Imaging of quantum-mechanical potentials

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In technical applications such as reflection seismics and nondestructive testing, imaging principles are successfully used for the reconstruction of inhomogeneities. In quantum-mechanical inverse problems one usually proceeds by parametrizing the unknown potential with some free parameters, which are fitted to the data. In this paper an imaging method is presented for the inversion of quantum-mechanical data. This method is derived by applying a gradient method to the minimization of the least-squares misfit of the data. This leads to an update of the model for the potential as a continuous function of the space variables in terms of the temporal correlation of two wave fields in this model. The theory is formulated in such a way that these wave fields can be computed using a finite-difference method. With current computers the method can be implemented for spherically symmetric potentials, which might include a spin-orbit interaction.

I. INTRODUCTION

The aim of quantum-mechanical measurements is ultimately the reconstruction of the potential which interacts with particles. In a typical experiment, one determines the scattering cross section when the potential is exposed to a particle beam. The scattering cross section is determined by measuring the particle intensity at a set of detectors. Possibly one performs different experiments where one exposes the potential to particle beams from different directions, and with different energies.

In practice, one performs the inversion by parametrizing the potential with a limited number of parameters. These parameters are usually fitted to the data using a least-squares criterion.[1] For example, one expands the potential in a (small) number of spherical Bessel functions, and one determines the expansion coefficients. Alternatively, one imposes a specific analytical form of the potential, such as the Saxon-Woods potential, with some free parameters which are fitted to the data. Specifying the functional form of the potential introduces a degree of subjectivity in the inversion. One would like to construct the potential without introducing possibly erroneous notions on the shape or the smoothness properties of the potential. Ideally one would use an imaging principle to determine the potential.

Analytical results show that in order to construct a potential for the one-dimensional Schrödinger equation using exact inverse scattering methods, one needs the reflection coefficient for all energies. Furthermore, bound states introduce a nonuniqueness in the inversion.[2] For the inverse problem of the Schrödinger equation in three dimensions, exact inverse scattering techniques require the scattered waves for all energies, all directions of incoming waves and all directions of outgoing waves, and bound states must not be present.[3] In real measurements one normally only measures the amplitude of the waves for only a finite range of energies and for a finite range of measurement directions.

This means that the solution of a realistic quantum-mechanical inverse problem is ill posed (as almost any other realistic inverse problem in physics). In practice, one needs a criterion to select the "best solution" from a multitude of possible solutions for a given data set. Specifying the functional form of the potential is one way to do this, but with such a method one has no idea what artifacts one introduces in the solution by this particular choice of the shape of the potential. We propose the following criterion for the best model. The best model of the potential is the model that gives the best fit of the data in the least-squares sense, and that is closest to the potential for a free particle (i.e., $V=0$).

This can be realized by formulating the inverse problem as a least-squares problem where one fits the observed data to the synthetic data for the potential. In this way, the inverse problem amounts to a minimization problem of the data misfit for the potential. The model space in which one performs this minimization is infinitely dimensional because the potential is assumed to be an arbitrary function of the space variables. Because of the large number of degrees of freedom in the inversion, and because of the requirement that one wants to be closest to the potential for a free particle, it is preferable to use a gradient method to achieve the minimization of the least-squares misfit. The formulation of this theory naturally leads to an imaging principle for quantum-mechanical potentials.

The presented method for data inversion has been very successful in reflection seismics. The resulting imaging principles have led to accurate and efficient algorithms for the reconstruction of the Earth's subsurface. Several formulations of seismic inversion using minimization methods have been formulated using both linearized[4] and nonlinear[5] versions of the theory. Given enough data, it is possible to locate the inhomogeneities at their correct position, and to a certain extent one can separate the heterogeneity of the elastic impedances and of the seismic velocities.[6]

The theory presented in this paper is the simplest formulation of an imaging principle for quantum-

mechanical potentials. In this way the physical principles are not obscured by unnecessary mathematical detail. The theory presented here only deals with scattering of spinless particles by a fixed potential. Extensions of the theory to more complicated situations can be formulated without much difficulty. For example, in the Appendix it is shown how spin-orbit interactions of spin-$\frac{1}{2}$ particles can be incorporated. *A priori* notions on the statistical properties of the model and the data can be incorporated in the inversion without essential modifications of the theory. In such an approach it is possible to prescribe *a priori* values for the model, as well as covariance functions for both the model and the data. In this way one can impose a smoothness constraint on the reconstructed model in a natural fashion by a suitable choice of the spatial covariance function of the model.[7]

II. LEAST-SQUARES FORMULATION OF THE INVERSE PROBLEM

In a typical problem one has observed data $d^{e,r}_{\text{obs}}$, which are gathered in different experiments, and which are recorded at different instruments (the data are labeled with the experiment index e and the receiver index r). From these data one wants to determine a model m, which is in a quantum-mechanical experiment, for example, the potential as a function of the space variables. One can only solve the inverse problem if a theory exists for the relation between the model and the data (the forward problem):

$$d^{e,r}=d^{e,r}(m) . \tag{1}$$

The inverse problem can be solved by minimizing the misfit between the observations $d^{e,r}_{\text{obs}}$ and the synthetic data $d^{e,r}(m)$. The misfit can be defined by a suitable norm such as the L_1 or L_2 norm. In this paper the following least-squares misfit $S(m)$ is used:

$$S(m)=\tfrac{1}{2}\sum_{e,r}[d^{e,r}(m)-d^{e,r}_{\text{obs}}]^2 . \tag{2}$$

The misfit is required to be minimized with respect to the model parameters m.[7] This is the simplest formulation of the least-squares problem, where one defines the best model m as the model which gives the best fit between the observations and the synthetics for this model.

In general, the relation (1) between the data and the model is nonlinear so that the misfit $S(m)$ is a nonquadratic function of the model m. In principle, there is a wide choice of optimization methods that can be used for the minimization of the misfit. In seismic inversion, gradient methods have proven to be extremely useful for the reconstruction of elastic impedances.[4-6] In such an approach one starts with an initial model m_0, and iteratively updates this model so that a sequence of models m_n is obtained which subsequently minimize the misfit $S(m_n)$. One can define the gradient γ_n of the misfit with respect to the model parameters by

$$S(m+\delta m)=s(m)+\gamma\delta m+O((\delta m)^2) . \tag{3}$$

The model can then be updated in the direction of this gradient

$$m_{n+1}=m_n-\alpha_n\gamma_n . \tag{4}$$

The step length α_n can be determined by trial and error, or can be estimated if the misfit function behaves locally quadratic.[8] In any case one should make sure that one uses a step length α_n such that the misfit function indeed decreases $[S(m_{n+1})<S(m_n)]$. After this, a new gradient can be computed, and this minimization process can be continued until convergence.

In such an approach the main difficulty is the computation of the gradient. The model m is, in general, a physical field, and it is therefore an arbitrary function. Rather than parametrizing this function, we aim to retrieve this field as an arbitrary function of the space variables. It is for this reason that methods of functional analysis are needed for the formulation of the inversion method.

For the computation of the gradient it is necessary to define the Fréchet derivative $D_{e,r}(m)$ by

$$d^{e,r}(m+\delta m)=d^{e,r}(m)+D_{e,r}(m)\delta(m)+O((\delta m)^2) . \tag{5}$$

Inserting this expression in (3) and (2), one finds that

$$\gamma_n=\sum_{e,r} D^{\dagger}_{e,r}(m_n)[d^{e,r}(m_n)-d^{e,r}_{\text{obs}}] . \tag{6}$$

In this expression $D^{\dagger}_{e,r}(m_n)$ is the Hermitian of the Fréchet derivative for model m_n. The term $(d^{e,r}(m_n)-d^{e,r}_{\text{obs}})$ is the misfit for the model m_n. For a perfect fit of the data $(d^{e,r}(m)=d^{e,r}_{\text{obs}})$ the gradient is, of course, zero.

III. PHYSICAL PROBLEM

Consider a scattering experiment where the wave function satisfies the Schrödinger equation

$$L\psi=0 , \tag{7}$$

where

$$L=i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\partial_j\partial_j-V , \tag{8}$$

with initial conditions

$$\psi(\mathbf{x},t_0) \tag{9}$$

is given. We shall see later that an overall phase change of the initial conditions does not alter the results. In order to ensure that the wave function remains normalized we assume that

$$|\psi(\mathbf{x},t)|^2|\mathbf{x}|^2\to 0 \quad \text{if } |\mathbf{x}|\to\infty . \tag{10}$$

In a typical scattering experiment one measures the number of particles at certain positions $\mathbf{x}_r$ using, for example, a photographic film or particle detectors. These instruments usually measure the total number of particles arriving at positions $\mathbf{x}_r$ during the experiment. It is therefore assumed that detectors at positions $\mathbf{x}_r$ measure the integrated amplitude for the duration of the experiment. The data $d^{e,r}_{\text{obs}}$ are thus given by

$$d^{e,r}_{\rm obs}=d^{e}_{\rm obs}(\mathbf{x}_r)=\int_{t_0}^{t_1}|\psi^{e}_{\rm obs}(\mathbf{x}_r,t)|^2dt\ . \tag{11}$$

The detectors are assumed to be pointlike devices. For detectors with a finite extent one should simply replace the sum over detectors by an integration of the detector coordinates $\mathbf{x}_r$. The model we are seeking is the potential as a function of the space coordinates:

$$m(\mathbf{x})=V(\mathbf{x})\ . \tag{12}$$

In the remainder of this paper the model is denoted by the potential V.

The forward problem (7)–(9) can numerically be solved using finite-difference methods. Of course, the computational domain must be of finite extent, and one needs to impose absorbing boundary conditions[9] at the edge of the computational domain. In this way it is possible to compute synthetic data $d^e(\mathbf{x}_r)$ for a given model of the potential.

IV. FRÉCHET DERIVATIVE D AND THE GRADIENT γ

Using the definition (11), the synthetics $d(\mathbf{x}_r;V)$ for the potential V are given by

$$d(\mathbf{x}_r;V)=\int_{t_0}^{t_1}|\psi(\mathbf{x}_r,t;V)|^2dt\ , \tag{13}$$

where $\psi(\mathbf{x}_r,t;V)$ is the solution of the forward problem (7)–(9) for the potential V. In expression (2) for the misfit and (6) for the gradient one applies a summation over all experiments e. For brevity the theory is developed for one experiment so that the index e is temporarily suppressed. The inversion scheme for multiple experiments can be found by a summation of the final results over all experiments.

In order to compute the Fréchet derivatives it is necessary to compute the effect of a perturbation of the potential on the wave function. Up to first order one finds that

$$|\psi(\mathbf{x},t;V+\delta V)|^2-|\psi(\mathbf{x},t;V)|^2 =\psi^*(\mathbf{x},t;V)\delta\psi(\mathbf{x},t;V)+\text{c.c.} \tag{14}$$

Throughout this paper c.c. stands for complex conjugation, and $\delta\psi(\mathbf{x},t;V)$ is the perturbation of the wave function due to a perturbation δV. From the definition (5) of the Fréchet derivative and the definition of the data (11) it follows that

$$D_r\delta V=\int_{t_0}^{t_1}\psi^*(\mathbf{x}_r,t;V)\delta\psi(\mathbf{x}_r,t;V)dt+\text{c.c.} \tag{15}$$

Knowledge of the perturbation $\delta\psi$ of the wave function therefore leads to the Fréchet derivative. It follows from the initial condition (9) that $\delta\psi$ satisfies the quiescent initial condition

$$\delta\psi(\mathbf{x},t_0;V)=0\ . \tag{16}$$

From the Schrödinger equation (7)–(9) one finds that $\delta\psi$ satisfies the following differential equation:

$$(L-\delta V)(\psi+\delta\psi)=0 \tag{17}$$

so that up to first order

$$L\delta\psi=\delta V\psi\ , \tag{18}$$

Now introduce the causal Green's function $\vec{G}(\mathbf{x},t,\mathbf{x}',t')$ which satisfies

$$L\vec{G}(\mathbf{x},t,\mathbf{x}',t')=\delta(\mathbf{x}-\mathbf{x}')\delta(t-t')\ , \tag{19}$$

and

$$\vec{G}(\mathbf{x},t,\mathbf{x}',t')=0\ \text{ for } t<t'\ . \tag{20}$$

[In this paper, an arrow over functions is used to denote causal (right arrow) and acausal (left arrow) functions, respectively.] Equation (18) with the initial condition (16) has the solution

$$\delta\psi(\mathbf{x},t)=\int\vec{G}(\mathbf{x},t,\mathbf{x}',t')\delta V(\mathbf{x}')\psi(\mathbf{x}',t')dV'dt'\ . \tag{21}$$

This finally gives the Fréchet derivative

$$D_r\delta V=\int dV'\int dt'\int dt\ \psi^*(\mathbf{x}_r,t)\vec{G}(\mathbf{x}_r,t,\mathbf{x}',t') \times\psi(\mathbf{x}',t')\delta V(\mathbf{x}')+\text{c.c.} \tag{22}$$

According to (6), the Hermitian of the Fréchet derivative is needed in the computation of the gradient. Applying the Hermitian of D_r to the misfit $(d^r-d^r_{\rm obs})$, one finds that

$$(D_r^\dagger\delta d^r)(\mathbf{x}')=\int dt\int dt'\psi(\mathbf{x}',t')\vec{G}^{\,\dagger}(\mathbf{x}',t',\mathbf{x}_r,t) \times\psi^*(\mathbf{x}_r,t)\delta d(\mathbf{x}_r)+\text{c.c.} \tag{23}$$

Using (6), this leads to the following expression for the gradient:

$$\gamma(\mathbf{x})=\sum_r\int dt\int dt'\psi(\mathbf{x},t')\vec{G}^{\,\dagger}(\mathbf{x},t',\mathbf{x}_r,t)\psi^*(\mathbf{x}_r,t) \times[d(\mathbf{x}_r)-d_{\rm obs}(\mathbf{x}_r)]+\text{c.c.} \tag{24}$$

More concisely this can be written as

$$\gamma(\mathbf{x})=\int dt\,\overleftarrow{\psi}(\mathbf{x},t)\vec{\psi}(\mathbf{x},t)+\text{c.c.} \tag{25}$$

In this expression $\vec{\psi}$ is the normal causal wave function

$$\vec{\psi}(\mathbf{x},t)=\psi(\mathbf{x},t)\ , \tag{26}$$

while $\overleftarrow{\psi}$ is defined by

$$\overleftarrow{\psi}(\mathbf{x},t')=\sum_r\int dt\,\vec{G}^{\,\dagger}(\mathbf{x},t',\mathbf{x}_r,t)\psi^*(\mathbf{x}_r,t) \times[d(\mathbf{x}_r)-d_{\rm obs}(\mathbf{x}_r)]\ . \tag{27}$$

This means that the gradient $\gamma(\mathbf{x})$ can be expressed as the temporal correlation of the wave fields $\vec{\psi}$ and $\overleftarrow{\psi}$. The causal wave field $\vec{\psi}$ which satisfies (7) with the initial conditions (9) can be computed using a finite-difference technique. The Hermitian of an integral operator follows by interchanging the integration variables and taking the complex conjugate.[10] This means that $\overleftarrow{\psi}$ can be computed once $\vec{\psi}$ and $\vec{G}$ are known. However, in this approach one needs to know $\vec{G}(\mathbf{x},t',\mathbf{x}_r,t)$ for all values of the arguments $(\mathbf{x},t')$ which is practically not feasible and not necessary. The introduction of the adjoint problem leads to an efficient method for the computation of $\overleftarrow{\psi}$.

V. ADJOINT PROBLEM

Consider the problem

$$L\vec{\phi}=q \ , \tag{28}$$

with initial condition

$$\vec{\phi}(\mathbf{x},t_0)=0 \ . \tag{29}$$

The adjoint problem is defined by

$$L^\dagger\overleftarrow{\phi}=q' \ , \tag{30}$$

where we leave the temporal boundary condition yet unspecified. Both $\vec{\phi}$ and $\overleftarrow{\phi}$ are supposed to satisfy the condition (10) at infinity.

For the operator L in (8) one has

$$L^\dagger=L \ . \tag{31}$$

A dot product can be defined by

$$\langle \phi\cdot\psi\rangle=\int dV\int_{t_0}^{t_1}dt\ \phi^*(\mathbf{x},t)\psi(\mathbf{x},t) \ . \tag{32}$$

Using this definition and expression (8) for L, one finds, using an integration by parts,

$$\begin{aligned}\langle\overleftarrow{\phi},L\vec{\phi}\rangle-\langle L^\dagger\overleftarrow{\phi},\vec{\phi}\rangle&=\frac{\hbar^2}{2m}\int dS\int_{t_0}^{t_1}dt\ \hat{\mathbf{n}}\cdot[\overleftarrow{\phi}^*(\mathbf{x},t)\nabla\vec{\phi}(\mathbf{x},t)-\text{c.c.}]\\&+i\hbar\int dV[\overleftarrow{\phi}^*(\mathbf{x},t_1)\vec{\phi}(\mathbf{x},t_1)-\overleftarrow{\phi}^*(\mathbf{x},t_0)\vec{\phi}(\mathbf{x},t_0)] \ .\end{aligned} \tag{33}$$

The terms on the right-hand side (r.h.s.) are the bilinear concomitant terms.[10] The surface integral vanishes because the wave function vanishes at infinity. The volume integral on the r.h.s. of (33) vanishes if we impose quiescent final conditions on $\overleftarrow{\phi}$:

$$\overleftarrow{\phi}(\mathbf{x},t_1)=0 \ . \tag{34}$$

With these conditions we have

$$\langle\overleftarrow{\phi},L\vec{\phi}\rangle=\langle L^\dagger\overleftarrow{\phi},\vec{\phi}\rangle \ . \tag{35}$$

The problem (28) with the quiescent initial conditions (29), and its adjoint problem (30) and (34), can conveniently be solved using the causal and acausal Green's functions $\vec{G}$ and $\overleftarrow{G}$ which satisfy

$$L\vec{G}(\mathbf{x},t,\mathbf{x}',t')=L^\dagger\overleftarrow{G}(\mathbf{x},t,\mathbf{x}',t')=\delta(\mathbf{x}-\mathbf{x}')\delta(t-t') \ , \tag{36}$$

and

$$\vec{G}(\mathbf{x},t,\mathbf{x}',t')=0 \quad \text{for } t<t' \ , \tag{37a}$$

$$\overleftarrow{G}(\mathbf{x},t,\mathbf{x}',t')=0 \quad \text{for } t>t' \ . \tag{37b}$$

The adjoint problem (30) and (34) has the solution

$$\overleftarrow{\phi}(\mathbf{x},t)=\int dV'\int dt'\overleftarrow{G}(\mathbf{x},t,\mathbf{x}',t')q'(\mathbf{x}',t') \ . \tag{38}$$

The Green's function $\overleftarrow{G}$ is the formal inverse of $L^\dagger$ so that

$$(L^\dagger)^{-1}=\overleftarrow{G} \ . \tag{39}$$

Furthermore, $\vec{G}$ is the inverse of L, which implies that

$$(L^{-1})^\dagger=\vec{G}^\dagger \ . \tag{40}$$

Since the Hermitian of the inverse is the inverse of the Hermitian $[(L^\dagger)^{-1}=(L^{-1})^\dagger]$ it follows from (39) and (40) that

$$\vec{G}^\dagger=\overleftarrow{G} \ . \tag{41}$$

VI. COMPUTATION OF THE GRADIENT γ

According to (25), the gradient γ follows from the temporal correlation between the wave fields $\vec{\psi}$ and $\overleftarrow{\psi}$. Using (41), Eq. (27) for $\overleftarrow{\psi}$ can be written as

$$\overleftarrow{\psi}(\mathbf{x},t)=\sum_r\int dt'\overleftarrow{G}(\mathbf{x},t,\mathbf{x}_r,t')\psi^*(\mathbf{x}_r,t')\times[d(\mathbf{x}_r)-d_{\text{obs}}(\mathbf{x}_r)] \ . \tag{42}$$

The wave field $\overleftarrow{\psi}$ needs to be computed for every experiment. Introducing the experiment index e once more, and comparing (38) with the adjoint problem (30) and (34), one finds that $\overleftarrow{\psi}^e$ satisfies

$$L\overleftarrow{\psi}^e(\mathbf{x},t)=q^e(\mathbf{x},t) \ , \tag{43}$$

with

$$q^e(\mathbf{x},t)=\sum_r\psi^{e*}(\mathbf{x}_r,t)[d^e(\mathbf{x}_r)-d^e_{\text{obs}}(\mathbf{x}_r)]\delta(\mathbf{x}-\mathbf{x}_r) \ , \tag{44}$$

and with quiescent final conditions

$$\overleftarrow{\psi}^e(\mathbf{x},t_1)=0 \ . \tag{45}$$

The wave fields whose temporal correlation produce the gradient can be computed with two finite difference computations for each experiment. These computations are performed for the current estimate of the potential (the current model). First, one computes the physical wave field ψ which is propagated forward in time from the initial condition (9). The values of the wave field are stored for all positions in space. This computation also gives the wave field at the receivers $[\psi^e(\mathbf{x}_r,t)]$ and the difference between the observations and the synthetics for the current model $[d^e(\mathbf{x}_r)-d^e_{\text{obs}}(\mathbf{x}_r)]$.

With these fields, the source term for the field $\overleftarrow{\psi}^e$ is obtained [see (44)]. With this source term the adjoint problem (43) for $\overleftarrow{\psi}^e$ with the quiescent final conditions (45) can be solved. In this computation one propagates the solution $\overleftarrow{\psi}$ backwards in time using a finite-difference technique. For this the same finite-difference code can be used as for the computation of the physical field ψ. The temporal correlation of these two wave fields yields for every position in space the value of the gradient

$$\gamma(\mathbf{x})=\sum_e\int\overleftarrow{\psi}^e(\mathbf{x},t)\vec{\psi}^e(\mathbf{x},t)dt+\text{c.c.} \tag{46}$$

For the computation of the gradient one thus needs to perform for each experiment two finite-difference computations, and one temporal correlation.

The term ψ^* in (44) plays an interesting role in the expression for the sources of $\overleftarrow{\psi}$. Suppose this term was absent. In that case the source q would be independent of time. Such a source does not radiate energy, so that there is no wave field backpropagated in the medium. The ψ^* term in (44) gives the source of $\overleftarrow{\psi}$ an oscillatory behavior,

which effectively radiates the field $\overleftarrow{\psi}$ and thus produces a nonzero gradient.

The same term also ensures that the procedure does not depend on an overall phase shift of the physical wave function ψ. If one applies an overall phase shift $\exp i\alpha$ to the initial conditions (9), then ψ will have this phase shift for all later times. The source of $\overleftarrow{\psi}$ then obtains a phase shift $\exp -i\alpha$; the same applies to the solution $\overleftarrow{\psi}$ for all earlier times. These opposing phase factors cancel in the final expression (46) for the gradient.

VII. PRACTICAL ASPECTS OF THE INVERSION

Due to practical limitations of the available computing power, the theory presented here cannot be used yet without modifications in practical implementations. At this point finite-difference computations in more than two dimensions require more computing power than is generally available. It is for this reason that in seismic inversion one frequently makes the assumption that the Earth does not vary perpendicular to the line along which a seismic profile has been shot.

There is a tremendous difference in the relative scale of a seismic experiment and a typical quantum-mechanical scattering experiment. In seismic inversion, the domain of interest generally has a size of approximately 100 wavelengths, while the duration of the experiment is, say, 100 periods. (These numbers fix the required computational domain.) In a quantum-mechanical experiment one may employ waves with a wavelength of, say, 10^{-10} m, and the apparatus may have a size of 10^{-3} m (or more), so that the wave field needs to be modeled on a domain of 10^7 wavelengths (or more). Similarly, the duration of a quantum-mechanical experiment in terms of the dominant period of the employed waves may be extremely large.

For practical applications it is therefore necessary to reduce the spatial and temporal size of the physical problem. The data (the average amplitude of the waves) depend in the far field only on the average particle flux in each direction. This means that given the measured intensity at distant receivers, one can infer the intensity that would be measured closer to the scattering region. In the far field zone this means that the measured intensity only needs to be corrected with a $1/r^2$ factor to account for geometrical spreading effects.

Similarly, the initial conditions (9) may specify the wave field a very large number of wavelengths from the scatterer. However, the wave field is only influenced by the scatterer if the wave field differs appreciably from zero near the scatterer. This means that in many situations one can replace the initial conditions (9) by equivalent initial conditions which specify the wave packet just before it comes into contact with the scatterer.

These tricks make it possible to reduce the spatial size of the computational domain. From an academic point of view this can be justified by remarking that this procedure effectively replaces a pure finite-difference modeling of the wave field by a hybrid modeling procedure where the vicinity of the scatterer is handled by a finite-difference method, and where the propagation between the computational domain and the area of observation is handled analytically.

The long temporal duration of the experiment in terms of the periods of the waves can be handled by using a reformulation of the theory in the frequency domain. Alternatively, in case one employs near-monochromatic beams, the intensity is almost constant in time. In that case one can replace the true experiment by a hypothetical experiment with a shorter duration and with the same average square-wave amplitude. In this way the temporal duration of the experiment may be reduced to a size which is computationally manageable.

Since finite-difference computations in three dimensions are currently too expensive to perform on a routine basis, the practical applications are at this point limited to situations where only two dimensions are relevant for the wave propagation. This is the case for spherically symmetric potentials for which

$$V(\mathbf{r})=V(r)\ . \tag{47}$$

Of course, the measurements are performed in three-dimensional space, but since the scattered waves depend only on the scattering angle and not on the azimuth one can reduce the number of dimensions to two. In that case the gradient γ depends only on the radius r. This can be incorporated by averaging the gradient as obtained in (46) over all angles:

$$\gamma(r)=\frac{1}{4\pi}\int_{\Omega}\gamma(r,\theta,\phi)d\Omega\ , \tag{48}$$

where θ and ϕ are the usual polar coordinates and Ω denotes the space angle. Mathematically, this procedure can be justified by introducing a spherically symmetric *a priori* covariance function for the potential.[7]

VIII. CONCLUSION

The imaging method presented here constitutes an unbiased method for the reconstruction of quantum-mechanical potentials. In this approach it is not necessary to specify the (possibly erroneous) functional form of the potential. At this point the method can be implemented for the reconstruction of spherically symmetric potentials.

The theory presented here is only the simplest formulation of imaging of quantum-mechanical potentials. The incorporation of *a priori* notions on the statistical properties of the data and the potential can be performed without essential modifications of the theory.[7] The theory is flexible and can be applied to more complicated situations; for example, in the Appendix it is shown how spin-orbit coupling can be taken into account.

The main difference of the proposed imaging technique with seismic applications is that in seismics one can directly measure the wave function, whereas in quantum mechanics one usually only measures the time-averaged amplitude of the waves. By analogy with the seismic case,[5] one can show that if one could measure ψ directly, instead of $\int|\psi|^2dt$, the source q of $\overleftarrow{\psi}$ in (44) needs to be replaced by

$$q^e(\mathbf{x},t)=\sum_r[\psi^e(\mathbf{x}_r,t)-\psi^e_{\text{obs}}(\mathbf{x}_r,t)]\delta(\mathbf{x}-\mathbf{x}_r)\ . \tag{49}$$

In this hypothetical situation one could use the phase information contained in ψ. However, one would have the additional problem that it is only possible to obtain meaningful results from ψ if one knew the position of the detectors with an accuracy smaller than a wavelength. In practice, this is hard to realize. In the situation where one uses (13) as the data one does not have this problem because $|\psi(\mathbf{x},t)|^2$ is in the far field a smooth function of $\mathbf{x}$.

Just as with seismic inversion, one cannot hope to reconstruct the true potential with arbitrary data because the null space of the inversion is nonzero. For example, if one only has measured the amplitude for near-forward scattering, for a finite range of energies, one can only hope to reconstruct a smoothed version of the true potential. If one only uses data for backscattering one can only hope to find the spectral components of the potential which match the wavelengths in the employed waves. This is not a drawback of the employed inversion scheme, but it is a consequence of the fact that for realistic data the inverse problem is ill posed. In seismic inversion using a gradient method one has a similar situation; transmission data only give the trend in the velocity, while reflection data only give spectral components of the elastic impedances which match the wavelengths of the employed waves.[11] However, the employed method allows both in reflection seismics as in quantum mechanics for the retrieval of the information of the medium that *is* contained in the data.

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APPENDIX: TREATMENT OF SPIN-ORBIT INTERACTION

In this appendix an extension of the proposed inversion scheme is presented for spin-orbit interactions as an example of the flexibility of the inversion method. The theory is presented for one experiment; for an inversion using data of different experiments one should sum the final result for the gradient over all experiments. For spherically symmetric interactions of particles with spin $\frac{1}{2}$, the spin-orbit interaction is incorporated in the operator L in the following way:[12]

$$L=i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\partial_j\partial_j-V(r)-W(r)(\mathbf{L}\cdot\boldsymbol{\sigma})+\frac{e\hbar}{2mc}(\mathbf{B}\cdot\boldsymbol{\sigma})\ . \tag{A1}$$

This matrix operator acts on the spinor ψ. The angular momentum operator is denoted by $\mathbf{L}$, and $\boldsymbol{\sigma}$ are the Pauli matrices. The magnetic field $\mathbf{B}$ is assumed to be given, and the aim of the inversion is to determine both $V(r)$ and $W(r)$.

The derivation of the expression of the gradient proceeds along the same lines as in Secs. II–VI. The only difference is that the gradient and the Fréchet derivative now have two components instead of one, since they describe the dependence of both V and W. Expression (22) for the Fréchet derivative is for the operator in (A1) given by

$$\begin{aligned}D_r(\delta V,\delta W)=&\int dV'\int dt'\int dt\ \psi^\dagger(\mathbf{x}_r,t)\vec{G}(\mathbf{x}_r,t,\mathbf{x}',t')\\&\times\psi(\mathbf{x}',t')\delta V(\mathbf{x}')\\&+\int dV'\int dt'\int dt\ \psi^\dagger(\mathbf{x}_r,t)\vec{G}(\mathbf{x}_r,t,\mathbf{x}',t')\\&\times(\mathbf{L}\cdot\boldsymbol{\sigma})\psi(\mathbf{x}',t')\delta W(\mathbf{x}')\ .\end{aligned} \tag{A2}$$

The gradient γ now has two components, which describe the derivative of the misfit S with respect to V and W, respectively,

$$\gamma(\mathbf{x})=\left[\frac{\partial S}{\partial V}(\mathbf{x}),\frac{\partial S}{\partial W}(\mathbf{x})\right]=(\gamma_V(\mathbf{x}),\gamma_W(\mathbf{x}))\ . \tag{A3}$$

By analogy with (6), the gradient is related to the Fréchet derivative and the misfit $(d^r-d^r_{\text{obs}})$ by

$$(\gamma_V(\mathbf{x}),\gamma_W(\mathbf{x}))=\sum_r D_r^\dagger(d^r-d^r_{\text{obs}})\ . \tag{A4}$$

Using (A2) and (A3), this gives by analogy with (24)

$$\begin{aligned}\gamma_V(\mathbf{x})=&\sum_r\int dt'\psi^T(\mathbf{x},t')\vec{G}^{\,\dagger}(\mathbf{x},t',\mathbf{x}_r,t)\\&\times\psi^*(\mathbf{x}_r,t)[d(\mathbf{x}_r)-d_{\text{obs}}(\mathbf{x}_r)]+\text{c.c.}\ ,\end{aligned} \tag{A5}$$

$$\begin{aligned}\gamma_W(\mathbf{x})=&\sum_r\int dt'\psi^T(\mathbf{x},t')(\boldsymbol{L}\cdot\boldsymbol{\sigma})^\dagger\vec{G}^{\,\dagger}(\mathbf{x},t',\mathbf{x}_r,t)\\&\times\psi^*(\mathbf{x}_r,t)[d(\mathbf{x}_r)-d_{\text{obs}}(\mathbf{x}_r)]+\text{c.c.}\ ,\end{aligned} \tag{A6}$$

where T indicates the transposed. In analyzing these expressions one should be careful with the spinor indices, and one should decide on what are the data d^r. We suppose here that the data d^r are the integrated amplitudes of the spinor components:

$$d_i^r=d_i(\mathbf{x}_r)=\int_{t_0}^{t_1}|\psi_i(\mathbf{x}_r,t)|^2dt\ . \tag{A7}$$

In that case a term like $\psi^T\vec{G}^{\,\dagger}\psi^*\delta\mathbf{d}$ is in an explicit component notation $\sum_{i,j}\psi_i\vec{G}^{\,\dagger}_{ij}\psi^*_j(\delta d_j)$, while $\psi^T(\boldsymbol{L}\cdot\boldsymbol{\sigma})^\dagger\vec{G}^{\,\dagger}\psi^*\delta\mathbf{d}$ stands for $\sum_{i,j,k}\psi_i(\boldsymbol{L}\cdot\boldsymbol{\sigma})^\dagger_{ij}\vec{G}^{\,\dagger}_{jk}\psi^*_k(\delta d_k)$.

Expression (A5) for γ_V is analogous to expression (24) and can be treated along the same lines with the provision that the wave function is now a two-component spinor. Thus one can define a spinor $\overleftarrow{\psi}$ which satisfies

$$\underline{L}\overleftarrow{\psi}(\mathbf{x},t)=\sum_r\psi^*(\mathbf{x}_r)[d(\mathbf{x}_r)-d_{\text{obs}}(\mathbf{x}_r)]\delta(\mathbf{x}-\mathbf{x}_r)\ , \tag{A8}$$

where $\underline{L}$ is the operator (A1) for the current model. The spinor $\overleftarrow{\psi}$ has quiescent final conditions:

$$\overleftarrow{\psi}(\mathbf{x},t_1)=0\ . \tag{A9}$$

By analogy with (46) it follows that

$$\gamma_V(\mathbf{x})=\int dt\ \vec{\psi}^{\,T}(\mathbf{x},t)\overleftarrow{\psi}_V(\mathbf{x},t)dt+\text{c.c.}\ , \tag{A10a}$$

with

$$\overleftarrow{\psi}_V(\mathbf{x},t)=\overrightarrow{\psi}(\mathbf{x},t)\ , \tag{A10b}$$

and where $\overrightarrow{\psi}(\mathbf{x},t)$ satisfies (A8) and (A9).

In the derivation it is tacitly assumed that $L=L^\dagger$. For the first terms in (A1) this follows from the same arguments as for the scalar Schrödinger equation (8). The magnetic interaction $(\sigma\cdot\mathbf{B})$ is Hermitian because the Pauli matrices are Hermitian, and the angular momentum operator is also Hermitian $(L=L^\dagger)$. Furthermore the boundary terms associated with this operator vanish because the boundary conditions on the sphere are periodic. This means that the operator L is indeed Hermitian.

The gradient γ_W is given by (A6). Going through the steps of the Secs. II–VI, and using that $(\mathbf{L}\cdot\sigma)$ is Hermitian, it follows that

$$\gamma_W(\mathbf{x})=\int dt\ \overrightarrow{\psi}^T(\mathbf{x},t)\overleftarrow{\psi}_W(\mathbf{x},t)dt+\text{c.c.}\ , \tag{A11a}$$

with

$$\overleftarrow{\psi}_W(\mathbf{x},t)=(L\cdot\sigma)\overleftarrow{\psi}(\mathbf{x},t)\ . \tag{A11b}$$

This means that, using Eqs. (A10) and (A11), one can compute the gradient of the misfit both with respect to $V(r)$ and $W(r)$. In order to do this it is only necessary to perform two finite-difference computations for the spinors $\overrightarrow{\psi}$ and $\overleftarrow{\psi}$ for the current model. The two components of the gradient γ follow by applying different operators to $\overleftarrow{\psi}$. After a temporal correlation with $\overrightarrow{\psi}$ this leads to the desired gradient.

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