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TIME-DEPENDENT PROBLEMS IN QUANTUM-MECHANICAL STATE RECONSTRUCTION[1]

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We study the state reconstruction of wave packets that travel in time-dependent potentials. We solve the problem for explicitly time-dependent harmonic oscillators and sketch a general adaptive technique for finding the wave function that matches an observed evolution.

1. Introduction

At the 4th of the series of splendid Central-European Workshops on Quantum Optics we discussed [1] how to extract the density matrix of a one-dimensional Schrödinger wave packet from position measurements of the corresponding "particles" evolving in time. We arrived at the compact reconstruction formula

$$\rho_{mn} \equiv \langle m | \hat{\rho} | n \rangle = \left\langle\!\!\left\langle \frac{\partial}{\partial x}\left[\psi_m^*(x,t)\,\varphi_n(x,t)\right] \right\rangle\!\!\right\rangle_{x,t} . \tag{1}$$

Here ρ_{mn} denotes the density matrix in energy representation, ψ_m is the regular and φ_n the irregular wave function of the energy eigenstate $|n\rangle$. The double brackets describe an average with respect to the experimentally measured positions x at all times t. Central to this result is the orthogonality of $d[\psi_m(x)\,\varphi_n(x)]/dx$ on products of wave functions $\psi_\mu(x)\,\psi_\nu(x)$ that obey the frequency (energy) condition $\omega_\mu - \omega_\nu = \omega_m - \omega_n$. Formula (1) was proven [1, 2, 3, 4, 5] for bound states in time-independent potentials. It turns out [6] that in the continuous part of the spectrum the order of regular and irregular wave functions is critical. We are entitled to use formula (1) only if the energy ω_n of $|n\rangle$ exceeds ω_m of $|m\rangle$. Otherwise we should replace (1) by

$$\rho_{mn} = \left\langle\!\!\left\langle \frac{\partial}{\partial x}\left[\varphi_m^*(x,t)\,\psi_n(x,t)\right] \right\rangle\!\!\right\rangle_{x,t} . \tag{2}$$

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What happens if the wave packet travels in a time-dependent potential? Why is this interesting?

Paul traps, for instance, require a time-dependent potential for trapping charged particles. If the parameters of the trap are chosen right the particle moves effectively in a stationary harmonic-oscillator potential, apart from a rapidly oscillating motion called the micromotion, cf. for example [7, 8]. The trap is quasi-one-dimensional if one component of the 3D binding force is very weak compared to the others. If the trap is large enough the spatial motion of the trapped particle is directly observable via detecting the fluorescence light [9]. In this case we do observe a quantum particle moving in a time-dependent potential.

There is another prominent physical system that can be reduced to a wave packet traveling in a time-dependent potential: A Bose-Einstein condensate is a trapped many-body system where all "particles" are approximately in identical pure states described by the wave function ψ. However, because of the collisional interactions between the condensed particles, the dynamical law of ψ is nonlinear

$$i\frac{\partial\psi}{\partial t} = \left(-\frac{1}{2m}\Delta + U + g\,|\psi|^2\right)\psi \ . \tag{3}$$

Here U denotes the trap potential, m is the particle mass, $\hbar$ equals unity and g quantifies the mutual particle interaction. We note that the density $|\psi(x,t)|^2$ can be measured by phase-contrast imaging [10] very much like a living cell is observed in phase-contrast microscopy. Can we reconstruct ψ at a time t_0 when $|\psi(x,t)|^2$ is given for all times? Looking at the nonlinear Schrödinger equation (3) (called the Gross-Pitayevski equation) we notice that

$$U_{\text{eff}} = U + g\,|\psi(x,t)|^2 \tag{4}$$

acts just as an effective potential in a linear Schrödinger equation. This potential is known if $|\psi(x,t)|^2$ is known, yet U_{eff} is clearly time-dependent. The problem of finding $\psi(x,t_0)$ from $|\psi(x,t)|^2$ is thus reduced to state reconstructions of wave packets moving in arbitrary time-dependent potentials. We also note that x is three-dimensional for a real Bose-Einstein condensate. This is indicated by the Laplacian in Eq. (3). So in addition to the time-dependence of the potential we are facing here a multidimensional problem, in general.

2. Time-dependent harmonic oscillators

Let us first approach the problem of a one-dimensional time-dependent potential. Let us study a simple and completely solvable model to see whether we can extend our reconstruction recipe (1) to this situation. Our model is, of course, a harmonic oscillator with a time-dependent frequency $\omega(t)$ denoted by the Hamiltonian

$$\hat{H} = \tfrac{1}{2}\hat{p}^2 + \tfrac{1}{2}\omega^2(t)\,\hat{q}^2 \ . \tag{5}$$

As we have mentioned in the introduction, a one-dimensional Paul trap is a physically relevant example of this model.

There are several ways to establish a theory of the state reconstruction for time-dependent harmonic oscillators. We have always the option of using a tomographic technique, because the motion of $\hat{q}$ and $\hat{p}$ is linear. Let us, however, pursue another approach that is based on a remarkable scaling property [11] of the Schrödinger equation

$$i\frac{\partial\Phi}{\partial t} = -\frac{1}{2}\frac{\partial^2\Phi}{\partial q^2} + \frac{\omega^2(t)}{2}q^2\,\Phi \ . \tag{6}$$

For describing the quantum motion of Φ we introduce a classical reference oscillator that obeys Hill's equation

$$\frac{d^2\varepsilon(t)}{dt^2} + \omega^2(t)\varepsilon(t) = 0 \tag{7}$$

with the initial condition

$$\varepsilon(0) = 1 \quad , \quad \dot{\varepsilon}(0) = i\omega_0 \ . \tag{8}$$

First, we notice that Hill's equation (7) conserves the Wronskian

$$\varepsilon(t)\dot{\varepsilon}(t)^* - \dot{\varepsilon}(t)\varepsilon(t)^* = \varepsilon(0)\dot{\varepsilon}(0)^* - \dot{\varepsilon}(0)\varepsilon(0)^* = -2i\omega_0 \ . \tag{9}$$

We introduce the phase θ and the reference amplitude q_0,

$$\theta \equiv \arg\varepsilon \quad , \quad q_0 \equiv \sqrt{\frac{\varepsilon^*\varepsilon}{\omega_0}} \ , \tag{10}$$

and see from the Wronskian (9) that the phase obeys

$$\dot{\theta} = q_0^{-2} \ , \tag{11}$$

i.e. θ is just the temporal integral of q_0^{-2}. We represent $\Phi(q,t)$ by the scaling ansatz

$$\Phi(q,t) = \phi(x,\theta)\,q_0^{-1/2}\exp\left(\tfrac{1}{2}i\dot{q}_0 q_0 x^2\right) \quad , \quad x = q/q_0 \tag{12}$$

and find that $\Phi(q,t)$ satisfies the time-dependent Schrödinger equation (6) if $\phi(x,\theta)$ solves

$$i\frac{\partial\phi}{\partial\theta} = -\frac{1}{2}\frac{\partial^2\phi}{\partial x^2} + \frac{x^2}{2}\phi \ . \tag{13}$$

In this way we have transformed the time-dependent problem to a familiar time-independent model.

The state reconstruction procedure [1] relies on an orthonormal system with respect to products of wave functions $\psi_\mu(q,t)\,\psi_\nu^*(q,t)$. The spatial derivatives of regular and irregular wave functions form such a system [2]. In particular, we obtain for the time-independent harmonic oscillator [3, 12] described by Eq. (13) the central relation

$$\delta_{\mu m}\delta_{\nu n} = \frac{1}{\pi}\int_0^\pi\int_{-\infty}^{+\infty}\psi_\mu(x,\theta)\,\psi_\nu^*(x,\theta)\frac{\partial}{\partial x}\left[\psi_m^*(x,\theta)\,\varphi_n(x,\theta)\right]dx\,d\theta \ . \tag{14}$$

We use the scaling property (12) and the phase equation (11) and find for the time-dependent harmonic oscillator

$$\begin{aligned}\delta_{\mu m}\delta_{\nu n} &= \frac{1}{\pi}\int_0^{\pi}\int_{-\infty}^{+\infty}\Psi_\mu(q,t)\,\Psi_\nu^*(q,t)\frac{\partial}{\partial q}\left[\Psi_m^*(q,t)\,\Phi_n(q,t)\right]dq\,q_0^2\,d\theta \\ &= \frac{1}{\pi}\int_0^{T}\int_{-\infty}^{+\infty}\Psi_\mu(q,t)\,\Psi_\nu^*(q,t)\frac{\partial}{\partial q}\left[\Psi_m^*(q,t)\,\Phi_n(q,t)\right]dq\,dt\,. \qquad (15)\end{aligned}$$

Therefore [1], the density matrix is given by the integral

$$\rho_{mn} = \frac{1}{\pi}\int_0^{T}\int_{-\infty}^{+\infty}\frac{\partial}{\partial q}\left[\Psi_m^*(q,t)\,\Phi_n(q,t)\right]\mathrm{pr}(q,t)\,dq\,dt \qquad (16)$$

with respect to the observed probability distribution $\mathrm{pr}(q,t)$ from time $t=0$ until a time T when the phase θ reaches π. This result indicates that we could extend formula (1) to one-dimensional time-dependent problems. However, the factor π^{-1} in front of the integral (16) suggests that the normalization will be different from the time-independent case [1]. Currently we are working on a proof to generalize our result to arbitrary potentials.

3. Nonlinear wave packets

Nonlinear atomic wave packets, for example traveling Bose-Einstein condensates, move in effective time-dependent potentials, as we have pointed out in the introduction. However, these atomic droplets are three-dimensional systems. Can we generalize our method to more than one dimension? Let us simply count the dimensionality of the problem. The density matrix in position representation $\rho(x,x')$ is a function of $2d$ variables. On the other hand, the probability distribution $\mathrm{pr}(x,t)$ depends on only $d+1$ variables. We find it hard to imagine how one could extract a $2d$-dimensional function from $d+1$ dimensional data if d exceeds unity. Therefore we expect that formula (1) is restricted to one-dimensional systems.

However, our principal goal for atomic wave packets is not the determination of the density matrix but the reconstruction of only the wave function. We know [13, 14, 15] that the measurement of $|\psi(x,t_0)|^2$ and of the first temporal derivative of $|\psi(x,t_0)|^2$ at a given time t_0 is *almost* [15, 16] sufficient to reconstruct $\psi(x,t_0)$. We expect that the observation of the motion for an extended period of time removes some ambiguities [15, 16]. Note also that forming a derivative usually enhances experimental errors. Therefore we believe that an extended observation is more practical than the minimalistic approach where only $|\psi(x,t_0)|^2$ and $\partial|\psi(x,t_0)|^2/\partial t_0$ are required.

How can we infer the wave function of a moving wave packet from position measurements? We assume that all external parameters are known, i.e. the equation of motion and the effective potential. We could, for example, start with a trial function φ and let it evolve according to the Schrödinger equation for ψ. Then we compare $|\varphi|^2$ and $|\psi|^2$ and vary φ in such a way that the evolution of $|\varphi|^2$ and $|\psi|^2$ coincides. But, of course, the Hilbert space of φ is quite roomy, and thus, the probability of finding φ by trial

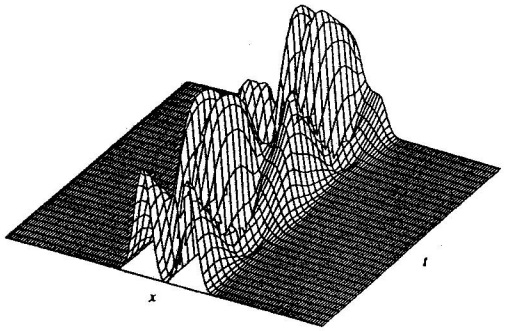

Fig. 1. One-dimensional evolution of a nonlinear Schrödinger-cat state (a double condensate [17]) in a harmonic potential $U(x)=\frac{1}{2}x^2$ with the additional nonlinear term $g|\psi(x,t)|^2$ and $g=10$.

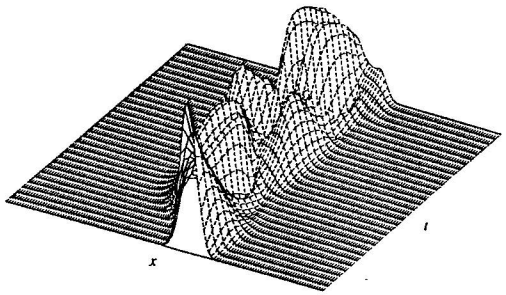

Fig. 2. Illustration how φ adapts to ψ when φ was initially a localized Gaussian wave packet. We have set the adaption rate k to the value of 7.

and error is rather low. A more intelligent approach would be adaptive. Knowing the evolution of $|\psi|^2$ we could constantly adapt φ to the measured wave packet. For this we must use a *nonlinear propagation* for φ. The simplest ansatz is

$$i\frac{\partial\varphi}{\partial t} = \left(-\frac{1}{2}\Delta + U_{\mathrm{eff}}\right)\varphi + ik\left(|\psi|^2 - |\varphi|^2\right)\varphi. \qquad (17)$$

If $|\psi|^2$ coincides with $|\varphi|^2$ at all times the evolution of φ decouples from ψ. At positions where $|\psi|^2$ is below $|\varphi|^2$ the modulus of φ is damped and where $|\psi|^2$ exceeds $|\varphi|^2$ it is amplified. Thus we expect that if $|\psi|^2$ deviates from $|\varphi|^2$ by a small quantity ε the evolution of φ converges to ψ. To be more precise, we represent φ as

$$\varphi(x,t) = \left[\psi(x,t) + \varepsilon(x,t)\right]e^{i\theta} \qquad (18)$$

with a constant overall phase θ. We obtain from the adaptive equation (17) the dynamical law for ε,

$$i\frac{\partial\varepsilon}{\partial t} = \left(-\frac{1}{2}\Delta + U_{\mathrm{eff}}\right)\varepsilon + ik\left(|\psi|^2 - |\varphi|^2\right)(\psi+\varepsilon)\,, \qquad (19)$$

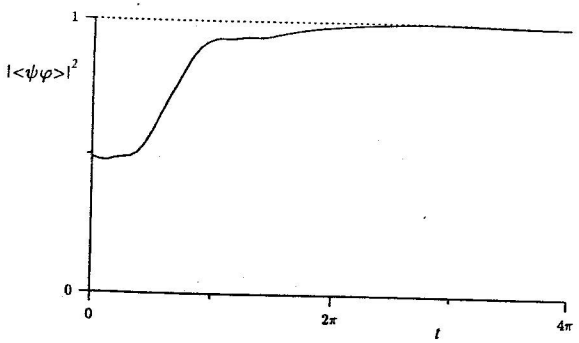

Fig. 3. Evolution of the modulus-squared scalar product, $\left|\int \psi^* \varphi \, dx\right|^2$, of ψ and φ. We see that after about one oscillation cycle φ coincides with ψ, apart from a trivial overall phase θ.

which implies

$$\begin{aligned} \frac{d}{dt}\int |\varepsilon|^2 \, dx &= -k \int \left[(\varepsilon^* \psi + \varepsilon \psi^* + |\varepsilon|^2)(\varepsilon^* \psi + \varepsilon \psi^* + 2|\varepsilon|^2)\right] dx \\ &\approx -k \int (\varepsilon^* \psi + \varepsilon \psi^*)^2 \, dx \\ &< 0 \end{aligned} \tag{20}$$

for a small ε. Consequently, ε must tend to zero if ε is small. In other words $\varphi = \psi e^{i\theta}$ is a *stable* solution of the adaptive equation (17).

An important point is that the nonlinear Hamiltonian in Eq. (17) is non-Hermitian. Therefore we have to normalize φ to unity after each temporal step,

$$\varphi(x, t + dt) \leftarrow \varphi(x, t + dt) \left[\int |\varphi(x, t + dt)|^2 \, dx\right]^{-1/2} . \tag{21}$$

So far we were not able to prove that φ converges with certainty to a solution that matches $|\psi|^2$ for all times. Our numerical tests indicate that this could be indeed true.

Fig. 1 shows the one-dimensional evolution of a nonlinear Schrödinger-cat state (a double condensate [17]) in a harmonic potential $U(x) = \frac{1}{2}x^2$ with the additional nonlinear term $g|\psi(x,t)|^2$ and $g = 10$. Fig. 2 illustrates how φ adapts to ψ with φ being initially a localized Gaussian wave packet. We have set the adaption rate k to the value of 7. Fig. 3 displays the modulus-squared scalar product, $\left|\int \psi^* \varphi \, dx\right|^2$, of ψ and φ. We see that after about one oscillation cycle φ coincides with ψ, apart from a trivial overall phase θ.

4. Summary

The example of an explicitly time-dependent harmonic oscillator indicates that the extension of the state-reconstruction recipe (1) to time-dependent problems seems possible. In addition, we can use a nonlinear adaptive technique to find the pure-sate *wave function* ψ from the evolution of $|\psi|^2$. We finally remark that the latter method is not restricted to one-dimensional geometries.

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