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Eigenvector continuation with subspace learning

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A common challenge faced in quantum physics is finding the extremal eigenvalues and eigenvectors of a Hamiltonian matrix in a vector space so large that linear algebra operations on general vectors are not possible. There are numerous efficient methods developed for this task, but they generally fail when some control parameter in the Hamiltonian matrix exceeds some threshold value. In this work we present a new technique called eigenvector continuation that can extend the reach of these methods. The key insight is that while an eigenvector resides in a linear space with enormous dimensions, the eigenvector trajectory generated by smooth changes of the Hamiltonian matrix is well approximated by a very low-dimensional manifold. We prove this statement using analytic function theory and propose an algorithm to solve for the extremal eigenvectors. We benchmark the method using several examples from quantum many-body theory.

We address the problem of finding the extremal eigenvalues and eigenvectors of a Hamiltonian matrix that is too large to store in computer memory. This problem occurs regularly in quantum many-body theory and all existing methods either use Monte Carlo simulations, diagrammatic expansions, variational methods or some combination. While these methods can be quite efficient, they can break down when one or more parameters in the Hamiltonian exceed some tolerance threshold. In Monte Carlo simulations the difficulty is caused by sign oscillations that cause positive and negative weights to cancel. In diagrammatic expansions the problem is the divergence of the series expansion, and in variational methods the obstacle is capturing the details of the wave function using a variational ansatz or truncated basis expansion. In this letter we introduce a new variational technique called eigenvector continuation that can be used to salvage the most difficult cases.

In the mathematical literature, the terms eigenvector continuation [1–3], subspace tracking [4], and successive constraint method for subspace acceleration [5] refer to the computation of smoothly-varying bases for invariant subspaces of parameter-dependent matrices. Although related, our approach is aimed at determining eigenvalues and eigenvectors in a vector space so large that linear algebra operations on general vectors are not possible. As a result, Krylov space methods as the Lanczos algorithm [6, 7] are not applicable in their usual formulation. Some examples of computational methods that can tolerate extremely large-dimensional spaces are quantum Monte Carlo simulations and many-body perturbation theory. We assume that we have a computational method that can perform a limited set of operations such as inner products between eigenvectors of different Hamiltonian matrices and amplitudes of eigenvectors sandwich-

ing specific matrices such as a Hamiltonian matrix. In order to obtain results using only this limited information, we must be careful to maintain numerical accuracy and robustness in the presence of collinearities among the eigenvectors.

In the following we demonstrate that when a control parameter in the Hamiltonian matrix is varied smoothly, the extremal eigenvectors do not explore the large dimensionality of the linear space. Instead they trace out trajectories with significant displacements in only a small number of linearly-independent directions. We prove this statement using the principles of analytic continuation. Since the eigenvector trajectory is a low-dimensional manifold embedded in a very large space, we can “learn” the eigenvector trajectory using data where the eigenvector is computable and apply eigenvector continuation to address problems where the computational method breaks down.

Let us consider a finite-dimensional linear space and a family of Hamiltonian matrices $H(c) = H_0 + cH_1$ where H_0 and H_1 are Hermitian. Let $|\psi_j(c)\rangle$ denote the eigenvectors of $H(c)$ with corresponding eigenvalues $E_j(c)$. Since $H(c)$ is Hermitian for real c and thus diagonalizable, $E_j(c)$ has no singularities on the real axis, and we can define $|\psi_j(c)\rangle$ so that it also has no singularities on the real axis. We now expand $|\psi_j(c)\rangle$ as a power series about the point $c = 0$. The series coefficients for c^n are $|\psi_j^{(n)}(0)\rangle/n!$, where the superscript (n) denotes the n^{th} derivative. An analogous series expansion can also be applied to the eigenvalue $E_j(c)$. These series converge for all $|c| < |z|$, where z and its complex conjugate \bar{z} are the closest singularities to $c = 0$ in the complex plane. In the following we discuss perturbation theory, which can be regarded as the calculation of these series expansions

in cases where the eigenvalues and eigenvectors of H_0 are known or readily computable.

In order to illuminate our discussion with a concrete example, we consider a quantum Hamiltonian known as the Bose-Hubbard model in three dimensions [8]. It describes a system of identical bosons on a three-dimensional cubic lattice. The Hamiltonian has a term proportional to t that controls the lattice hopping of each boson, a term proportional to U that controls the pairwise interactions between bosons on the same site, and a chemical potential μ . The full details of the model are given in Supplementary Materials. We consider a system of four bosons with $\mu = -6t$ on a $4 \times 4 \times 4$ lattice. We first try to use perturbation theory to compute the ground state energy eigenvalue E_0 in units of the hopping parameter t . In panel **a** of Fig. 1 we show E_0/t versus interaction strength U/t . The red asterisks indicate the exact energies. The lines (1 = red dashed, 2 = magenta dotted, 3 = grey dashed-dotted, 4 = blue solid, 5 = black long-dashed-dotted, 6 = orange long-dashed) denote the first six orders for the expansion of E_0/t as a power series around $U/t = 0$. We see that perturbation theory fails to converge when U/t is less than about -3.8 .¹ This is caused by branch point singularities at nearby points in the complex plane where the ground state eigenvalue is merging with another eigenvalue.

The failure of perturbation theory is not surprising considering that the physical character of the ground state eigenvector changes significantly. It is a Bose gas for $U/t > 0$, a weakly-bound state for $-3.8 < U/t < 0$, and then a tightly-bound cluster for $U/t < -3.8$. Although the eigenvector makes these changes in a linear space with hundreds of thousands of dimensions (before symmetrization), the eigenvector traces out a path with significant displacement in only a few independent directions. To demonstrate this we compute the ground state eigenvectors at three sampling points, $U/t = -5.0, -1.5, 2.0$. These three vectors span a three-dimensional subspace. We project the Hamiltonian for general U/t onto this subspace and find the lowest eigenvalue and eigenvector. This technique is an example of an approach we call eigenvector continuation. In panel **a** of Fig. 1 the black solid line shows E_0/t computed using eigenvector continuation (EC) with the three sampling points shown as black diamonds. The agreement with the exact energies is quite good, and the same level of accuracy is found when comparing the eigenvector computed using EC to the exact eigenvector.

Eigenvector continuation can be used to “learn” sampling data from the region $-3.8 < U/t < 0$ and extrapo-

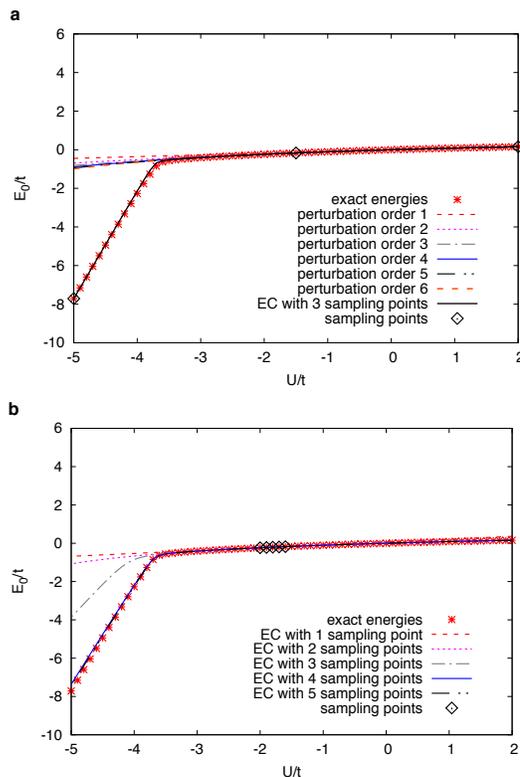


FIG. 1: **Ground state energy versus coupling.** In each panel **a** and **b** we plot the ground state energy E_0/t versus coupling U/t for four bosons in the three-dimensional Bose-Hubbard model on a $4 \times 4 \times 4$ periodic lattice. The red asterisks are the exact energies. In panel **a** the lines (1 = red dashed, 2 = magenta dotted, 3 = grey dashed-dotted, 4 = blue solid, 5 = black long-dashed-dotted, 6 = orange long-dashed) denote the first six orders of the expansion of E_0/t as a power series around the point $U/t = 0$. For comparison, the black solid line shows E_0/t computed using eigenvector continuation (EC) with the three sampling points shown as black diamonds. In panel **b** the black diamonds show the five sampling points, and the lines (1 = red dashed, 2 = magenta dotted, 3 = grey dashed-dotted, 4 = blue solid, 5 = black long-dashed-dotted) denote the eigenvector continuation (EC) results for E_0/t when projecting onto 1, 2, 3, 4, or 5 vectors.

late to the regions $U/t < -3.8$ and $U/t > 0$. To demonstrate this we sample the ground state eigenvectors at five points, $U/t = -2.0, -1.9, -1.8, -1.7, -1.6$. The results are shown in panel **b** of Fig. 1. The red asterisks are the exact energies. The black diamonds show the five sampling points, and the lines (1 = red dashed, 2 = magenta dotted, 3 = grey dashed-dotted, 4 = blue solid, 5 = black long-dashed-dotted) denote the EC results for E_0/t when projecting onto 1, 2, 3, 4, or 5 vectors. We see that the method converges rapidly and is able to capture the abrupt change in slope near $U/t = -3.8$.

Why eigenvector continuation works and how fast it converges can be understood using analytic function theory. We return back to the series expansion for $|\psi_j(c)\rangle$.

¹ From the first six orders of the expansion, the series might seem to converge to the wrong value for $U/t < -3.8$. However the series is divergent at higher orders.

Although the series expansion about $c = 0$ fails to converge for points $|c| > |z|$, we can define an analytic extension by constructing a new series about another point $c = w$, where w is real and $|w| < |z|$. For this second series the coefficients of $(c - w)^n$ are $|\psi_j^{(n)}(w)\rangle / n!$. We can use the original series to express each $|\psi_j^{(n)}(w)\rangle$ in terms of $|\psi_j^{(m)}(0)\rangle$. In this way we can approximate $|\psi_j(c)\rangle$ to arbitrary accuracy as a linear combination of the vectors $|\psi_j^{(n)}(0)\rangle$ in the region $|c - w| < |z - w|$ centered at w . Using this process of analytic continuation repeatedly, we can reach any value of c and express any $|\psi_j(c)\rangle$ to arbitrary accuracy as a linear combination of a finite number of vectors $|\psi_j^{(n)}(0)\rangle$. The number of required vectors is determined by the number of different expansion centers needed in the analytic continuation and the rate of convergence of each series expansion. This explains why the trajectory traced out by $|\psi_j(c)\rangle$ moves in a small number of linearly-independent directions.

The basic strategy of eigenvector continuation is to “learn” the low-dimensional subspace that contains the eigenvector trajectory $|\psi_j(c)\rangle$. We start with the lowest eigenvalue and eigenvector in a given symmetry class. We then sample several values $c = c_i$ with $i = 1, \dots, K$ and compute the corresponding eigenvectors $|\psi_j(c_i)\rangle$. The sampling values c_i are chosen in the domain where the computational method of choice is accurate. The target value $c = c_\odot$, where we want to determine $E_j(c_\odot)$ and $|\psi_j(c_\odot)\rangle$, will often lie in a region where direct calculation is no longer feasible. We then compute the inner products $N_{i',i} = \langle \psi_j(c_{i'}) | \psi_j(c_i) \rangle$ and matrix elements $H_{i',i} = \langle \psi_j(c_{i'}) | H(c_\odot) | \psi_j(c_i) \rangle$ and solve the generalized eigenvalue problem. This consists of finding the eigenvalues and eigenvectors of the K -dimensional matrix $N^{-1/2} H N^{-1/2}$, where $N^{-1/2}$ is the inverse square root of the positive matrix N . For the lowest eigenvalue and eigenvector of each symmetry class, it suffices to compute the lowest eigenvalue and eigenvector of the K -dimensional matrix. We then proceed to the next-lowest eigenvalue and eigenvector in the symmetry class with the additional constraint that it is orthogonal to the lowest eigenvector. Continuing on in this manner, any eigenvalue and eigenvector can in principle be calculated. In cases where there are singularities near the real axis, the convergence of the method can be accelerated by including several eigenvectors $|\psi_j(c_i)\rangle, |\psi_{j'}(c_i)\rangle, \dots$ for each c_i . This procedure and the connection to Riemann sheets at branch point singularities is discussed in Supplementary Materials.

We now test the eigenvector continuation in a many-body quantum Monte Carlo calculation. We consider lattice simulations of pure neutron matter at leading order in chiral effective field theory. Instead of using the lattice actions used in recent work [9, 10], we purposely use the computationally difficult action described in Ref. [11]. Due to severe sign oscillations, it is not

possible to do accurate simulations for more than four neutrons. Even extrapolation methods such as those discussed in Ref. [12, 13] provide no significant improvement due to the rapid onset of sign cancellations. The leading-order action consists of the free neutron action, a single-site contact interaction between neutrons of opposite spins, and the two-body potential generated from the exchange of a pion. This one-pion exchange potential is proportional to g_A^2 , the square of the axial-vector coupling constant. In contrast with the lattice actions used in Ref. [9, 10], the short distance behavior of this one-pion exchange potential is not softened and, as a result, causes severe sign oscillations in the Monte Carlo simulations. We will consider the one-parameter family of lattice Hamiltonians $H(g_A^2)$ which results from varying g_A^2 . The desired target value of g_A^2 is the value 1.66 used in Ref. [11]. Details of the lattice action are presented in Supplementary Materials.

The systems we calculate are the ground state energies of six and fourteen neutrons on a $4 \times 4 \times 4$ lattice with spatial lattice spacing 1.97 fm and time lattice spacing 1.32 fm. We are using natural units where \hbar and the speed of light are set to 1. We use projection Monte Carlo with auxiliary fields to calculate the ground state energy. Details of the simulation are presented in Supplementary Materials, and some reviews of the lattice methods can be found in Ref. [11, 14]. We first attempt to compute the ground state energies by direct calculation. The errors are quite large due to sign oscillations. For six neutrons the ground state energy is $E_0 = 12({}_{-4}^{+3})$ MeV, and for fourteen neutrons $E_0 = 42({}_{-15}^{+7})$ MeV.

Next we use eigenvector continuation for the same systems with sampling data $g_A^2 = c_1, c_2, c_3$, where $c_1 = 0.25$, $c_2 = 0.60$, and $c_3 = 0.95$. We use Monte Carlo simulations to calculate the ground state eigenvectors for c_1, c_2, c_3 . In Table I we show the EC results using just one of the three vectors, two of the vectors, or all three vectors. The error bars are estimates of the stochastic error and extrapolation error when taking the limit of infinite projection time. For comparison we also show the direct calculation results. We see that the EC results converge quite rapidly with the number of vectors included. The results are also consistent with the direct calculation results, though with an error bar that is smaller by an order of magnitude.

Our calculations demonstrate the potential value of eigenvector continuation for quantum Monte Carlo simulations. One can use eigenvector continuation for interactions that produce sign oscillations or noisy Monte Carlo simulations. Eigenvector continuation can also be used to significantly extend the convergence of perturbation theory, and this will be demonstrated in a forthcoming publication. While eigenvector continuation would not improve a Lanczos calculation using a truncated basis with fixed dimensions, eigenvector continuation can be used to extend the reach of techniques that remove ba-

g_A^2 values	$E_0(N=6)$ [MeV]	$E_0(N=14)$ [MeV]
c_1	14.0(4)	48.8(6)
c_2	13.7(4)	48.5(7)
c_3	13.8(6)	48.8(8)
c_2, c_3	13.7(4)	48.4(7)
c_3, c_1	13.8(4)	48.8(6)
c_1, c_2	13.7(4)	48.4(7)
c_1, c_2, c_3	13.7(4)	48.4(7)
direct calculation	12($^{+3}_{-4}$)	42($^{+7}_{-15}$)

TABLE I: Eigenvector continuation results for the ground state energy for six and fourteen neutrons using sampling data $g_A^2 = c_1, c_2, c_3$, where $c_1 = 0.25$, $c_2 = 0.60$, and $c_3 = 0.95$. For comparison we also show the direct calculation results.

sis truncation errors[15]. The method is expected to be particularly useful for bound state calculations. For continuum states one should consider all low-lying continuum states in a finite volume together rather than picking out one continuum eigenvector at a time. This can be done using a framework such as the adiabatic projection method [16, 17], which constructs continuum states for all possible relative displacements between clusters.

If the inner products $N_{i',i}$ and matrix elements $H_{i',i}$ can be computed with sufficient accuracy, then any eigenvector problem can be solved in this manner. However, there are practical limits to the accuracy one can achieve for any computational method, and this sets limits on how far eigenvector continuation can be pushed. In future work we will discuss machine learning techniques for optimizing the eigenvector continuation process [18–20]. While we have emphasized the use of eigenvector continuation to perform extrapolations in the control parameter c , there are also fascinating quantum systems where interpolation is the most interesting question. One example is the phenomenon known as “BCS-BEC crossover” in degenerate fermionic systems at large scattering length [21]. There are variational wave functions that work very well for the weak-coupling BCS side, and other variational wave functions that accurately describe the strong-coupling BEC side. Our results here suggest that the crossover transition can be well represented using linear combinations of the different variational wave functions. In the same manner, eigenvector continuation could also be used to study shape phase transitions in atomic nuclei [22].²

We look forward to seeing future applications of eigenvector continuation when paired with computational methods such as quantum Monte Carlo simulations, many-body perturbation theory, and variational methods. We anticipate that eigenvector continuation can

serve as a new theoretical tool to study quantum correlations, BEC-BCS crossover, shape transitions, entanglement, geometric phases, and quantum phase transitions at finite volume.

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