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On the inversion of quantum mechanical systems: determining the amount and type of data for a unique solution

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The inverse problem of extracting a quantum mechanical potential from laboratory data is studied from the perspective of determining the amount and type of data capable of giving a unique answer. Bound state spectral information and expectation values of time-independent operators are used as data. The Schrödinger equation is treated as finite dimensional and for these types of data there are algebraic equations relating the unknowns in the system to the experimental data (e.g., the spectrum of a matrix is related algebraically to the elements of the matrix). As these equations are polynomials in the unknown parameters of the system, it is possible to determine the multiplicity of the solution set. With a fixed number of unknowns the effect of increasing the number of equations on the multiplicity of solutions is assessed. In general, if the number of the equations matches the number of the unknowns, the solution set is denumerable. A result on the solvability of polynomial equations is extended to the case where the number of equations exceeds the number of unknowns. We show that if one has more equations than the number of unknowns, generically a unique solution exists. Several examples illustrating these results are provided.

KEY WORDS: Schrödinger equation, quantum mechanical systems

1. Introduction

Unlike the forward problem of determining the state of the system, the inverse problem of determining parameters in the system (via observation of some functional of

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the state) is generally ill-posed in the Hadamard sense. One finds that, either the solution does not exist, or the solution is not unique or, it is unstable with respect to errors in the data. We assume there is no error in the data so that existence of a solution is assured. For a particular system, classifying the type and amount of data to identify unknown parameters (lumped or distributed) is of paramount importance. The identification algorithm must be stable and the solution must be unique for it to be useful. Our interest centers on the identification of the potential in quantum mechanical systems. A quantum mechanical system is governed by Schrödinger's equation and data is in the form of a quadratic functional of the state (wavefunction).

The determination of the potential within the Born–Oppenheimer approximation is generally pursued by two different approaches: (1) perform *ab initio* quantum chemistry calculations and (2) the inversion of appropriate experimental data. High quality computational quantum chemistry approaches to produce *ab initio* potentials are limited to relatively small systems of a few atoms and these potentials often do not have the accuracy to explain modern laser-spectroscopic data. On the other hand, most of the existing numerical procedures to extract potentials from laboratory data may be characterized as parameter-fitting [1,2]. Direct inversion methods exist for special problems: for example, the Rydberg–Klein–Rees (RKR) [3] method can extract potentials for diatomic molecules from spectroscopic data. A method of inversion for excited state potentials using spectroscopic data and knowledge of the ground state potential is presented in [4]. The identification of the coefficient function $q(x)$ in a Sturm–Liouville problem

$$\begin{aligned} &-y'' + q(x)y = \lambda y, \\ &y'(0) - ay(0) = 0, \\ &y'(1) + by(1) = 0, \end{aligned} \tag{1}$$

using complete spectral information $\{\lambda_i\}_{i=1}^{\infty}$ is a well-known inverse problem. It is known [5,6] that this spectral information is insufficient to retrieve the potential uniquely unless the function q is symmetric with respect to mid-point of the interval $[0, 1]$. However, two sets of spectra obtained by changing the boundary conditions (i.e., changing a and b) is sufficient to recover q uniquely [7–10]. The finite-dimensional version of this inverse eigenvalue problem aims to construct the diagonal matrix V from knowledge of the spectrum of the matrix $H_0 + V$, where H_0 is a real Hermitian matrix [11–14]. A single spectrum again is insufficient to determine the matrix V, and additional data must be incorporated for a unique inversion. Expectation value data of observable operators may be exploited for this purpose, including time-dependent data arising from starting in a non-stationary initial state. Exploration of this issue is the main motivation of the paper.

We assume that the system is restricted to bound-state dynamics, i.e., spectrum is discrete and finite. The Hamiltonian of the system is represented in a basis where the potential matrix is diagonal. We assume that spectroscopic information is available and also that we can measure the expected value of appropriate observables in a bound-state or in a superposition of bound states. This latter data augmentation consists of time-dependent expectation values. Various cases will be considered using different types of

data. Since the number of unknowns is fixed, the goal is to assess whether this augmentation is capable of reducing the multiplicity of solutions to one. When only spectral data is used the number of polynomial equations matches the number of unknowns. It may be shown that generically the solution set is not unique when the number of equations matches the number of unknowns [11]. We will show that if the number of equations exceeds the number of unknowns, then the multiplicity of the solution is almost always reduced to one. The method presented here can classify the type and amount of data in relation to the number of unknowns. The unknowns are those of the potential matrix and/or an eigenvector. Extracting an eigenvector and its eigenvalue will also determine the potential matrix elements, since the latter is assumed to be diagonal.

The paper is organized as follows. Section 2 formulates the inverse problem. We present a theorem [11] concerning the multiplicity of the solution set of a polynomial system of equations and introduce a lemma to generalize and extend the theorem for our purposes. The theorem and lemma will be employed to indicate what kind and amount of data may be used for inversion to provide a unique solution. The conditions stated in the lemma must be strictly satisfied for its rigorous application to the inverse problem. Several examples are considered with different types of data. Section 3 addresses error analysis and numerical issues as experimental data inevitably contains error. Concluding remarks and future perspectives are presented in section 4. Finally, in the context of dynamic computer vision, Holt and Netravali [15–17] follow a similar approach to that taken here. In principle, other inverse problems that reduce to solving polynomial equations could also be analyzed with the same tools exploited in this work.

2. Inverse problem and the identification algorithm

Consider the time-dependent Schrödinger equation:

$$\begin{aligned} \mathrm{i}\,\frac{\partial|\psi(t)\rangle}{\partial t} &= (H_0 + V)\big|\psi(t)\big\rangle, \\ \big|\psi(0)\big\rangle &= |\psi_0\rangle, \end{aligned} \tag{2}$$

with $\hbar = 1$. H_0 and V represent the kinetic and potential energy operators, respectively. The inverse problem is expressed as follows. Laboratory data is assumed available, which is a functional of the state $|\psi(t)\rangle$. The data may be either time-independent (e.g., spectral data or the expectation values of time-independent operators in a particular eigenstate) or time dependent as the expectation value of an operator with respect to $|\psi(t)\rangle$, where $|\psi(0)\rangle$ is not an eigenstate. We may construct algebraic equations relating the data to the unknown potential. The state is projected into a finite-dimensional subspace spanned by an orthonormal set $\{|\phi_k\rangle\}_{k=1}^{n}$. We assume that the state is adequately described as residing in this subspace:

$$\big|\psi(t)\big\rangle = \sum_{k=1}^{n} a_k(t)|\phi_k\rangle. \tag{3}$$

This assumption implies that sufficient *a priori* information about the potential exists so that we can deduce a suitable basis $\{|\phi_k\rangle\}_{k=1}^n$ to support the state at all times of observation. The representation of equation (2) under this basis is

$$\mathrm{i}\dot{\vec{a}}_t = H\vec{a}_t, \tag{4}$$

where

$$\begin{aligned} \vec{a}_t &\equiv \big[a_1(t)\ a_2(t)\ \ldots\ a_n(t)\big], \\ H_{ij} &= \langle\phi_i|H_0 + V|\phi_j\rangle, \quad i, j = 1, 2, \ldots, n. \end{aligned} \tag{5}$$

The inverse problem considered here seeks to deduce whether the data uniquely determines the unknown elements in V. V is assumed to be diagonal unless otherwise stated, and this circumstance could arise either from physical considerations or due to the choice of the basis $\{|\phi_k\rangle\}_{k=1}^n$.

In the following analysis, inverting the potential reduces to solving a system of nonlinear polynomial equations. The unknowns in these equations will be either the unknowns of the potential or the coefficient vector $\vec{a}_t$. In either case we may denote the vector $x \equiv [x_1, x_2, \ldots, x_n]$ as representing all of the unknowns and we have the following equations

$$\begin{aligned} f_1(x_1, x_2, \ldots, x_n) &= d_1, \\ f_2(x_1, x_2, \ldots, x_n) &= d_2, \\ &\vdots \\ f_k(x_1, x_2, \ldots, x_n) &= d_k, \end{aligned} \tag{6}$$

where $k \geqslant n$ and $f_i(\cdot) : \mathbb{R}^n \to \mathbb{R}^k$. The quantities d_i on the right-hand side of the equations are the data. We seek to determine under what conditions the solution to the above system is unique. When the unknowns are those of the potential, then the solution of (6) will directly yield the potential. If the unknowns are the coefficient vector $\vec{a}_t$ at different times, the potential is determined by using equation (4). If the number of unknowns exactly matches the number of equations, then the following theorem [11] explains why the solution is a subset of $\mathbb{R}^n$ rather than a single point.

Let $f(x)$ be a polynomial over $\mathbb{C}^n$, the n dimensional complex Euclidean space. Denote by x the point $(x_1, x_2, \ldots, x_n)$ in $\mathbb{C}^n$. By $d(f)$ we denote the degree of f, i.e., the degree of the polynomial $f(tx_1, \ldots, tx_n)$ with respect to t. The principal part $f_\pi(x)$ is the highest homogeneous term appearing in $f(x)$. That is, f_π is uniquely determined by the conditions

$$f_\pi(tx_1, \ldots, tx_n) = t^{d(f)} f_\pi(x_1, \ldots, x_n), \tag{7}$$

$$d(f - f_\pi) < d(f) \tag{8}$$

for any nonconstant polynomial f; if $f \equiv$ *constant*, then $f_\pi \equiv 0$. Define

$$\begin{aligned} \phi &= (f_1, \ldots, f_n), \\ \phi_\pi &= (f_{1\pi}, \ldots, f_{n\pi}). \end{aligned} \tag{9}$$

The degree $d(\phi)$ of ϕ is defined by

$$d(\phi) = \prod_{j=1}^{n} d(f_j). \tag{10}$$

The following theorem provides a sufficient condition for the solvability of the system

$$\phi(x) = d. \tag{11}$$

Theorem. Let $\phi = (f_1, \ldots, f_n)$ be a polynomial map of $\mathbb{C}^n$ into $\mathbb{C}^n$. Assume that the system

$$\phi_\pi(x) = 0 \tag{12}$$

has only a trivial solution $x = 0$. Then for any given $d = (d_1, \ldots, d_n)$ the system (11) is always solvable. The number of distinct solutions is always finite and does not exceed $d(\phi)$. Moreover, for almost all d the number of distinct solutions is exactly $d(\phi)$.

Remark. If $\phi : \mathbb{R}^n \to \mathbb{R}^n$ where $\mathbb{R}^n$ is the n-dimensional Euclidean space, the system $\phi(x) = d$ may not have a solution at all, i.e., the equations are inconsistent. However, if the system has at least one solution, the number of solutions is at most $d(\phi)$. In the ideal case of error-free data, there is at least one solution to the equations above since the data in the laboratory is generated by the underlying potential. Thus we always are assured of the existence of solutions in this case; the issue of concern is the possible multiplicity of solutions. It would be desirable if the number of solutions to the system (11) could be reduced to just one by adding a single observation equation. The following lemma states under what conditions and in which sense this operation reduces the solution set to a single unique point in $\mathbb{R}^n$.

Lemma. Let $\psi = (f_1, f_2, \ldots, f_{n+1})$ be a polynomial map of $\mathbb{R}^n$ into $\mathbb{R}^{n+1}$. Suppose that the only solution to the system

$$\psi_\pi^{(n)}(x) = 0 \tag{13}$$

is the null solution, where $\psi_\pi^{(n)}(x)$ is the principal part of the polynomial vector function $\psi^{(n)}(x) = (f_1, f_2, \ldots, f_n)$. Suppose further that the system

$$\psi(x) = d \tag{14}$$

has at least one solution. Then the system (14) has no other solution for almost all polynomial functions $f_{n+1} : \mathbb{R}^n \to \mathbb{R}$.

Proof. Since the system $\psi(x) = d$ is consistent, it has at least one solution $X_0 \in \mathbb{R}^n$. Let $\mathcal{C} = \{X_0, X_1, \ldots, X_N\}$ be the solution set of the first n equations of the system (14). The claim is that in the space of all polynomial mappings $f_{n+1} : \mathbb{R}^n \to \mathbb{R}$ which satisfy $f_{n+1}(X_0) = d_{n+1}$, the subspace of functions which also pass through any other

point in $\mathcal{C}$ has measure zero. We proceed as follows to prove this statement. For $Y = (x_1, x_2, \ldots, x_n)$, $f_{n+1}(Y)$ is written as a linear combination of the monomials:

$$f_{n+1}(x_1, x_2, \ldots, x_n) = \sum_{i_1+i_2+\cdots+i_n \leqslant m} a_{i_1 i_2 \ldots i_n} {x_1}^{i_1} {x_2}^{i_2} \cdots {x_n}^{i_n}. \tag{15}$$

We have

$$M = 1 + \sum_{k=1}^{m} \frac{n(n+1)\cdots(n+k-1)}{k!} = 1 + \frac{(m+n)!}{m!n!}$$

numbers $a_{i_1 i_2 \ldots i_n}$. Define $\alpha \in \mathbb{R}^M$ as the vector of coefficents above and $\beta_Y \in \mathbb{R}^M$ as the vector of monomials ${x_1}^{i_1} {x_2}^{i_2} \cdots {x_n}^{i_n}$ so that

$$f_{n+1}(Y) = \alpha \cdot \beta_Y, \tag{16}$$

where $(\cdot)$ denotes the inner product in the Euclidean space $\mathbb{R}^M$. Note that $f_{n+1}(X_0) = \alpha \cdot \beta_{X_0} = d_{n+1}$. Now, define

$$\begin{aligned} \Lambda_0 &= \left\{\alpha \in R^M \mid \alpha \cdot \beta_{X_0} = d_{n+1}\right\}, \\ \Lambda_j &= \left\{\alpha \in \Lambda_0 \mid \alpha \cdot \beta_{X_j} = d_{n+1}\right\}, \quad j = 1, 2, \ldots, N, \end{aligned} \tag{17}$$

with $N + 1$ as the cardinality of the set $\mathcal{C}$. Λ_0 is a hyperplane in $\mathbb{R}^M$ and being so, it is an $(M-1)$-dimensional differentiable submanifold of $\mathbb{R}^M$ and each Λ_j is a hyperplane in Λ_0 and being so it is an $(M-2)$-dimensional submanifold of $\mathbb{R}^M$. From differential geometry [18] we know that if $A \subset B$ is a submanifold of codimension greater than zero, then A has measure zero in B. Since each $\Lambda_j \subset \Lambda_0$ is of codimension 1 in Λ_0 then Λ_j, $j = 1, 2, \ldots, N$, has measure zero in Λ_0, and thus so does their arbitrary intersections.

This result shows that for a polynomial that belongs to space Λ_0, the chance of it being in any subspace Λ_j (or in their arbitrary intersections) is essentially zero. This is equivalent to saying that system (14) has a unique solution for almost all polynomial functions $f_{n+1} : \mathbb{R}^n \to \mathbb{R}$.

The above lemma states that for the nonlinear polynomial system of equations defined above (n polynomials in n unknowns), if the number of solutions is finite, then adding another consistent polynomial equation (which is independent of the original set) shrinks the number of solutions to one with overwhelming likelihood. Thus, the set of functions which make the above system have multiple solutions has zero measure in the larger space of the functions which make the above system consistent. The key issue is for there to be a finite number of solutions to the first n equations, and then the number of solutions will be reduced to one for almost all consistent polynomial equations added as the last equation.

Armed with the theorem and lemma, we have a powerful criterion to judge whether a set of polynomial inverse equations have multiple solutions or not. In each case below we specify the data and analyze whether the potential (or equivalently an eigenstate) may be inverted from it. We used numerical searching algorithms to find the solutions. In no case did we find a false solution. However, as with any numerical algorithm, at times the

iterative procedure may not converge. In all the cases the physical system is assumed to be of finite dimension or the expansion in equation (3) is adapted to this effect. □

2.1. *Expectation values in a specific eigenstate as data*

The following $n+1$ time-independent data d_k is assumed available:

$$\langle\psi|O_k|\psi\rangle = d_k, \quad k = 1, 2, \ldots, n+1, \tag{18}$$

where ψ denotes one of the eigenstates of the Hamiltonian $H_0 + V$ and $\{O_k\}_{k=1}^{n+1}$ are independent Hermitian operators. We also assume that the eigenvalue E corresponding to this eigenstate is known. As ψ is an eigenstate, the coefficients $\{a_\ell\}_{\ell=1}^{n}$ are constants. Denoting by $\widetilde{O}_k$ the matrix representation of the operator O_k in the basis $\{|\phi_k\rangle\}_{k=1}^{n}$ and defining the real vector $\vec{a} = [a_1\ a_2\ \ldots\ a_n]$ we get the following equations:

$$\begin{aligned} \vec{a}^{\dagger}\widetilde{O}_1\vec{a} &= d_1, \\ \vec{a}^{\dagger}\widetilde{O}_2\vec{a} &= d_2, \\ &\vdots \\ \vec{a}^{\dagger}\widetilde{O}_{n+1}\vec{a} &= d_{n+1}. \end{aligned} \tag{19}$$

Here † denotes the transpose operation. The matrices must be independent, otherwise the number of equations can be reduced. Note that one of the matrices is taken as the identity matrix to specify the norm of the eigenstate $\langle\psi|\psi\rangle = 1$. This relation assures that equation (12) is satisfied which, in turn, guarantees that the system (19) has a finite number of solutions. So, we have $n+1$ consistent equations in n variables. The lemma says that for almost all independent Hermitian operators O_{n+1}, the system (19) has a unique solution.

For illustration we numerically tested the following example. Six random 5×5 Hermitian matrices $\widetilde{O}_k$, $k = 1, 2, \ldots, 6$, were chosen and a random normalized real vector $\vec{a}$ of dimension five generated the data $\{d_1, d_2, \ldots, d_6\}$. Then, by construction the data set is consistent and there is at least one solution to the observation equations. Powell's method (see [19, chapter 10]) was used as a nonlinear algorithm to search for the solutions to these equations. Fifteen random initial conditions were chosen to initiate numerical searches. Each search either found the solution $\vec{a}$ or ended up with a vector which did not solve the system of equations. In no case was another solution found which satisfied the equations. The above procedure starting with a new random set of six matrices O_k was repeated 25 times. In all cases the same conclusion was found. Those cases where no solution at all was found indicate a failure of the numerical algorithm since we know that $\vec{a}$ is always a solution. The lack of finding a false solution demonstrates the lemma statement that such false solutions, if they exist, do so with zero measure.

2.2. Time-dependent expectation values as data

Consider time-dependent data generated by $n+1$ observable expectation values where the initial state is assumed to be a mixture of at least two eigenstates. The equation system (19) becomes:

$$\begin{aligned} \vec{a}_t^{\dagger}\widetilde{O}_1\vec{a}_t &= d_1(t), \\ \vec{a}_t^{\dagger}\widetilde{O}_2\vec{a}_t &= d_2(t), \\ &\vdots \\ \vec{a}_t^{\dagger}\widetilde{O}_{n+1}\vec{a}_t &= d_{n+1}(t). \end{aligned} \tag{20}$$

This system satisfies the condition in the theorem and lemma since the norm of the state is always unity. As t only acts as a parameter in these equations one can determine coefficient vector $\vec{a}_t$ at any time during the observation interval $[0, T]$ uniquely and use this to invert the potential. In principle an inversion at times t and $t+\delta t$ would yield $|\psi(t)\rangle$ and $|\psi(t+\delta t)\rangle$ such that $|\dot{\psi}(t)\rangle$ could be determined as well, as $\delta t \to 0$ (see section 2.4 below). This information at any time t should permit full estimation of V by substitution into equation (2). It is evident that $n+1$ such equations over time carry excess information to identify the potential uniquely. This redundancy of information can be valuable, as at any time t we expect that $|\psi(t)\rangle$ will only have significant amplitude in a localized spatial region. Thus, one can only expect to determine V reliably in that region. The full scope of the potential could be resolved by concatenating many such pieces of V. This case also does not require that the potential matrix be diagonal in the chosen basis.

2.3. Augmented spectral data

Spectral data is often relatively easy to obtain and it is typically very accurate. Suppose the spectrum $E = \{E_1, E_2, \ldots, E_n\}$ of the matrix $(H_0 + V)$ is available; the goal is to determine if this data can uniquely identify the potential function . This case is referred to as the additive inverse eigenvalue problem [11,13], and it is known that there is not a unique solution if the matrix V is diagonal (e.g., consider V evaluated at discrete points in its diagonal coordinate representation). The theorem states that there are up to $n!$ solutions. This number may be deduced from the fact that the characteristic polynomial of the Hamiltonian matrix must be equal to the characteristic polynomial of the eigenvalue matrix and this gives n polynomial equations in n unknowns of the potential matrix with degrees from 1 to n. These equations satisfy the condition of equation (12). Since spectral information is not enough to invert the potential we may augment it with additional information to realize the inversion. We assume that the additional data is one expectation value of an observable operator in one of the specified eigenstates of the Hamiltonian. Below we show the generic uniqueness of the solution to this extended system of equations using the lemma.

Let $f_i(x_1, x_2, \ldots, x_n)$ be the ith coefficient of the characteristic polynomial of the matrix $H_0 + V$, where $x \equiv [x_1, x_2, \ldots, x_n]$ denotes the unknowns in the diagonal potential matrix. This gives the following n equations:

$$\begin{aligned} f_1(x_1, x_2, \ldots, x_n) &= \sum_{i=1}^{n} E_i, \\ f_2(x_1, x_2, \ldots, x_n) &= \sum_{i \neq j}^{n} E_i E_j, \\ f_3(x_1, x_2, \ldots, x_n) &= \sum_{i \neq j \neq k}^{n} E_i E_j E_k, \\ &\vdots \\ f_n(x_1, x_2, \ldots, x_n) &= \prod_{i=1}^{n} E_i. \end{aligned} \tag{21}$$

The additional data is $\psi^\dagger \widetilde{O} \psi = d$, where ψ is an eigenvector associated with the known eigenvalue E (i.e, one member of the set $E_1, E_2, \ldots, E_n$). Then we have the following additional equations:

$$\begin{aligned} \psi^\dagger \psi &= 1, \\ (H_0 + V)\psi &= E\psi, \\ \psi^\dagger \widetilde{O} \psi &= d. \end{aligned} \tag{22}$$

Regarding the elements of the vector ψ as additional unknowns, altogether we have $2n$ unknowns with $2n + 2$ nonlinear polynomial equations relating them with the experimental data. These equations satisfy the condition in equation (12) of the theorem and the lemma states that for almost all Hermitian operators $\widetilde{O}$ there is a unique solution to the above system of data equations. As an illustration consider the following example:

$$H_0 = \begin{bmatrix} 0.4 & -0.2 & & & & \\ -0.2 & 0.4 & -0.2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & & & -0.2 & \\ & & & -0.2 & 0.4 & \end{bmatrix},$$

V is diagonal with elements {1.1650 0.6268 0.0751 0.3516 −0.6965}, $\widetilde{O}$ is diagonal with elements {0.2500 1.0000 2.2500 4.0000 6.2500}, $\psi = [0.2988\ 0.2309\ 0.4401\ 0.2331\ -0.7806]^\dagger$.

The data in (22) was generated by the above entities. The resultant nonlinear equation system (21) and (22) was solved by a root-searching algorithm. The correct potential is recovered starting from a wide range of initial guesses.

2.4. Time-dependent data

In contrast to case 2.2, we now explore whether a unique inversion can be produced using the expectation value of a single observable with respect to a time-dependent wavefunction. If the initial state is a mixture of *all* the eigenstates we can decompose the wavefunction as in (3) at all times. Then one can determine the eigenvalues from the following data. $\widetilde{O}_1$ is a Hermitian operator:

$$d_1(t) = \langle \psi(t) | \widetilde{O}_1 | \psi(t) \rangle. \tag{23}$$

Fourier transforming equation (23) we get

$$\mathcal{F}\{d_1(t)\} = \sum_{k,l} (\widetilde{O}_1)_{kl} b_k b_l \delta(\omega - (E_k - E_l)), \tag{24}$$

where $\psi(0) = [b_1\ b_2\ \ldots\ b_n]$ and ω is the frequency. If the spectral transitions are non-degenerate, i.e.,

$$E_k - E_l \neq E_i - E_j \quad \text{for any pair } \{(k,l),(i,j)\}, \tag{25}$$

then the eigenvalues can be determined up to a constant. The latter indeterminacy is of no consequence since identifying the potential up to an additive constant is sufficient. From the analysis in section 2.3 we conclude that potential can be retrieved with data from equation (23) augmented by

$$d_2 = \langle \psi | \widetilde{O}_2 | \psi \rangle, \tag{26}$$

where $|\psi\rangle$ in (26) is an eigenstate. Note that knowledge of the initial condition is not necessary here.

2.5. Time-dependent data and knowledge of the initial state

If the initial wavefunction is a known mixture of the *all* bound-states, then we can generate additional algebraic equations for the unknown elements of the potential matrix. We will show that under these conditions we may obtain the potential with only one set of time-dependent data,

$$d(t) = \langle \psi(t) | \widetilde{O} | \psi(t) \rangle, \quad \psi(0) = \psi_0. \tag{27}$$

As in section 2.4 by Fourier transforming this data we may determine the spectrum. This information gives n equations in the n unknowns of the diagonal potential matrix. To generate the additional equation we take the derivative of the time-series $d(t)$,

$$\mathrm{i}\,\dot{d}(t) = \langle \psi(t) | [H, O] | \psi(t) \rangle, \quad \psi(0) = \psi_0, \tag{28}$$

where $H = H_0 + V$ and $[H, O] = HO - OH$. If ψ_0 is a real function then

$$\mathrm{i}\,\dot{d}(0) = \langle \psi_0 | [H, O] | \psi_0 \rangle = 0. \tag{29}$$

In this case we may take one more derivative and get

$$-\ddot{d}(0) = \langle\psi_0|\big[H, [H, O]\big]|\psi_0\rangle \tag{30}$$

to give an additional quadratic equation for the unknowns of the potential. Since the initial state is assumed known, the only unknowns in this last equation are those of the potential. As an illustration consider the same example as in section 2.3 for H and O with the initial condition being

$$\psi(0) = [0.6224\ -0.2748\ 0.1051\ -0.7031\ -0.1779]^{\dagger}. \tag{31}$$

The data (27) was generated consistent with the initial condition $\psi(0)$. The equations were solved by a root-searching algorithm repeatedly starting with a random initial guess. The correct potential is recovered when iterations converge.

3. Error analysis

There are two general sources of error in the inversion process discussed above. First equation (3) was assumed to be an identity (i.e., the wavefunction at all times could be represented in a finite dimensional basis so that there was no truncation error involved). Second, the inversion scheme described in section 2 assumed that there is no error in the data. The first of these error sources is difficult to assess, however, it can be treated in principle by increasing the basis set until convergence is achieved. The second case will be analyzed below. Since the inversion problem was reduced to finding the unique solution to a system of polynomial equations, we may analyze the stability of the solutions with respect to small perturbations ε_k in the data:

$$\begin{aligned} f_1(x_1, x_2, \ldots, x_n) &= d_1 + \varepsilon_1, \\ f_2(x_1, x_2, \ldots, x_n) &= d_2 + \varepsilon_2, \\ &\vdots \\ f_{n+1}(x_1, x_2, \ldots, x_n) &= d_{n+1} + \varepsilon_{n+1}. \end{aligned} \tag{32}$$

Each perturbation is of the same order, i.e., $\varepsilon_k \sim \mathcal{O}(\varepsilon)$ for a small parameter ε. Let X_0 be the desired unique solution and $X_0, X_1, \ldots, X_N$ be the solutions to the first n equations of the original unperturbed system. By the same reasoning presented in the proof, generally there is no solution to the above system as the perturbation makes the system inconsistent. However, we expect that X_0 *almost* satisfies the equations. Thus we transform the goal of finding an exact solution to a minimization problem over equation (32):

$$\min_x \big\| \boldsymbol{f}(x) - \boldsymbol{d} + \boldsymbol{\varepsilon} \big\|, \tag{33}$$

$\|\cdot\|$ indicates the Euclidean norm in the appropriate space. If $X^{\star}$ solves (33), then

$$\big\| \boldsymbol{f}\big(X^{\star}\big) - \boldsymbol{f}(X_0) \big\| \leqslant \mathcal{O}(\varepsilon). \tag{34}$$

If the Jacobian matrix of the first n equations is not ill-conditioned at the points $X_0, X_1, \ldots, X_N$, then $X^\star$ will be inside an order-ε neighborhood of one of these points. If $X^\star$ is in the neighborhood of X_0, the system is stable with respect to perturbations. In contrast consider whether $X^\star$ can be in the order-ε neighborhood of the point X_j, $j \neq 0$, which gives:

$$\left\| \boldsymbol{f}(X_0) - \boldsymbol{f}(X_j) \right\| \leqslant \mathcal{O}(\varepsilon). \tag{35}$$

Inequality (35) is true for the first n elements since $f_i(X_j) = f_i(X_0)$, $i = 1, 2, \ldots, n$. However, it is not true for the last element since otherwise $f_{n+1}(X_0)$ would be arbitrarily close to $f_{n+1}(X_j)$, which is not true due to uniqueness of the solution to the unperturbed system.

Thus, the solution to equation (33) will be close to X_0 which is the unique solution to the unperturbed system. This analysis shows that the inversion is stable with respect to small errors in the data.

4. Conclusion and future perspectives

This paper addressed the problem of bound-state potential function inversion in quantum mechanics where the potential is time independent. It is important to consider what can be practically measured in the laboratory for inversion, and spectral data is generally very accurate and readily available. In this paper we considered inversion with both spectral data and time-dependent data which is the expectation value of an observable. Although time-dependent data is currently more difficult to obtain, this situation will likely improve. Large numbers of accessible observable operators is also a problem that needs addressing. After projecting the wavefunction to an n-dimensional subspace, the problem of inverting the potential reduced to solving a system of nonlinear polynomial equations. If the solution to these equations is unique then the resulting potential is unique. The main aim of the paper is to quantify the number and type of data that will give rise to a unique solution. For n polynomial equations in n unknowns the number of solutions is finite if the system satisfies a condition stated in the theorem of section 2. Adding another equation which is consistent with the rest of the equations will generically reduce the number of solutions to one. We showed that for a specified finite set of points, if a polynomial passes through one of them, it is very unlikely that it will also pass any other point in this set. This is shown in a measure-theoretic sense and details are presented in the proof of lemma in section 2. If there is an abundance of data then the uniqueness of the sought after potential is assured by adding extra measurements.

Several classes of inversion problems were analyzed in the paper. The first data set presented in section 2.1 considered for the n dimensional system was expectation values of $n + 1$ observables in a single eigenstate of the Hamiltonian along with the corresponding eigenvalue for that state. It was shown that in this case the potential may be extracted uniquely. The data set in section 2.2 was the expectation values of $n + 1$ observables where the initial state is a mixture of the eigenstates rather than only one of them. Although in principle the potential could be fully generated everywhere in

this case, in practice the potential will likely only be extracted to reasonable accuracy in the region sampled by the wavefunction during the observation interval. The data set in section 2.3 is the spectral data augmented with the expectation of an observable in an eigenstate of the Hamiltonian. The potential is extracted uniquely in the region spanned by that eigenstate. The data set in section 2.4 was the expectation values of two observables: the initial state was a mixture of eigenstates for the first observable and it was a pure eigenstate for the second observable. The former data set is used to extract eigenvalues when the non-degeneracy condition (25) is satisfied. Then, inversion reduces to the same situation as in the previous problem. Lastly in section 2.5, we considered the expectation value of one observable with an initial mixture state where we also knew this initial state. Inversion is again shown to be unique by employing the result of the lemma. An error analysis given in section 3 showed that a slight perturbation in the data does not cause a large deviation in the solution if the polynomials behave sufficiently well. This case is always true if the Jacobian of the first n polynomials is not ill-conditioned at the solutions to these n equations. Note also that nothing is special about the choice of the first n polynomials, if any combination of n equations satisfy this requirement, the result mentioned above is true. For noise contaminated data we have inconsistent set of equations. The task of finding a solution then becomes a minimization problem.

The system analyzed in this paper involved inversion to extract the potential where the Hamiltonian is time-independent. Introducing an external time-dependent field may provide a means to aid in the inversion of the potential. As the system becomes time-dependent the notion of spectral information is lost. However by adjusting this field by design, time-dependent expectation data can be employed to invert potential. Controlling the system by an external electric field can be exploited [20] to track a prescribed output. The external field is designed in such a way that the time-dependent expected value of an observable is tracked. A similar paradigm can be used to invert potential. The problem of quantifying the amount and best type of such time-dependent expectation data sets awaits further research. Although inversion to obtain the potential is an important problem per se, its application to control of quantum dynamical systems is of considerable interest: control of molecular motion with optical electric fields is an active area of research [21]. One obstacle to achieving effective control is a serious lack of information on the underlying Hamiltonian and in particular the intramolecular potential function describing the interaction among the atoms of the molecule. To realize the control objective one can envision a sequential scheme in which a portion of potential is identified and control theory is used to manipulate the dynamics of the system followed by additional inversion and control until the final objective is met [22].

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