Can even-order laser harmonics exhibited by Bohmian trajectories in symmetric potentials be observed?

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Abstract: Strong-field laser-atom interactions provide extreme conditions that may be useful for investigating the de Broglie-Bohm quantum interpretation. Bohmian trajectories representing bound electrons in individual atoms exhibit both even and odd harmonic motion when subjected to a strong external laser field. The phases of the even harmonics depend on the random initial positions of the trajectories within the wave function, making the even harmonics incoherent. In contrast, the phases of odd harmonics remain for the most part coherent regardless of initial position. Under the conjecture that a Bohmian point particle plays the role of emitter, this suggests an experiment to determine whether both even and odd harmonics are produced at the atomic level. Estimates suggest that incoherent emission of even harmonics may be detectable out the side of an intense laser focus interacting with a large number of atoms.

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References and links

1. X. Y. Lai, Qing-Yu Cai, and M. S. Zhan, "Bohmian mechanics to high-order harmonic generation," Chin. Phys. B **19** 020302 (2010).
2. X. Oriols, *Applied Bohmian Mechanics: From Nanoscale Systems to Cosmology* (Pan Stanford Publishing, 2012).
3. J. Wu, B. B. Augstein, and C. Figueira de Morisson Faria, "Local dynamics in high-order-harmonic generation using Bohmian trajectories," Phys. Rev. A **88**, 023415 (2013).
4. Yang Song, Su-Yu Li, Xue-Shen Liu, Fu-Ming Guo, and Yu-Jun Yang, "Investigation of atomic radiative recombination processes by the Bohmian-mechanics method," Phys. Rev. A **88**, 053419 (2013).
5. A. L'Huillier, P. Balcou, S. Candel, K. J. Schafer, and K. C. Kulander, "Calculations of high-order harmonic-generation processes in xenon at 1064 nm," Phys. Rev. A **46**, 2778–2790 (1992).
6. J. Peatross, J. P. Corson, and G. Tarbox, "Classical Connection between Near-Field Interactions and Far-Field Radiation and the Relevance to Quantum Photoemission," Am. J. of Phys. **81**, 351–358 (2013).
7. J. Peatross, C. Müller, K. Z. Hatsagortsyan, and C. H. Keitel, "Photo-Emission of a Single-Electron Wave-Packet in a Strong Laser Field," Phys. Rev. Lett. **100**, 153601 (2008).
8. J. P. Corson, J. Peatross, C. Müller, and K. Z. Hatsagortsyan, "Scattering of Intense Laser Radiation by a Single-Electron Wave Packet," Phys. Rev. A **84**, 053831 (2011).
9. Gunadya Bandarage, Alfred Maquet, Thierry Menis, Richard Taieb, and Valerie Veniard, J. Cooper, "Harmonic generation by laser-driven classical hydrogen atoms," Phys. Rev. A **41**, 380–390 (1992).
10. J. Johansen, E. Cunningham, D. Black, and J. Peatross, "Bohmian Perspective on High Harmonic Generation," presented at Super Intense Laser-Atom Physics (SILAP), Zion National Park, Utah, 21-23 Sept. 2009.
11. J. D. Jackson, *Classical Electrodynamics*, 3rd ed. (Wiley, New York, 1998), pp. 407–411.
12. S. Backus, J. Peatross, E. Zeek, A. Rundquist, G. Taft, M. M. Murnane, and H. C. Kapteyn, "16 Femtosecond, 1μJ Ultraviolet Pulses Generated by Third-Harmonic Conversion in Air," Opt. Lett. **21**, 665–667 (1996).

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13. J. Peatross, S. Backus, J. Zhou, M. M. Murnane, H. C. Kapteyn, "Spectral-Spatial Measurements of Fundamental and Third-Harmonic Light of Intense 25-fs Laser Pulses Focused in a Gas Cell," J. Opt. Soc. Am. B **15**, 186–192 (1996).
14. D. J. Griffiths, *Introduction to Quantum Mechanics*, 2nd ed. (Pearson, Upper Saddle River NJ, 2005) pp. 5, 15.
15. D. Bohm and B. J. Hiley, *The undivided Universe*, (1993) pp. 28–30.

1. Introduction

Recently, the de Broglie/Bohm interpretation of quantum mechanics has been applied to laser high-harmonic generation [1–4]. In the Bohmian formalism, one is invited to conceptualize a point particle piloted by the electron quantum wave (as well as by external potentials). These studies emphasize insights into the harmonic generation process that the Bohmian approach offers, without necessarily promoting the Bohmian interpretation per se. In any case, Bohmian-like language is widely used when speaking of a three-step model: an electron breaks free of the atom, makes a laser assisted excursion in the continuum, and re collides with the nucleus. This description is used even though the greater portion of an electron wave packet remains bound to the atom throughout the process, with only a tiny fraction of the overall wave function undergoing the motion spoken of.

Ironically, Bohmian trajectories that remain close to the core generally exhibit stronger high-harmonic motion than the ones that accompany the part of the wave packet that breaks away and returns. In this context, an ensemble of Bohmian trajectories makes a set of useful markers of local wave-function behavior. Indeed, the average motion of a very large ensemble of Bohmian trajectories (statistically chosen to match the Born probability distribution) recovers the behavior of the wave-packet position expectation $\langle \mathbf{r} \rangle$ [4].

In this paper, we entertain the possibility that $\langle \mathbf{r} \rangle$ in general is insufficient to describe single-atom behavior when an atom is subjected to a strong laser field, in spite of the fact that the term "single-atom" is sometimes invoked in this context [5]. Within an atom, the quantum probability current often develops spatial structure across the laser-driven electron wave packet, owing to interactions with both the applied laser and the atomic potential. Much of this structure 'washes out' when Maxwell's equations are sourced with $\langle \mathbf{r} \rangle$, or when sourced with the probability current directly. Might the local behavior within a wave packet (as opposed to its overall structure) be important to single-atom light emission? Can Bohmian trajectories, taken individually (as opposed to averaged ensembles), predict spectral features in emitted light?

We will treat the scattered light classically and consider the probability of measuring photons to be proportional to light intensity. We emphasize that sourcing Maxwell's equations with $\langle \mathbf{r} \rangle$ effectively permits emission from different parts of the same electron wave function to interfere. In this sense, representing a single atom with $\langle \mathbf{r} \rangle$ conjures the (discredited) Schrödinger interpretation where the electron is treated as a charge distribution smeared across the wave function [6]. In contrast, the Born probabilistic interpretation considers the wave packet to be an indication of where a point-like electron might be found if a measurement is performed.

We recently demonstrated, using quantum electrodynamics (QED), that a free electron in a laser field scatters radiation at a rate independent of wave-packet size [7, 8]. When an electron wave packet is large compared to the driving laser wavelength, such that different parts of the same electron wave packet oscillate out of phase, there is no interference/suppression of the scattered light field. The scattered light maintains the same strength as that from a classical point emitter. In contrast, light emission based on $\langle \mathbf{r} \rangle$ depends crucially on wave-packet size, allowing emission from different parts of the wave packet to interfere. Alternatively, the de Broglie-Bohm interpretation (i.e. of a point trajectory somewhere within the electron wave function) lends intuition to this QED result, but from the semiclassical framework.

Strong-field laser-atom interactions provide extreme conditions that may prove useful for probing the de Broglie-Bohm interpretation of semiclassical quantum physics. We hypothesize that individual Bohmian trajectories can be used to source emitted radiation. As will be shown, a Bohmian trajectory calculated for a wave function bound to an atomic potential can exhibit both even and odd harmonic motion when subjected to a strong external laser field. The phases of the even harmonics depend on the random initial position of the trajectory within the wave function, indicating that even harmonics would be emitted incoherently (i.e. extremely faint).

2. Bohmian Mechanics for a single-electron atom in a strong laser field

Following the standard Bohmian formalism, one solves the Shrödinger equation

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

in the usual way. With Ψ in hand, a point-like trajectory piloted by the wave is then computed from

$$\frac{d\mathbf{r}}{dt} = \frac{\hbar}{m}\mathrm{Im}\left\{\frac{\nabla\Psi}{\Psi}\right\} \tag{2}$$

This differential equation requires an initial position, which is selected (at random) consistent with the conventional initial probability distribution $\rho = |\Psi|^2$ at $t = 0$. A brief overview of Bohmian mechanics is provided in appendix A.

We study the behavior of Bohmian trajectories using a one-dimensional single-electron model ‘atom’ subject to a strong field. The potential is given by

$$V(x,t) = -\frac{e^2}{4\pi\varepsilon_0\sqrt{x^2+a^2}} - exE_0(t)\cos\omega t \tag{3}$$

where $a = \sqrt{2}a_0$ is a smoothing parameter chosen to make the ground-state binding energy match that of hydrogen; a_0 is the Bohr radius. We neglect possible magnetic effects and treat the wave function as being much smaller than an applied laser wavelength.

Figure 1(a) shows an array of possible Bohmian trajectories associated with the ground-state wave function, computed via (2). Although it is interesting to look simultaneously at multiple trajectories, presumably only one trajectory would inhabit any individual atom. Figure 1(b) shows a representative Bohmian trajectory with initial position $x = 1$ atomic unit (i.e. a_0). During the applied Gaussian laser pulse, which reaches a peak field strength of $E_0 = 0.03$ atomic units (i.e. $0.03\hbar^2/\left(ema_0^3\right) \leftrightarrow I = 3\times10^{13}$ W/cm^2), the bound wave function undergoes a modest amount of sloshing from side to side while interacting with the laser field. Figure 1(c) plots the position of the representative Bohmian trajectory together with the position expectation $\langle x\rangle = \int\Psi^* x\Psi dx$ as a function of time. The frequency is set to $\omega = 0.055$ atomic units (i.e. $0.055\hbar/\left(ma_0^2\right) \leftrightarrow \lambda = 800$ nm). During the course of the entire pulse, about 0.5% ionization occurs, as evidenced by the outer trajectories in Fig. 1(a) escaping from the atom.

The behavior of the majority of individual Bohmian trajectories looks qualitatively similar to the behavior of $\langle x\rangle$. However, on close inspection of Fig. 1(c), it is noticed that the oscillations of the representative Bohmian trajectory are not symmetric about the initial position $x = 1$. (The trajectory approaches closer to $x = 1.5$ than to $x = 0.5$.) This is because the Bohmian trajectory oscillates on only one side of the potential well. The spacing between the different possible trajectories, as seen in Fig. 1(a) stretch and compress as they travel farther from and closer to the potential minimum. This asymmetry gives rise to even harmonic motion, reminiscent of those produced by eccentric classical Kepler orbits studied by Bandarage et al. [9].

Figure 1(d) shows the Fourier transform of both the representative Bohmian trajectory and the position expectation $\langle x\rangle$. The Bohmian trajectory exhibits both even- and odd-order harmonics with roughly equal strength, whereas the position expectation exhibits only odd harmonics.

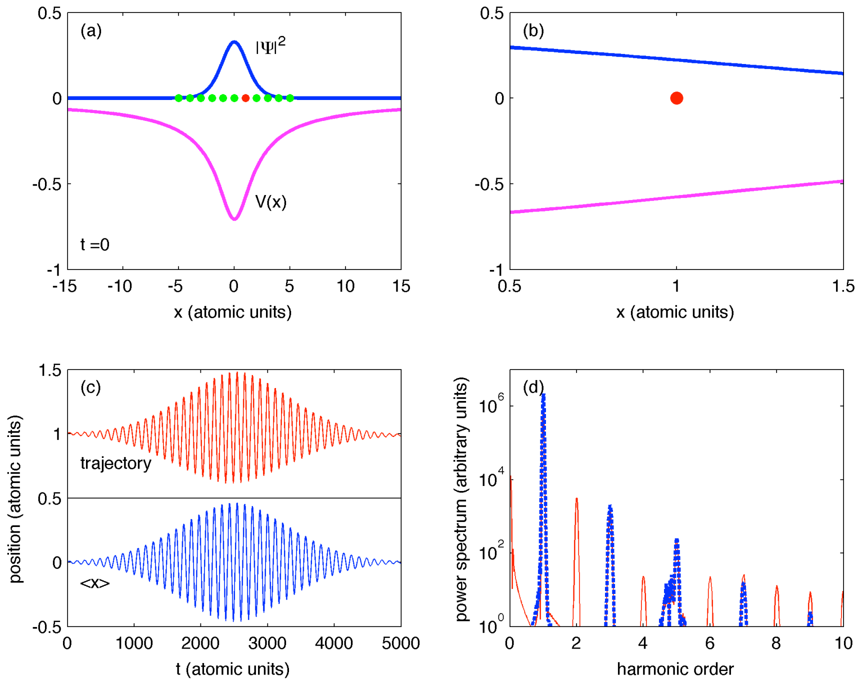

Fig. 1. (a) Media 1 of possible Bohmian trajectories with equally spaced initial positions ranging from x=-5 to x=5 atomic units during atomic exposure to a Gaussian laser pulse. The wave function and potential well are also shown. (b) Close up view of a representative Bohmian trajectory with initial position $x = 1$. (c) Position of the Bohmian trajectory in (b) plotted as a function of time together with the conventional position expectation $\langle x \rangle = \int \Psi^* x \Psi dx$. (d) Power spectrum of curves in (c), Bohmian trajectory (solid) and $\langle x \rangle$ (dotted), showing harmonic components.

As mentioned, when a statistical ensemble of Bohmian trajectories is averaged, the result begins to resemble $\langle x \rangle$ [4]; the even harmonics cancel away while the odd harmonics reinforce. The even harmonics exhibited by individual Bohmian trajectories were first noticed by Lai et al. [1] and discovered independently by us [10]. Lai et al. called the even harmonics "unphysical" and advocated averaging multiple trajectories to achieve their removal. In this paper, we entertain the possibility that the even harmonics are physical.

We outline an experiment to test whether both even and odd harmonics are emitted from individual atoms. This represents a novel testable 'prediction' of the Bohmian interpretation (albeit qualified by the conjecture that an individual Bohmian trajectory effectively acts as a source of emission). Since the incoherent signal is expected to be weak, it will be necessary to employ a very large ensemble of atoms.

3. Ensemble emission and phase matching

Consider a single radiating dipole $\mathbf{p}_n = \hat{z} p_0 \cos(-\omega t + \varphi_n)$, oriented along the z-direction, oscillating with frequency $\omega = ck$. The parameters p_0 and φ_n represent the amplitude and phase. This dipole might represent a particular oscillating component, such as the second harmonic, associated with a Bohmian trajectory within an individual atom located at $\mathbf{r}_n$.

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In the far field, the electric field radiating from the dipole is [11]

$$\mathbf{E}_n(\mathbf{r},t) = -\frac{p_0}{4\pi\varepsilon_0}\left((\hat{z}\cdot\hat{\boldsymbol{\imath}})\hat{\boldsymbol{\imath}}-\hat{z}\right)\frac{k^2\cos(k\boldsymbol{\imath}-\omega t+\varphi_n)}{\boldsymbol{\imath}} \tag{4}$$

where $\boldsymbol{\imath} \equiv \mathbf{r}-\mathbf{r}_n$ and $\hat{\boldsymbol{\imath}} \equiv \boldsymbol{\imath}/\imath$. In the far field, we may also write $\imath \cong r-\mathbf{r}_n\cdot\hat{r}$ in the cosine and $\imath \cong r$ in the denominator. Further, $(\hat{z}\cdot\hat{\boldsymbol{\imath}})\hat{\boldsymbol{\imath}}-\hat{z} \cong (\hat{z}\cdot\hat{r})\hat{r}-\hat{z} = \hat{\theta}\sin\theta$ in spherical coordinates.

If we add together the fields from many dipole oscillators, the time-averaged Poynting flux from the distribution becomes

$$\langle S\rangle_t = c\varepsilon_0\left\langle\left|\sum_{n=1}^{N}\mathbf{E}_n(\mathbf{r},t)\right|^2\right\rangle_t = \frac{cp_0^2\sin^2\theta}{2(4\pi)^2\varepsilon_o}\frac{k^4}{r^2}\left[N+\sum_{n=1}^{N}\sum_{m\neq n}^{N}\cos\left[k(\mathbf{r}_n-\mathbf{r}_m)\cdot\hat{r}-(\varphi_n-\varphi_m)\right]\right] \tag{5}$$

For simplicity, we have taken the strength of each dipole in the population to be p_0.

In the limit of many dipoles (i.e. $N\to\infty$), if there exists any coordination between the phases ϕ_n and positions $\mathbf{r}_n$, the double summation in (5), which has approximately N^2 terms, tends to dominate over the term N. Coordination between ϕ_n and $\mathbf{r}_n$ is commonly referred to as phase matching. For example, if $\phi_n = 3k_L x$, and $k = 3k_L$, where k_L is associated with a stimulating laser field, we say that third-harmonic emission is phase matched in the x-direction. In this case, for the x-direction only, it is as though all dipoles are collocated and oscillating with the same phase. On the other hand, emission in other directions can be dramatically suppressed if the dipoles are distributed throughout a finite volume. (Endowing ϕ_n additionally with the Gouy shift, perhaps played against index variations in k and k_L or intensity-dependent intrinsic phases, makes little difference to arguments made here.)

An incoherent signal, on the other hand, has random phase ϕ_n, even if spatial structure is additionally inscribed onto ϕ_n. This would be the case for even harmonics generated by Bohmian trajectories. The double summation in (5) in this case has an expectation of zero (albeit with fluctuations), making the overall signal proportional to N, regardless of emission direction. Incoherent emission from an ensemble of N atoms is therefore essentially the same as the accumulated signal from N measurements on a single atom. Since the majority of individual Bohmian trajectories exhibit even and odd harmonics with roughly equal strengths, one can estimate the strength of even-harmonic emission by simply dividing phase-matched odd-harmonic signal (proportional to N^2) by the number of atoms N participating in the emission.

4. Feasibility of an even-harmonic measurement

It has been observed that 1 μJ of third harmonic light can be produced in approximately 200 torr of argon using a 1-mJ, 25-fs, 800-nm laser pulse [12]. The narrow beam of third harmonic light (comprised of 10^{12} photons) emerges in the direction of the residual laser beam with a solid angle of approximately 10^{-4} steradians [13]. If the phase-matched generating volume has radius 50 μm and length 1 cm, this would suggest as many as $N = 10^{15}$ atoms participate in the observed coherent signal. Helium has a somewhat lower conversion efficiency.

Dividing the number of photons 10^{12} by the number of atoms $N = 10^{15}$ suggests a disappointing one-photon-per-1000-laser-shots. Fortunately, this can be improved by collecting photons from, say, 10^{-1} steradians as opposed to the 10^{-4} steradians in the pencil-like 3rd-harmonic beam mentioned above. Moreover, since phase matching plays no role in an incoherent signal, the atomic density can be increased as well as the laser pulse energy (employing larger focal volume and/or longer pulse duration). To avoid potential noise from plasma effects, it will likely be necessary to work with ultra pure targets at intensities well below the ionization threshold. Fortunately, the onset of ionization is an extremely nonlinear process, whereas the reduction in second harmonic signal presumably follows a more gentle I^2 law.

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With the above considerations, it appears plausible that an incoherent even-harmonic signal, if it exists, may be observed out the side of a laser focus during the course of a scan involving many laser shots. In particular, a high-quantum-efficiency detector might be employed in a search for the second harmonic of an 800 nm laser in a gas target such as argon or helium. The second harmonic signal should have a bandwidth somewhat narrower than the laser bandwidth, and it should shift when the center frequency of the laser is shifted.

5. Summary

To date, only odd-order harmonics have been observed to be emitted from atoms subject to a strong laser field. What we are calling into question is whether this result is truly a single-atom effect or whether it arises from ensemble averaging. After all, it is common for quantum textbooks to describe $\langle \mathbf{r} \rangle$ as being representative of *ensemble* behavior [14].

If even harmonics from symmetric atomic potentials are observed, it would suggest that the de Broglie/Bohm interpretation possesses a certain predictive power within the semiclassical framework, which aims for consistency with QED. The ramifications might impact how we view quantum wave functions and associated notions such as 'wave-function collapse' [14]. We expect that regardless of the outcome of a search for even harmonics, the result will align with QED, although a QED calculation appears to be difficult at this time.

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A. Appendix: Underpinnings of Bohmian mechanics

Equation (2) is motivated as follows [15]: We write the wave function as $\Psi = |\Psi| e^{iS/\hbar}$, where S is real, and substitute into (1). Equating separately the real and imaginary parts, one obtains the continuity equation

$$\nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t} = 0 \quad \text{where} \quad \mathbf{J} \equiv \frac{|\Psi|^2 \nabla \mathrm{S}}{\mathrm{m}} \quad \text{and} \quad \rho \equiv |\Psi|^2 \tag{6}$$

coupled with

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V + Q = 0 \quad \text{where} \quad \mathrm{Q} \equiv -\frac{\hbar^2}{2\mathrm{m}} \frac{\nabla^2 |\Psi|}{|\Psi|} \tag{7}$$

Equations (6) and (7) taken together are nothing more than the Schrödinger equation in the new (real) variables $|\Psi|$ and S. However, the latter resembles the Hamilton-Jacobi equation for classical motion of a point particle. In this context, the phase of the wave-function S is interpreted as an *action*. Accordingly, one is inspired to visualize a point particle responding to the potential V as well as to a *quantum potential* Q, which presumably describes the influence of de Broglie's 'pilot-wave' on the particle. The usual quantum uncertainty stems from a lack of information regarding the initial position of the trajectory.

To review the Hamilton-Jacobi formalism, one may describe a classical point particle's motion using Newton's second law $d^2\mathbf{r}/dt^2 = -\nabla V(\mathbf{r},t)/m$, or, alternatively, using

$$\frac{d\mathbf{r}}{dt} = \frac{\nabla S(\mathbf{r},t)}{m} \tag{8}$$

Equation (8), which is the basis for (2), relates a particle's velocity to the action S. To obtain S from a prescribed potential V, (8) can be substituted into Newton's second law to remove $d^2\mathbf{r}/dt^2$ and $d\mathbf{r}/dt$. This leads to (7) in the absence of Q, which is the Hamilton-Jacobi equation for a classical point particle. In the quantum context (where Q exists), if the Schrödinger equation has been solved, then (7) has been solved as well. Moreover, there is no need to extract S from Ψ since its gradient may be found directly from (2).

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