  $H$  and the reference trial state  $|\psi_0\rangle$ , or the similarity between the correlators  $h_i = \langle \psi | H_i | \psi \rangle$  and  $h_{0,i} = \langle \psi_0 | H_i | \psi_0 \rangle$ . [When we applied the method to the NACSL [12], our point was to show that we can find a local, approximate Hamiltonian with a gap between the three (in the thermodynamic limit topologically degenerate) ground states and the remaining spectrum. The size of this gap was hence a parameter we considered as well.]

In most applications we studied, the most naive application of the method designed for the identification of an exact parent Hamiltonian provided us with remarkably accurate approximations whenever no exact solutions were available. If one then desires to optimize the Hamiltonian specified by the set of parameters  $[a_i] \equiv (a_0, a_1, \dots, a_L)$  further, one may apply a Newton scheme as follows. We illustrate the method here for an optimization of the similarity in the correlators, as this usually optimizes variance and overlap as well. To begin with, we choose a set of weights  $[w_i]$ , and another set  $[w'_i]$ , where only a single weight  $w_j$  differs by a small parameter  $\delta_j$ . We then evaluate the corresponding coefficients  $[a_i]$  and  $[a'_i]$ , and from there  $[h_i]$  and  $[h'_i]$ . This yields the  $j$ th row of the derivative matrix

$$\frac{\partial h_i}{\partial w_j} \equiv \frac{h'_i - h_i}{\delta_j}.$$

As a next step, we solve the linear equation

$$\sum_{j=0}^L \frac{\partial h_i}{\partial w_j} \Delta w_j = h_{0,i} - h_i$$

for the shifts  $\Delta w_j$  we would require if we assume a linear dependence. The procedure can then be repeated with the adjusted weights  $[w_i + \Delta w_i]$  until it has converged. In the examples we considered, however, a single iteration was sufficient. Whenever adjustments of the weights  $[w_i]$  are insufficient to induce the desired changes in the correlators, one possible route is to follow the same steps with infinitesimal variations in the coefficients  $[a_i]$ . Usually, one needs to adjust nuances of the method to the problem one is considering. For example, it is sometimes better to include  $w_0$  and  $a_0$  in the optimization, while in other situations it is better to take  $a_0$  constant, if not zero to start with. We have also encountered examples where the optimization worked better when we adjusted the weights not on a linear, but on a logarithmic scale, a change which is fully implemented by taking  $e^{w_i} H_i$  instead of  $w_i H_i$  for the renormalized operators in  $H = \sum_i a_i w_i H_i$  and  $|\psi_i\rangle = w_i H_i |\psi_0\rangle$ . The procedure we have outlined here hence should be taken mostly as an inspiration to find an adequate algorithm for the problem one is interested in.

The approximate method we just outlined is heuristic and crude, but has been highly successful in our experience. The reader might ask at this point whether a more scholarly approach does not offer itself. One possible avenue we have explored is to minimize the variance (20) by maximizing  $\langle \psi_0 | H | \psi_0 \rangle^2$  subject to the constraints  $\langle \psi_0 | \psi_0 \rangle = \langle \psi_0 | H^2 | \psi_0 \rangle = 1$  with  $H$  given by (1). This yields

$$\sum_{i=1}^L M_{ji} a_i = -M_{j0} a_0 \quad \text{for } j = 1, \dots, L, \quad (21)$$

where  $a_0$  is now a normalization constant given by

$$a_0^{-2} = \sum_{i,j=1}^L M_{0i} (M^{-1})_{ij} M_{j0}. \quad (22)$$

Note that since  $a_0$  only affects the overall normalization of the parent Hamiltonian, we do not need to evaluate (22) in practical applications. Instead, we may set  $a_0 = 1$  in (21). In some of the examples we have investigated, the Hamiltonian corresponding to the solution of (21) for  $a_i$  was more accurate than the one obtained with the previous method, i.e., via the lowest nonzero eigenvalue of (5). In general, however, this method has not been as stable and robust as the previous one.

*Conclusion.* We have introduced a method to identify where available exact, but in general approximate, parent Hamiltonians for known trial wave functions. It is particularly useful when the trial states describe paradigms of fractionally quantized or topologically ordered, many-particle states. In the examples we studied, the most naive application of the method provided us already with compelling approximative Hamiltonians whenever exact Hamiltonians did not exist within the space of the interaction terms we considered. Since the effort required to optimize these approximations is very manageable, we explained and illustrated one optimization procedure in detail. Different physical problems usually require different approximations, and the procedure we outline is not universally applicable. We do believe, however, that the method in general will be of vital use in many different areas of physics that concern themselves with trial states, and yet unknown microscopic models associated with them.

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