Three Dimensional Quantum Delay Time Tomography

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Quantum delay time tomography data obtained from the intensity of a Gaussian wave packet are used to approximately construct the 3D scattering potential of the time dependent Schrödinger's equation by a least action tomography algorithm which decouples into multiple 2D x-ray tomography algorithms when the mean energy of the wave packet is sufficiently high. We obtain two "miracle" identities for the characterization of admissible quantum delay time tomography data. The first is related to Newton's miracle identity. The second is a new curved miracle identity.

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The main goal of 3D inverse quantum scattering is to determine the 3D scattering potential from scattering data. The usual scattering data have been the magnitude and phase of the scattering amplitude [1–8]. Whereas the magnitude of the scattering amplitude (the square root of the differential cross section) can be measured, the phase of the scattering amplitude cannot be measured. Newton [4] suggests to solve the phase problem prior to solving the 3D inverse quantum scattering problem, i.e., to determine the phase of the scattering amplitude from the measured differential cross section by solving numerically an integral equation [2] whose uniqueness and numerical solution have not been established yet. We formulate the 3D inverse quantum scattering problem with different scattering data, where the phase of the quantum wave function is not used. We use quantum delay time tomography data corresponding to the time of advance of the maximum of the intensity (not the phase) of a quantum Gaussian wave packet. Our formulation is based on the time dependent Schrödinger's equation, in contrast to the exclusive use of the time independent Schrödinger's equation in previous 3D inverse quantum scattering studies [1–8]. We obtain two different "miracle" identities for the characterization of admissible quantum delay time tomography data. The first is related to Newton's miracle identity of 3D inverse quantum scattering [4,6,9]. The second is a new curved miracle identity.

We first derive an approximate 3D quantum Gaussian wave packet in the space time domain whose probability density has the correct classical limit. Then we show how to approximately construct the 3D scattering potential within a bounded volume from quantum delay time tomography data on the surface that bounds this volume. We show that when the mean energy of the quantum Gaussian wave packet is sufficiently high, the 3D scattering potential can be rapidly constructed by multiple applications of the 2D x-ray tomography algorithm.

The 3D quantum wave function $\Psi(t,\vec{r})$ for a particle of mass m and charge q in the presence of general 3D electrostatic field is governed by the time dependent Schrödinger's equation

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + q\phi\Psi\,, \tag{1}$$

where $\phi = \phi(\vec{r})$ is the electrostatic potential, $\vec{r}$ is a position vector in 3D, t is time, ∇^2 is the 3D Laplacian, $i^2 = -1$, and $\hbar = h/2\pi$ is Planck's constant. This equation also holds for any other conservative field of force if $q\phi(\vec{r}) = V(\vec{r})$ is its corresponding potential. Born showed that the intensity $|\Psi(t,\vec{r})|^2$ is a measurable quantum attribute and it corresponds to the relative probability density of finding the particle at position $\vec{r}$ at time t. Our goal is to find a simple approximate relationship between $|\Psi(t,\vec{r})|^2$ on the surface of a bounded volume and $\phi(\vec{r})$ within this volume. This is discussed next. The time t can be transformed to the energy E by Fourier transform and the wave function $\Psi(t,\vec{r})$ transforms to $\hat{\Psi}(E,\vec{r})$ which satisfies $[\nabla^2 + P^2/\hbar^2]\hat{\Psi} = 0$, where $P = [2m(E - q\phi)]^{1/2}$. We use a modified semiclassical approximation $\hat{\Psi} = C\exp[iU/\hbar]$, where $U = U(E,\vec{A},\vec{r}) = \int_{\vec{A}}^{\vec{r}} P\,ds$ satisfies the Hamilton-Jacobi equation $\nabla U\cdot\nabla U = P^2$, $\vec{A}$ is a reference position vector, ds is a differential arc length along the least action trajectory, and C is a Gaussian function of energy. This approximation is adequate provided that the de Broglie's wavelength $\lambda = h/P$ does not change appreciably over its de Broglie's wavelength or equivalently $|\nabla\lambda| \ll 2\pi$, which we assume to hold till the end of this Letter. We next transform our approximation back to the time domain using inverse Fourier transform; this results in

$$\Psi(t,\vec{r}) = \frac{1}{\sqrt{2\pi\hbar}} \times \int_{-\infty}^{\infty} \frac{e^{-(1/2)[(E-E_0)/d]^2}}{\sqrt{\sqrt{\pi}\,d}}\, e^{iU(E,\vec{A},\vec{r})/\hbar - iEt/\hbar}\,dE\,, \tag{2}$$

where E_0 and d are positive constants. This particular scaling of the Gaussian function was chosen so that $|\hat{\Psi}(E,\vec{r})|^2$ is a proper probability density function for any fixed position $\vec{r}$. The mean energy of this Gaussian is E_0 whose uncertainty is $d^2/2$. This choice of the Gaussian will further result in a minimum uncertainty wave packet

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with the correct classical limit. A quantum wave packet is "almost monoenergetic" so that we choose $d \ll E_0$, and the major contribution to the integral in (2) comes from those E values in the vicinity of E_0. Consequently we approximate $U(E, \vec{\mathrm{A}}, \vec{\mathrm{r}})$ by the first two terms of its Taylor's expansion about E_0 and then we evaluate the resulting standard integral exactly. This results in a 3D quantum Gaussian wave packet whose intensity or equivalently its probability density is given by

$$|\Psi(t, \vec{\mathrm{r}})|^2 = (\sqrt{\pi}\, \hbar/d)^{-1} \exp\left[-\left(\frac{t - U'(E_0, \vec{\mathrm{A}}, \vec{\mathrm{r}})}{\hbar/d}\right)^2\right], \tag{3}$$

where the prime denotes the derivative with respect to energy. In the classical limit we set $\hbar$ to zero and then we set d to zero (the order is important); this results in the classical probability density function $|\Psi_c(t, \vec{\mathrm{r}})|^2 = \delta[t - U'(E_0, \vec{\mathrm{A}}, \vec{\mathrm{r}})]$ where $\delta[\cdot]$ is the Dirac delta function and the subscript c denotes classical limit. Note that $U'(E_0, \vec{\mathrm{A}}, \vec{\mathrm{r}})$ is deterministically the time of advance of the maximum of the intensity (3), statistically it is the mean time whose uncertainty is $\hbar^2/[2d^2]$ and classically it is the mean time whose uncertainty is zero, i.e., total certainty. We next show that $U'(E_0, \vec{\mathrm{A}}, \vec{\mathrm{r}})$ corresponds to the time of flight of a classical particle. The solution of the Hamilton-Jacobi equation is given by $U(E_0, \vec{\mathrm{A}}, \vec{\mathrm{r}})$. Consequently

$$U'(E_0, \vec{\mathrm{A}}, \vec{\mathrm{B}}) = \int_{\vec{\mathrm{A}}}^{\vec{\mathrm{B}}} \frac{m\, ds}{\sqrt{2m(E_0 - q\phi(\vec{\mathrm{r}}))}} \tag{4}$$

which also equals to $\int_{\vec{\mathrm{A}}}^{\vec{\mathrm{B}}} v^{-1}\, ds$, where v is the classical particle velocity. We have thus demonstrated that $U'(E_0, \vec{\mathrm{A}}, \vec{\mathrm{B}})$ is the time taken by a classical particle of mass m and charge q and energy E_0 to move from $\vec{\mathrm{A}}$ to $\vec{\mathrm{B}}$ in the presence of the general 3D electrostatic potential $\phi(\vec{\mathrm{r}})$ along the least action trajectory. So, the correspondence principle and the uncertainty principle are both satisfied by our approximation (3).

Equation (4) and the Hamilton-Jacobi equation are the required relationships between the quantum delay time $U'(E_0, \vec{\mathrm{A}}, \vec{\mathrm{B}})$ and the potential $\phi(\vec{\mathrm{r}})$. In the forward problem, when the potential is known and the quantum delay time is sought, we first find the least action trajectory and then we use (4) to determine the quantum delay time. This relationship between the quantum delay time and the potential is nonlinear. In the inverse problem, the quantum delay time is measured at many $\vec{\mathrm{A}}$ and $\vec{\mathrm{B}}$ positions on the surface Γ of a bounded volume D for a single mean energy or many mean energies, and the potential within this volume is sought such that (4) is satisfied. This is a nonlinear integral equation in geometrical mechanics similar to the corresponding nonlinear integral equation of first arrival time tomography in geometrical optics [10]. We note that the resolution of our method is zero in classically inaccessible regions similar to the white holes [11] of first arrival time tomography. The size of these white holes can be shown to decrease as the mean energy E_0 of the Gaussian wave packet increases. In the limit of very high mean energy, i.e., $E_0 \gg |q\phi|$, our nonlinear 3D quantum delay time tomography problem simplifies to multiple 2D x-ray tomography problems. In this limit (4) simplifies to

$$U'(E_0, \vec{\mathrm{A}}, \vec{\mathrm{B}}) = \frac{m|\vec{\mathrm{B}} - \vec{\mathrm{A}}|}{\sqrt{2mE_0}} + \frac{mq}{2E_0\sqrt{2mE_0}} \int_{\vec{\mathrm{A}}}^{\vec{\mathrm{B}}} \phi\, ds\,, \tag{5}$$

where ds is a differential arc length along the straight line joining $\vec{\mathrm{A}}$ and $\vec{\mathrm{B}}$. The first term in (5) is the time needed by a free particle to move from $\vec{\mathrm{A}}$ to $\vec{\mathrm{B}}$. The second term in (5) is proportional to the projection of the 3D potential ϕ onto the straight line joining $\vec{\mathrm{A}}$ and $\vec{\mathrm{B}}$. If $\vec{\mathrm{A}}$ and $\vec{\mathrm{B}}$ are located on the boundary of a circle $|\vec{\mathrm{r}}| = a$, where a is its radius, then from many such $\vec{\mathrm{A}}$ and $\vec{\mathrm{B}}$ positions we can obtain by (5) most of the fan beam projections of $\phi(\vec{\mathrm{r}})$ for $\vec{\mathrm{r}}$ on the plane of this circle. Using the fast convolution algorithm of 2D x-ray tomography [12], we can recover approximately $\phi(\vec{\mathrm{r}})$ on this slice and similarly for all other slices. One can numerically produce these 2D slices from the fan beam projections or from the parallel beam projections. The latter will require to first transform all the fan beam projections to the parallel beam projections or alternatively, the parallel beam projections can be obtained directly from a plane quantum Gaussian wave packet.

Our formulation of the 3D inverse quantum scattering problem using the time dependent Schrödinger's equation yielded two practical inverse scattering algorithms for the approximate construction of the 3D potential from quantum delay time tomography data, obtained from the intensity of a wave packet without using its phase. The first algorithm is similar to the first arrival time tomography within the geometrical optics approximation where the least action trajectories are curved as are the geometrical optics rays. The second algorithm is similar to computerized x-ray tomography where the least action trajectories are approximately straight lines for sufficiently high energy as are x rays. Our first algorithm could have been "sensed" from Hamilton's [13] relationship between the classical particle trajectory in a conservative field of force and the geometrical optics ray in inhomogeneous and isotropic medium, which played a major role in the development of quantum mechanics and the electron microscope. Alternatively, if one applies the "optical thinking" of Born and Wolf [14] to the 3D quantum scattering problem, then our first algorithm is "obvious" as soon as one establishes that the quantum delay time is "equivalent" to the first arrival time of classical waves within the short wavelength approximation. My initial difficulty in using this concept was that the group velocity and the phase velocity of the classical wave are identical whereas for quantum waves they are different (the "group velocity" of the quantum wave has nothing to do with the structure called "quantum groups" which are obtained from groups such as SO(N), SU(N), SP(N), $G/2$, $A/2$, and $F/2$). A simpler algorithm results from quantum phase delay tomography data, but the phase of a quantum wave is an unmeasurable quantum attribute (our second algorithm could have been predicted from [15]). In [15] the 3D inverse Radon transform is used to solve the inverse scattering problem for the 3D plasma wave equation which in the absence of bound states can be also used for the 3D inverse quantum scattering problem [16] provided that the phase of the quantum scattered waves can be computed by solving an integral equation [2]. We can approximately construct the phase of our quantum Gaussian wave packet from its intensity if needed for other applications. The phase of our wave packet is $\alpha/\hbar$, where α is the time integral of the classical Lagrangian along the least action trajectory for the "corresponding" particle as the phase used by Feynman [17] in computing the probability density using his version of quantum mechanics. From the constructed potential (from the intensity of the wave packet) we can compute the least action trajectory and then we can compute the phase of the quantum Gaussian wave packet. We should emphasize however that in the presence of classically inaccessible regions, the uniqueness of the potential distribution obtained by our first algorithm is questionable as the quantum delay time tomography data cannot "feel" that part of the potential within the geometrical mechanics white hole [11]. As the mean energy of the quantum wave packet increases these "ambiguous" regions shrink but not entirely in regions where the repulsive potential is singular. Thus, the resolution of the constructed potential by both of our algorithms is expected to be poor or zero in such regions. Furthermore, it is not expected that our algorithms will be able to construct microscopic details of the potential distribution when the measurements are taken at macroscopic distances in the presence of "noise." This is also the characteristic of the solutions given in [15] and [16] using phase information in addition to intensity information. In our second algorithm the 3D inverse quantum scattering problem is decoupled into multiple 2D x-ray tomography problems which can be solved numerically on a standard work station. This will be discussed elsewhere.

In [4] and [6] the phase and magnitude of the scattering amplitude are input data for the 3D Newton-Marchenko integral equation whose solution is $\eta(\tau, \hat{\theta}, \vec{\mathrm{r}})$, where $\hat{\theta}$ is a unit vector corresponding to the direction of the plane wave incidence and τ is the time variable of a corresponding plasma wave equation. The potential $V(\vec{\mathrm{r}})$ is obtained from η by $-2\hat{\theta} \cdot \nabla\eta(0^+, \hat{\theta}, \vec{\mathrm{r}}) = V(\vec{\mathrm{r}})$. This is called a miracle [4,6,9], because the left-hand side is a function of five variables whereas the right-hand side is a function of only three variables. Physically this means that the potential is independent of the direction of the incoming plane wave. This miracle identity is used by Newton for the characterization of admissible quantum scattering data, which is another goal of inverse scattering. We have two similar miracle identities for the characterization of quantum delay time tomography data. Our first miracle identity is obtained as follows: First we construct the potential using multiple applications of the 2D x-ray tomography algorithm [12] to the quantum delay time tomography data obtained from sufficiently high mean energy. Using (5) we can compute the quantum delay time interior to the surface where the measurements were taken. If we define $\hat{\theta} = (\vec{\mathrm{r}} - \vec{\mathrm{A}})/|\vec{\mathrm{r}} - \vec{\mathrm{A}}|$ and

$$\lim_{E_0\to\infty}\left[U'(E_0, \vec{\mathrm{A}}, \vec{\mathrm{r}}) - \frac{m|\vec{\mathrm{r}} - \vec{\mathrm{A}}|}{\sqrt{2mE_0}}\right]\left(\frac{2E_0\sqrt{2mE_0}}{mq}\right) \equiv \xi_H(\vec{\mathrm{A}}, \vec{\mathrm{r}}), \tag{6}$$

then our first miracle identity is

$$\hat{\theta} \cdot \nabla\xi_H(\vec{\mathrm{A}}, \vec{\mathrm{r}}) = \phi(\vec{\mathrm{r}}), \tag{7}$$

where the left-hand side is a function of five variables and the right-hand side is a function of only three variables. Physically this means that the potential is independent of the reference position vector $\vec{\mathrm{A}}$ or equivalently the potential is independent of the direction $\hat{\theta}$. Our second miracle identity is obtained as follows: We construct the potential by numerically solving the nonlinear integral equation (4) using methods related to first arrival time tomography for classical waves within the geometrical optics approximation [10]. Then we insert this potential into (4) and we can compute the quantum delay time inside the volume that is interior to the surface where the measurements were taken. This produces our second miracle identity

$$\frac{E_0}{q} - \frac{1}{\frac{2q}{m}[\hat{s} \cdot \nabla U'(E_0, \vec{\mathrm{A}}, \vec{\mathrm{r}})]^2} = \phi(\vec{\mathrm{r}}), \tag{8}$$

where the left-hand side is a function of six variables, and the right-hand side is a function of only three variables. Physically the potential is independent of energy and also independent of the reference position vector or alternatively, the potential at any given position is independent of the particular curved least action trajectory that crosses this position. This is a curved miracle identity because the least action trajectories are curved in contrast to our first miracle identity and Newton's miracle identity which are both straight miracle identities because they correspond to straight line trajectories. Both of our miracle identities can be verified numerically and will be discussed further elsewhere.

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