On a dual representation of the Goldstone manifold

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(Dated: April 13, 2020)

An intrinsic wavefunction with a broken continuous symmetry can be rotated with no energy penalty leading to an infinite set of degenerate states known as a Goldstone manifold. In this work, we show that a dual representation of such manifold exists that is sampled by an infinite set of non-degenerate states. A proof that both representations are equivalent is provided. From the work of Peierls and Yoccoz (Proc. Phys. Soc. A 70, 381 (1957)), it is known that collective states with good symmetries can be obtained from the Goldstone manifold using a generator coordinate trial wavefunction. We show that an analogous generator coordinate can be used in the dual representation; we provide numerical evidence using an intrinsic wavefunction with particle number symmetry-breaking for the electronic structure of the Be atom and one with $\hat{S}^z$ symmetry-breaking for a H$_5$ ring. We discuss how the dual representation can be used to evaluate expectation values of symmetry-projected states when the norm $|\langle \Phi | P^q | \Phi \rangle|$ becomes very small.

I. INTRODUCTION

In finite fermion systems, exact solutions to the Schrödinger equation can be labelled by quantum numbers associated with the symmetries of the Hamiltonian. Approximate solutions may break some of those symmetries in order to develop some of the physical correlations in the system within the constraint imposed by the form of the trial wavefunction. As a typical example, the $U(1)$ particle-number symmetry is spontaneously broken in the Hartree–Fock–Bogoliubov (HFB) framework in order to account for pairing correlations [1]. When continuous symmetries are broken, Goldstone’s theorem establishes that the trial state can be rotated with no energy penalty (see, e.g., Ref. [2]). The infinite set of all degenerate, gauge-rotated states constitutes the Goldstone manifold (GM).

In finite systems, symmetry breaking in approximate solutions is artificial. In fact, symmetry-broken solutions can be seen as intrinsic or deformed states from which exact symmetries should still be restored. It is possible to obtain symmetry-adapted states from the intrinsic solutions using symmetry-projection operators. Commonly used projection techniques exploit the degeneracy within the GM in order to restore those symmetries broken in mean-field trial states (see, e.g., Refs. [3][5], as first proposed by Peierls and Yoccoz [6].

When some of us studied the stability matrix of symmetry-projected mean-field states [7] we realized that, for each continuous broken symmetry, there are two directions in which the intrinsic wavefunction can be deformed such that the resulting symmetry-projected state is actually equivalent. While one of the directions was expected, as it points along the GM, the other direction came as a surprise.

The redundancy of symmetry-projected states has been observed in different contexts. For instance, in our own work we described how the inclusion of a chemical potential during the optimization of trial number-projected HFB states in a variation-after-projection framework did not change the final result [3]. In related work, Jensen et al. [8] described an optimization method for the antisymmetrized geminal power (AGP) wavefunction (equivalent to number-projected HFB). The authors noted that the AGP energy is the ratio of two homogeneous functions of the same degree and, as such, the parameters in the AGP wavefunction are non-unique. Some of us recently pointed out [9] that in fact all of the reduced density matrices of the AGP wavefunction are invariant with respect to a multiplicative factor rescaling the geminal parameters. Rescaling the geminal parameters is equivalent to modifying the underlying intrinsic determinant from a number-projected HFB point of view but this only results in a change of normalization of the resulting AGP wavefunction (see Sec. III A for a more detailed discussion).

The aim of this work is to unambiguously identify the source of this redundancy in symmetry-projected states. Namely, we provide a proof that an equivalent representation of the GM exists. This is generated by a set of non-degenerate states, generated from the parent broken symmetry state using a rotation involving a purely imaginary angle.

The rest of the manuscript is organized as follows.
In Sec. II A we introduce the GM associated with symmetry-broken trial wavefunctions. In Sec. II B we provide a short introduction to the Generator Coordinate Method (GCM), which we use in Sec. II C to extract symmetry-adapted states from the GM. In Sec. II D we provide a short discussion of how the double projection method relates to the dual representation of the GM. In Sec. IV we make some concluding remarks, including how the dual representation can be used, in certain cases, to improve the numerical precision in the evaluation of matrix elements between symmetry-projected states.

II. THEORY

A. Symmetry Breaking and the Goldstone Manifold

Continuous symmetries of the Hamiltonian can be either Abelian or non-Abelian, depending on the number of generators involved and their commutation properties. For the sake of simplicity, we will limit ourselves in this work to Abelian groups, that is, $U(1)$ symmetries. Nonetheless, the dual representation described below also exists in non-Abelian symmetries.

Consider an operator $Q$ associated with a continuous symmetry of the Hamiltonian such that $[Q, H] = 0$. Note that $Q$ must be Hermitian in order to be associated with an observable. Exact eigenstates of $H$ can always be chosen as eigenstates of $Q$. Approximations to eigenstates need not, however, preserve the symmetry. If a trial state $|\Phi\rangle$ is not an eigenfunction of $Q$, then the states

$$|\Phi_{\theta}\rangle = \exp(i\theta \hat{Q}) |\Phi\rangle$$

constitute the GM. We label this representation as direct in the rest of this manuscript. It is trivial to show that the unitary operator $\exp(i\theta \hat{Q})$ preserves the norm and Hamiltonian expectation values

$$\langle \Phi_{\theta} | \Phi_{\theta} \rangle = \langle \Phi | \Phi \rangle,$$

$$\langle \Phi_{\theta} | \hat{H} | \Phi_{\theta} \rangle = \langle \Phi | \hat{H} | \Phi \rangle.$$  

That is, all states in the direct representation are degenerate. A rotation in the GM can therefore be performed with no energy penalty.

The central premise of this manuscript is that there exists a dual representation of the same GM. This is generated by the set of states

$$|\Phi_{\theta}\rangle = \mathcal{N} \exp(\theta \hat{Q}) |\Phi\rangle,$$

where $\mathcal{N}$ is a normalization factor. (We use, for convenience, different symbols for rotations in the direct ($\theta$) and dual ($\vartheta$) representations.) Note that $\exp(\vartheta \hat{Q})$ is not unitary and therefore the norm and Hamiltonian expectation values are not preserved. We refer the reader to App. A for a proof of the equivalence of the manifolds.

B. Generator Coordinate Method (GCM)

In this section we provide a short introduction to the GCM, with only the necessary elements to follow the discussion below. For more details about the GCM, we refer the reader to Refs. 1 and 10. In the GCM, a variational ansatz for the wavefunction is written as

$$|\psi\rangle = \int da |\phi_a\rangle f(a).$$

The wavefunction $|\psi\rangle$ is written as a superposition, with a weight function $f(a)$, of the intrinsic wavefunctions $|\phi_a\rangle$ along the deformation parameter $a$. Most commonly, $|\phi_a\rangle$ are chosen as mean-field states, but this need not always be the case.

The function $f(a)$ can be determined by the variational principle leading to the Griffin-Hill-Wheeler (GHW) equation:

$$\int da' [\mathcal{H}(a', a') - E \mathcal{S}(a, a')] f(a') = 0,$$

with $\mathcal{H}(a, a') = \langle \phi_a | \hat{H} | \phi_a' \rangle$ and $\mathcal{S}(a, a') = \langle \phi_a | \phi_a' \rangle$. The state $|\psi\rangle$ can be normalized as

$$\langle \psi | \psi \rangle = 1 = \int da \int da' f^*(a) \mathcal{S}(a, a') f(a').$$

Because of this normalization choice, the function $|f(a)|^2$ cannot be associated with a probability distribution. On the other hand, it is possible to construct

$$g(a) = \int da' \mathcal{S}^{1/2}(a, a') f(a').$$

It follows that $|g(a)|^2$ can actually be associated with a probability distribution:

$$\int da |g(a)|^2 = 1.$$  

Here, $\mathcal{S}^{1/2}$, the operational square root of the norm kernel, can be formally defined through

$$\mathcal{S}(a, a') = \int da'' \mathcal{S}^{1/2}(a, a'') \mathcal{S}^{1/2}(a'', a').$$

It will also prove useful to introduce the function

$$h(a) = \int da' \mathcal{S}(a, a') f(a') = \langle \phi_a | \psi \rangle.$$

Here, $h(a)$ gives the projection of $|\psi\rangle$ onto the component $|\phi_a\rangle$. As described in the next section, a GCM ansatz can be used along the GM to yield symmetry-adapted states.
C. GCM on the Goldstone manifold

Peierls and Yoccoz [6] proposed the use of a GCM ansatz among the states in the GM. (See also Refs. [1] and [11] for a more detailed presentation.) Namely, they proposed a variational optimization of an ansatz of the form

$$|\Psi\rangle = \int d\theta |\Phi_\theta\rangle \tilde{f}(\theta), \quad (12)$$

with $|\Phi_\theta\rangle$ given by Eq. 1.

Note that all the states $|\Phi_\theta\rangle$ are spanned by the same set of symmetry-adapted states (see App. A). A representation of the Hamiltonian among such symmetry-adapted states is necessarily diagonal given that $\hat{Q}$ is a symmetry of $\hat{H}$. It follows that the eigenstates of the Hamiltonian among the overcomplete set $\{\Phi_\theta\}$ correspond to the symmetry-adapted states. In other words, symmetries can be restored by a wavefunction of the form of Eq. 12. We can therefore rewrite the ansatz as

$$|\Psi\rangle = \int d\theta |\Phi_\theta\rangle \hat{f}(\theta), \quad (13)$$

which explicitly indicates that the weight function $\hat{f}(\theta)$ depends parametrically on the quantum number $q$ to yield the symmetry-adapted state $|\Psi_q\rangle$.

The same justification can be established by a GCM ansatz on the dual GM. Namely, the ansatz

$$|\Psi\rangle = \int d\vartheta |\Phi_\vartheta\rangle \tilde{f}(\vartheta),$$

with $|\Phi_\vartheta\rangle$ given by Eq. 4, can also be used and will yield the same set of symmetry-adapted states. The amplitudes $f(\vartheta)$ can be obtained from a solution to the corresponding GHW equation.

In the direct representation, it is possible to deduce the form of the amplitudes in the GCM ansatz of Eq. 12 without solving the corresponding GHW equation. For instance, in the case of a $U(1)$ symmetry, the GCM amplitudes are given by (see App. B)

$$\hat{f}(\theta) = \frac{1}{2\pi} e^{-iq\theta}.$$ \hspace{1cm} (15)

This can be used to deduce the form of the projection operator for an Abelian symmetry as

$$\hat{P} = \frac{1}{2\pi} \int d\theta \exp(i\theta(\hat{Q} - q)).$$ \hspace{1cm} (16)

In the dual representation one cannot generally deduce the shape of the weight functions $f(\vartheta)$ a priori. These have to be obtained by a numerical solution to the GHW equations. We note that, in practical calculations, one can use a discretized sampling of the domain $\vartheta$. In particular, it can be easily shown that the exact Hamiltonian eigenvalues can be obtained as long as the number of grid points sampled is sufficient to obtain all quantum numbers. For $\hat{N}$ projection, this is equal to $M + 1$, where $M$ is the number of orbitals available.

D. Comparison with Double Projection

In Ref. [12] Peierls and Thouless introduced the double projection (DP) method or double GCM (DGCM). In DGCM, the deformation parameter is generalized from a real to a complex one. This extension allowed the authors to obtain the correct kinetic energy associated with translational motion in nuclei.

In Sec. II A we established that the manifold generated by a real or a purely imaginary deformation parameter are equivalent. Therefore, there is no additional variational flexibility gained by letting the generator coordinate become complex.

This, however, does not apply to DGCM. In particular, the idea of Peierls and Thouless was to define a manifold of intrinsic states $|\Phi_\vartheta\rangle$ where these are obtained by minimization of $\langle \hat{H} \rangle$ subject to the constraint $\langle \hat{Q} \rangle = x$. (In DGCM, the authors additionally restore the symmetry $Q$, for each $|\Phi_\vartheta\rangle$, using the direct representation of the GM.) The manifold $\{\Phi_\vartheta\}$ is not equivalent to the dual representation of the GM, where the states $|\Phi_\theta\rangle$ are generated by a simple rotation of $|\Phi\rangle$. In particular, it will not be generally true that $\exp(\vartheta \hat{Q}) |\Phi\rangle$ is a minimizer of $\langle \hat{H} \rangle$, even though it does satisfy the constraint imposed.

III. RESULTS AND DISCUSSION

A. $\hat{N}$ projection on Be

Due to the repulsive nature of electron-electron interactions, spontaneous symmetry breaking of particle number does not occur in mean-field solutions to the electronic Schrödinger equation in molecular and atomic systems [13]. An intrinsically deformed state can still be obtained when the wavefunction is optimized in the presence of a projection operator (i.e., a variation-after-projection approach). We work with a number-projected HFB solution to the neutral Be atom ($n = 4$) using a standard cc-pVDZ basis set [14].

The intrinsic wavefunction used corresponds to an HFB state with singlet pairing and can be written, in the natural orbital basis as

$$|\Phi\rangle = \prod_k \left( 1 + \frac{u_k}{v_k} a_k^\dagger a_k^\dagger \right) |\rangle, \quad (17)$$

where $|\rangle$ is the bare vacuum. We have optimized the wavefunction under the constraint $\langle \hat{N} \rangle|\Phi\rangle/\langle \Phi | \Phi \rangle = 4$.

The dual representation of the GM corresponds to the set of states

$$|\Phi_\vartheta\rangle = \mathcal{N} \exp(\vartheta \hat{N}) |\Phi\rangle, \quad (18)$$

where $\mathcal{N}$ is a normalization factor [15]. The set $\{\Phi_\vartheta\}$ is composed of HFB states of the same form as that of Eq. 17 expanded in the same set of natural orbitals, but
with parameters \(v_k\) that depend on the angle \(\vartheta\). This dependence is shown in Fig. 1.

We show in Fig. 2 the expectation values of \(\hat{N}\) and \(\hat{H}\) among the states \(\{\Phi_{\vartheta}\}\), with

\[
N_{\vartheta} = \langle \Phi_{\vartheta} | \hat{N} | \Phi_{\vartheta} \rangle / \langle \Phi_{\vartheta} | \Phi_{\vartheta} \rangle, \tag{19}
\]

\[
H_{\vartheta} = \langle \Phi_{\vartheta} | \hat{H} | \Phi_{\vartheta} \rangle / \langle \Phi_{\vartheta} | \Phi_{\vartheta} \rangle. \tag{20}
\]

As it is evident from the figure, expectation values are not conserved in this dual representation. \(N_{\vartheta}\) varies monotonically between 0 and 28 (the basis set used has 14 basis functions). \(H_{\vartheta}\) has a minimum near \(\vartheta = 0\), as expected, given that \(\vartheta = 0\) was defined such that \(N_{\vartheta} = 4\), corresponding to a neutral Be atom.

The wavefunctions obtained from the solution of the GHW equation in the dual representation of the GM are shown in Fig. 3. On the right, we show the probability distributions \(|g(\vartheta)|^2\). Note that, in solving for the GHW equation, we have pre-normalized each intrinsic state, such that the norm kernel has a unit diagonal.

The form of \(g(\vartheta)\) depends on the domain chosen for \(\vartheta\), as shown in the inset of Fig. 3. Here, we should clarify that the domain of \(\vartheta\) can be formally truncated to a finite one: as long as the domain samples the states of all symmetries \(q\), enlarging the domain just adds redundant information. Using an infinite domain for \(\vartheta\) renders some states (in this case, those with \(n = 0\) or \(n = 28\)) non-normalizable. Unlike \(g(\vartheta)\), the representation \(h(\vartheta)\) is unique, given that this is the projection of the eigenstates onto the manifold \(\{\Phi_{\vartheta}\}\). This can be obtained, even without solving the GHW equation, using the known representation of the symmetry-adapted states in the direct manifold.

Because \(N_{\vartheta}\) varies monotonically with \(\vartheta\), the deformation parameter \(\vartheta\) can be mapped onto \(N_{\vartheta}\). The resulting amplitudes, as a function of \(N_{\vartheta}\), are shown in Fig. 4. As one would expect, \(h(N_{\vartheta})\) peaks at \(N_{\vartheta} = n\). For \(n \geq 6\) the functions have a Gaussian-like profile, suggesting that a numerical integration with an appropriate Gaussian quadrature can yield a good description of such states.

**B. \(\hat{S}^z\) projection on \(H_5\) ring**

We next consider a system with five hydrogen atoms equally spaced placed around a circle such that the distance between nearest neighbor atoms is 1.8 a.u. A standard cc-pVDZ basis set was used in the calculations (5 basis functions per H atom). The lowest-energy Hartree–Fock (HF) solution for a ring of hydrogen atoms produces an anti-ferromagnetic alignment of the spins; when the rings have an odd number of atoms, this leads to spin frustration and a generalized HF (GHF) ground state with a coplanar spin arrangement. In the case of \(H_5\), the lowest energy solution has nearest-neighbor spins rotated by 144 degrees, as illustrated schematically in Fig. 5.

As discussed in Ref. 17 a HF solution with a coplanar but not collinear spin arrangement is not an eigenfunction of \(\hat{S}^z\), for any direction \(q\). In what follows, we consider the restoration of \(\hat{S}^z\) as a symmetry from a solution with spins oriented as shown in Fig. 5. (Note that results would be different had we chosen to restore \(\hat{S}^x\) or \(\hat{S}^y\).

The intrinsic wavefunction used corresponds to a GHF state which can be written in a corresponding orbital basis (with the spin-up orbitals being different than the spin-down ones, even when they are spanned by the same basis functions) as

\[
|\Phi_{\vartheta}\rangle = N \exp(\vartheta \hat{S}^z) |\Phi\rangle.
\]

where \(N\) is the number of electrons. As it should be evident from the scheme the intrinsic wavefunction satisfies \(\langle \Phi | \hat{S}^z | \Phi \rangle / \langle \Phi | \Phi \rangle = 0\).

The dual representation of the GM is generated in this case through

\[
|\Phi_{\vartheta}\rangle = N \exp(\vartheta \hat{S}^z) |\Phi\rangle,
\]

where \(N\) is a normalization factor. Fig. 6 shows the dependence of the expectation values of \(\hat{H}\) and \(\hat{S}^z\) on the deformation parameter \(\vartheta\). Note that in this case \(H_{\vartheta}\) is even while \(S^z_{\vartheta}\) is odd about \(\vartheta = 0\).

The wavefunctions obtained from the solution of the GHW equation in the dual representation of the GM are shown in Fig. 7. In this case, the wavefunctions are only shown with the deformation parameter \(\vartheta\) mapped onto \(S^z_{\vartheta}\). The wavefunction amplitudes for \(\pm S^z\) are reflections of each other through \(S^z_{\vartheta} = 0\), as one would have expected. Note that the decomposition of \(\langle \Phi_{\vartheta} | \Phi\rangle\) in terms of symmetry-adapted states can be extracted from the profile of \(h(S^z_{\vartheta})\) in Fig. 7.

**IV. CONCLUSIONS**

In this work, we have shown that a dual representation exists for the Goldstone manifold of symmetry-broken states. This is a general conclusion that is not restricted to the mean-field states considered in the results section. That is, it holds regardless of the form of the approximate solution to the Schrödinger equation used.

The use of the dual representation in the context of symmetry-projected techniques requires a numerical solution of the GHW equations, as opposed to the direct representation where the amplitudes are known a priori. The dual representation, however, can still be useful in other contexts. As an example, one typically faces numerical difficulties in evaluating expectation values of the state \(P^\vartheta |\Phi\rangle\) whenever \(\langle \Phi | P^\vartheta | \Phi \rangle\) is very small. In such a case, one can first rotate along a dual representation
FIG. 1. (Left) Coefficients $|v_k|$ in the intrinsic wavefunction along the deformation parameter $\vartheta$. Note that some levels, corresponding to $p$ or $d$ orbitals, are multiply degenerate: $v_3 = v_4 = v_5$, $v_7 = \cdots = v_{11}$, and $v_{12} = v_{13} = v_{14}$. (Right) Ratios $|v_k/u_k|$ in the intrinsic wavefunction.

FIG. 2. (Left) Expectation value of the number operator $\hat{N}$ along the deformation parameter $\vartheta$. (Right) Expectation value of the Hamiltonian operator $\hat{H}$. The inset zooms into the low-energy region; it also shows the energies of the symmetry-restored states (with the value of $n$ indicated) which are equivalent to the eigenvalues obtained from a solution of the GHW equation in the dual GM.

to an intrinsic state $|\Phi_\chi\rangle$ chosen such that it maximizes $|\langle \Phi_\vartheta | \hat{P}_q | \Phi_\vartheta \rangle |$.

The existence of the dual representation of the GM also suggests caution when trying to read significance into the structure of the deformed states optimized in symmetry-projected methods: there are multiple intrinsic states, with different deformation parameters, that all lead to the same symmetry-projected wavefunction.

V. ACKNOWLEDGMENTS

CAJH is grateful for support from a Wesleyan University start-up package. The work at Rice University was supported by the U.S. National Science Foundation under Grant No. CHE-1762320. GES is a Welch Foundation Chair (Grant No. C-0036).

Appendix A: On the equivalence of the Goldstone manifold representations

Consider a symmetry broken state $|\Phi\rangle$ and its expansion in terms of normalized symmetry-adapted states $\{\chi\}$:

$$|\Phi\rangle = \sum_q |\chi_q\rangle c_q, \quad (A1)$$
FIG. 3. (Left) GCM wavefunctions $h(\theta)$ obtained as solutions to the GHW equation for $n = 0, 2, \ldots, 10$. (Right) Probability distributions $|g(\theta)|^2$ obtained with a deformation domain $\theta \in (-10, 8)$. The inset shows, in thin lines, the behavior for large $-\theta$ when the deformation domain is reduced to $\theta \in (-8, 6)$.

FIG. 4. Same as Fig. 3 but mapping the deformation parameter $\theta$ onto $N_\theta$.

FIG. 5. Coplanar spin arrangement in the HF solution for H$_5$. The axis system in the lower corner indicates the convention used for the spin axis.

with $c_q = \langle \chi_q | \Phi \rangle$. Here, the subscript $q$ on $|\chi_q\rangle$ labels the symmetry of the states, such that

$$\hat{Q} |\chi_q\rangle = q |\chi_q\rangle. \quad (A2)$$

As shown below, $\exp(i\theta \hat{Q}) |\Phi\rangle$ is expanded in terms of the same set of symmetry-adapted states as $|\Phi\rangle$:

$$\exp(i\theta \hat{Q}) |\Phi\rangle = \sum_q \exp(i\theta \hat{Q}) |\chi_q\rangle c_q = \sum_q |\chi_q\rangle d_q \quad (A3)$$

with $d_q = \exp(i\theta q) c_q$.

A similar reasoning applies in the case of the dual representation. The states $\exp(\vartheta \hat{Q}) |\Phi\rangle$ are also expanded in the same set of symmetry-adapted states as $|\Phi\rangle$:

$$\exp(\vartheta \hat{Q}) |\Phi\rangle = \sum_q \exp(\vartheta \hat{Q}) |\chi_q\rangle c_q = \sum_q |\chi_q\rangle b_q \quad (A4)$$
FIG. 6. (Left) Expectation value of $\hat{S}_z$ along the deformation parameter $\vartheta$. (Right) Expectation value of the Hamiltonian operator $\hat{H}$. The energies of the symmetry-restored states are also shown (with the value of $s^z$ indicated); states with $\pm s^z$ are exactly degenerate.

FIG. 7. (Left) GCM wavefunctions $h(S_z^\vartheta)$ obtained as solutions to the GHW equation where the deformation parameter $\vartheta$ has been mapped onto $S_z^\vartheta$. (Right) Probability distributions $|g(S_z^\vartheta)|^2$.

with $b_q = \exp(\vartheta q) c_q$. It follows that the direct and dual representations are spanned by the same set of symmetry-adapted states and are therefore equivalent.

As a corollary, note that

$$\hat{P}^q \exp(i\vartheta Q) |\Phi\rangle = |\chi_q\rangle c_q \exp(i\vartheta q), \quad (A5)$$

$$\hat{P}^q \exp(\vartheta Q) |\Phi\rangle = |\chi_q\rangle c_q \exp(\vartheta q). \quad (A6)$$

That is, the same symmetry-projected states (up to arbitrary phase and normalization factors) are obtained from the direct and dual representations of the GM.

**Appendix B: Structure of the GCM kernels in $U(1)$ symmetry**

In this section we provide a brief discussion of the structure of the norm and Hamiltonian kernels associated with $U(1)$ symmetry restoration in both the direct and dual representations.

In the direct representation, the overlap kernel $S$ among the states of Eq. (1) defined by

$$S(\vartheta', \vartheta) \equiv \langle \Phi_{\vartheta'} | \Phi_{\vartheta} \rangle, \quad (B1)$$

satisfies a translation symmetry

$$S(\vartheta', \vartheta) = S(\theta - \theta'). \quad (B2)$$

This, along with the periodicity of the $\vartheta$ domain, implies that a Fourier transform of the norm kernel brings it to
diagonal form. The same holds true for the Hamiltonian kernel. In a discretized, equi-spaced grid the norm kernel has a matrix structure of the form
\[
\begin{pmatrix}
a & b & c & d \\
b & c & d & a \\
c & d & a & b \\
d & a & b & c \\
\end{pmatrix}.
\]
That is, the norm (and Hamiltonian) matrix is circular and its eigenvectors are given by a discrete Fourier transform.

In the dual representation, the overlap kernel $S$ among unnormalized states $| \tilde{\Phi}_\vartheta \rangle = \exp(\vartheta \hat{Q}) | \Phi \rangle$, defined by
\[
S(\vartheta', \vartheta) \equiv \langle \tilde{\Phi}_{\vartheta'} | \tilde{\Phi}_\vartheta \rangle, \quad (B3)
\]
satisfies a translation symmetry
\[
S(\vartheta', \vartheta) = S(0, \vartheta + \vartheta'). \quad (B4)
\]
In this case, however, the domain of $\vartheta$ is not periodic. In a discretized, equi-spaced grid the norm (and Hamiltonian) kernel has a matrix structure of the form
\[
\begin{pmatrix}
a & b & c & d \\
b & c & d & e \\
c & d & e & f \\
d & e & f & g \\
\end{pmatrix}.
\]
The eigenvectors of such a matrix do not have an analytic representation that is independent of the specific matrix elements. Note, however, that the full matrix can be constructed from evaluation of a linear (and not quadratic) number of terms.

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