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Manipulation of quantum particles in rapidly oscillating potentials by inducing phase hops

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Analytical calculations show that the mean-motion of a quantum particle trapped by a rapidly oscillating potential can be significantly manipulated by inducing phase hops, i.e., by instantaneously changing the potential’s phase. A phase hop can be visualized as being the result of a collision with an imaginary particle which can be controlled. Several phase hops can have accumulating effects on the particle’s mean-motion, even if they transform the particle’s Hamiltonian into its initial one. The theoretical predictions are verified by numerical simulations for the one-dimensional Paul-trap.

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I. INTRODUCTION

Potentials which oscillate rapidly relative to the motion of particles inside them are widely used to trap charged and neutral particles. Most notably, this is because rapidly oscillating potentials (ROPs) allow trapping in cases where static potentials cannot. Well-known paradigms are the Paul-trap for charged particles and the electro- and magneto-dynamic traps for high-field seeking polar molecules and neutral atoms. It is not clear if this can strongly influence the particle’s mean-motion, even if it is in the ground state of the effective trapping potential. The experimental ability to prepare single and ensembles of quantum particles in ROPs in specific states would allow to apply this tool in a controlled fashion.

The model used to describe both the time-dependent and the effective system is given in Sec. I In Sec. II it is shown that the effect of a phase hop can be visualized as being the result of a collision with an imaginary particle. In Sec. III it is demonstrated that phase hops offer a powerful tool to manipulate quantum particles, whose application, in particular, does not affect the effective trapping potential.

II. QUANTUM MOTION IN A RAPIDLY OSCILLATING POTENTIAL

The Schrödinger equation for a quantum particle in a time-periodic potential $V(x, \omega t)$ reads

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \hat{H}(x, \omega t)\psi(x, t),$$

with the time-dependent, periodic Hamiltonian

$$\hat{H}(x, \omega t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_0(x) + V_1(x, \omega t),$$

where the last two terms represent a separation of $V$ into a time-averaged part $V_0$ and an oscillating part $V_1$ with a vanishing period-average. Two experimentally relevant examples for the considered type of potentials are

$$V^\text{PT}(x, \omega t) = \frac{1}{2} m \omega_\text{osc}^2 x^2 \cos \omega t,$$

$$V^\text{OT}(x, \omega t) = \frac{1}{2} m \omega_\text{osc}^2 (x - x_0 \cos \omega t)^2,$$
The last two terms of Eq. (1) represent a time-independent effective potential \( V_{\text{eff}}(x) \equiv V_0(x) + \frac{\hbar^2}{2m} F(x, \tau)^2 \). For the above examples one has \( V_{\text{eff}}^{\text{PT}}(x) = m \Omega \omega_{\text{osc}}^2 x^2 / 2 \), \( V_{\text{eff}}^{\text{OT}}(x) = m \Omega^2 x^2 / 2 + c \), with a constant \( c \) (see Fig. 3). The solution of Eq. (3) is

\[
\phi(x, t) = e^{-i \hat{H}_{\text{eff}}(x)t / \hbar} e^{i F(x, 0)} \psi(x, 0),
\]

where \( \psi(x, 0) \) is the particle’s state at \( t = 0 \). \( \phi \) approximately describes the particle’s mean-motion, since it is \( \langle x \rangle \equiv \langle \psi | x | \psi \rangle \approx \langle \phi | x | \phi \rangle \) and \( \langle p \rangle \equiv \langle \psi | p | \psi \rangle \approx \langle \phi | p | \phi \rangle \). The difference between \( \phi \) and \( \psi \) is approximately given by the oscillating phase factor \( e^{-iF} \) (Eq. (4)), which has a small amplitude as \( F \) scales with \( \omega^{-1} \) (Eq. (3)), and thus describes a micromotion \( \psi^{\text{eff}} \), since it is \( \langle \psi | x | \psi \rangle \approx \langle \phi | x | \phi \rangle \approx 0 \) and \( \langle \psi | p | \psi \rangle \approx \langle \phi | p | \phi \rangle \). In the following we consider the limit \( \omega \to \infty \), where the approximations become exact. We consider the case of a trapped particle, which can be expressed in terms of eigenstates of the effective Hamiltonian (the stationary mean-motion states), i.e., for the above examples (Eqs. (3) and (4)), of the harmonic oscillator.

III. EFFECTS OF PHASE HOPS: COLLISIONS WITH IMAGINARY PARTICLES

Suppose now that, at a time \( t_{\text{ph}} \), the phase of the potential \( V(x, \tau) \) is instantaneously changed from \( \tau_{\text{ph}} = \omega t_{\text{ph}} + \Delta \varphi \). Then, for \( t > t_{\text{ph}} \) the particle is moving in the ROP \( V_{\text{new}}(x, \tau) \equiv V(x, \tau + \Delta \varphi) \) and its mean-motion wave function \( \phi_{\text{new}} \) is governed by Eq. (3), with an effective Hamiltonian \( \hat{H}_{\text{new}} \). As the effective Hamiltonian of a ROP consists only of period-averaged terms (Eq. (3)), it is independent of the phase of the ROP, implying \( \hat{H}_{\text{new}} = \hat{H}_{\text{eff}} \). Thus the equation of motion for the particle’s mean-motion wave function remains unchanged. However, the mean-motion wave function itself changes due to the natural continuity of the particle’s real wave function at \( t = t_{\text{ph}} \): For \( t \neq t_{\text{ph}} \) the latter is a product of a phase factor and the mean-motion wave function (Eq. (3)). As the phase factor \( e^{-iF} \) depends on the phase of \( V \) through \( F \) (Eq. (3)), it changes instantaneously and thus involves a corresponding change of the mean-motion wave function. In the first instance one might, however, naively expect that this change is negligible since for large \( \omega \) the change of the phase factor is very small (\( F \) scales with \( \omega^{-1} \)). But, as we show in the following, the change of the particle’s mean-motion can be indeed significant and even for arbitrarily large \( \omega \).

To demonstrate this, we calculate \( \phi_{\text{new}} \) and derive the resulting changes of the mean-motion observables. The condition of continuity for the particle’s real wave function yields

\[
\phi_{\text{new}}(x, t_{\text{ph}}) = e^{-i \Delta F(x, \tau_{\text{ph}})} \phi(x, t_{\text{ph}}),
\]

(10)

(the notation \( \lim_{t_{\text{ph}} \to t_{\text{ph}} -, t_{\text{ph}} > t_{\text{ph}}} \phi(x, t) = \phi(x, t_{\text{ph}}) \) is used), where \( \Delta F(x, \tau_{\text{ph}}) \equiv \int_{t_{\text{ph}}}^{t_{\text{ph}} + \Delta \varphi} F(x, \tau) d\tau \). Applying Eq. (3), leads to

\[
\phi_{\text{new}}(x, t) = e^{-i (t - t_{\text{ph}})} \hat{H}_{\text{eff}}(x) / \hbar e^{i \Delta F(x, \tau_{\text{ph}})} \phi(x, t_{\text{ph}}),
\]

(11)

Combined with Eq. (3), Eq. (11) allows to completely describe the phase hop, as the particle’s mean-motion wave function is known for all times.
The effect of the phase hop on $\phi$ involves an instantaneous change of some mean-motion observables, which, for a given mean-motion observable $\hat{O}$, is given by $\Delta \langle \hat{O} \rangle = \langle \phi_{\text{new}}(x, t_{\text{ph}}) | \hat{O} | \phi_{\text{new}}(x, t_{\text{ph}}) \rangle - \langle \phi(x, t_{\text{ph}}) | \hat{O} | \phi(x, t_{\text{ph}}) \rangle$. Using Eqs. (9) and (10) we find

$$\Delta \langle x \rangle = 0,$$

$$\Delta \langle p \rangle = \hbar \int_{-\infty}^{\infty} \langle \phi(x, t_{\text{ph}}) | \Delta F(x, t_{\text{ph}}) \rangle \, dx.$$  (13)

Inspection of the right-hand side (rhs) of Eq. (13) shows that $\Delta \langle p \rangle$ equals the change of momentum of the particle’s micromotion, which is taking place at the same time, demonstrating that the phase hop causes a momentum transfer between the micromotion and the mean-motion. The fact that the phase hop can change the particle’s mean-motion instantaneously, but not its mean-position, shows that its effect on the particle’s mean-motion can be visualized as being the result of a collision with an imaginary particle [22].

Inspection of the rhs of Eq. (14) shows that $\Delta \langle \phi \rangle$ is at rest, $\Delta \langle \phi \rangle = 0$, since it is $\phi^* \phi_n = \phi_n^* \phi_n$. Using the picture of the imaginary collision, Eq. (15) also directly follows from the fact that stationary mean-motion states $\phi_n$ have $\langle \hat{p} \rangle = 0$. For the Paul trap potential [3] the fact that the energy change $\Delta \langle \epsilon \rangle$ can be non-zero (and even be very large as shown in Sec. III) marks a difference to the classical regime, since for a classical particle whose mean-motion is at rest, $\Delta \langle \epsilon \rangle_{\text{class}}$ is always zero [22]. This difference is a direct consequence of Heisenberg’s uncertainty principle which implies that in the quantum regime the particle’s mean-position is spread around zero, leading — contrary to the classical regime — to a non-vanishing micromotion (since $e^{iF} \neq 1$ for $x \neq 0$), thus giving rise to an effect of the phase hop. If the quantum particle is not in a stationary mean-motion state its mean-energy can be found in Eq. (16) be both increased and decreased:

$$\Delta \langle \epsilon \rangle \geq 0.$$  (16)

(see also the appendix).

IV. PHASE HOPS CAN HAVE SIGNIFICANT IMPACT

In order to demonstrate that the phase hop can have a strong effect we compare $\Delta \langle \epsilon \rangle$ to the particle’s initial mean-energy $\langle \epsilon \rangle$. Experimentally relevant are particles that are in stationary mean-motion states $\phi_n$ with mean-energy $\epsilon_n$. For the Paul-trap [3] we find

$$\Delta \langle \epsilon \rangle \text{PT} = \omega_0^2 \left( \sin(\tau_{\text{ph}} + \phi) - \sin(\phi_{\text{ph}}) \right)^2,$$  (17)

with $\omega_0 = \hbar \Omega / (n + 1/2)$ and the reference frequency $\omega_{\text{ref}} = \sqrt{m \omega_0 / 2 \hbar}$. Here, the relative change $\Delta \langle \epsilon \rangle / \epsilon_n \text{PT}$ can take values between 0 and 4. This demonstrates that in the Paul-trap a phase hop can have a strong effect on the particle’s mean-motion, even for arbitrarily large $\omega$. For the rapidly scanning optical tweezers [4] we find

$$\Delta \langle \epsilon \rangle \text{PT} = \omega_0^2 \left( \sin(\tau_{\text{ph}} + \phi) - \sin(\phi_{\text{ph}}) \right)^2,$$  (18)

with $\epsilon_0 = \hbar \omega_{\text{ref}} / (n + 1/2)$ and the reference frequency $\omega_{\text{ref}} = \sqrt{m \omega_0 / 2 \hbar}$ and thus becomes negligible for $\omega \to \infty$. However, as an inspection of $\omega_0\phi_{\text{ph}}$ shows, $\Delta \langle \epsilon \rangle / \epsilon_n \text{PT}$ can still be large even if $\omega$ is as large as required by the validity condition of the underlying effective theory (i.e., for $\omega \gg \omega_{\text{osc}}$, cf. Sec. III).

To generalize the above findings, consider first an arbitrary ROP with a vanishing time-average. The mean potential energy of a particle in a stationary mean-motion state $\phi_n$ then is $\epsilon_n \text{PT} = \langle \phi_n | V_{\text{eff}} | \phi_n \rangle$ with $V_{\text{eff}}(x) = \hbar^2 / 2 m (F(x, \tau)^2)$ and the following relation holds:

$$\epsilon_n \text{PT} < \max_{\tau_{\text{ph}}, \Delta \phi} \left[ \langle \phi_n(x) | \Delta \langle \epsilon \rangle \text{PT} | \phi_n(x) \rangle \right]$$

$$= \max_{\tau_{\text{ph}}, \Delta \phi} \left[ \Delta \langle \epsilon \rangle \text{PT} \right].$$  (19)

Therefore a time $\tau_{\text{ph}}$ exists (within each period of $V$) for which a phase hop of a size $\Delta \phi$ (with $0 \leq \Delta \phi < 2\pi$) induces a change $\Delta \langle \epsilon \rangle$ of the particle’s mean-energy $\epsilon_n$, which is greater than its mean potential energy $\epsilon_n \text{PT}$. Since $\epsilon_n \text{PT}$ is in general a significant fraction of $\epsilon_n$, Eq. (19) shows that the phase hop can always be induced such that $\Delta \langle \epsilon \rangle$ is large with respect to $\epsilon_n$, even for arbitrarily large $\omega$. An intuitive explanation of the very fact that in ROPs with a vanishing time-average a phase hop can always significantly change the particle’s mean-energy (when it is induced in a correct moment), can be given as follows: For ROPs with a vanishing time-average the particle’s mean potential energy equals the average kinetic energy that is stored in the particle’s micromotion (since $\langle \phi | V_{\text{eff}} | \phi \rangle = \langle \langle p^2 | | \psi \rangle \rangle - \langle \langle p^2 | | \phi \rangle \rangle ) / (2m)$. A phase hop causes a momentum transfer between the particle’s
micromotion and mean-motion, whose maximum value is given by the peak-to-peak amplitude of the (oscillating) momentum of the micromotion (Eq. (13)). Since the momentum of the particle’s micromotion is oscillating around zero, this momentum transfer can, due to the equivalence of the micromotion’s average kinetic energy and the mean potential energy, lead to a change of the particle’s mean-energy which is comparable to its mean potential energy and which thus is significant.

In ROPs with a non-vanishing time-average a phase hop can only then lead to a significant change of the particle’s mean-energy if ω is not too large, since for such ROPs the fraction of the particle’s mean potential energy which equals the average kinetic energy stored in the particle’s micromotion scales with ω−2. This is expressed by Eq. (13), which yields that for stationary mean-motion states ∆⟨E⟩ scales with ω−2 (cf. Eq. (13)).

We have seen that the phase hop can affect the particle’s mean-motion wave function and observables. The phase hop thus can induce transitions between stationary mean-motion states, φn → φm, whose probabilities are given by pn,m ≡ |⟨φm(x)|φn(x)⟩|2 (implying pn,m = μnm, where φm denotes the particle’s mean-motion state after the phase hop. For the potentials (3) and (4), the pn,m can be calculated analytically. In particular, the pn,m are of experimental relevance as the mean-motion ground state φ0 can be prepared with a high precision and can be easily probed. For the Paul-trap (3) we find

\[ p_{0,m}^{PT} = \left( \frac{m!}{2^m (\frac{m}{2})! (\frac{m}{2})!} \right) \frac{\delta^m}{(1 + \delta^2)^{m/2}}, \]

for m = even,

\[ p_{0,m}^{PT} = 0, \quad \text{for } m = \text{odd}, \]

with δ = sin(τph + ∆φ) − sin(τph). In typical single ion experiments, the p0,m could be directly measured using resolved Raman sideband spectroscopy [1, 2]. Figure 3 shows the probability for a particle to remain in the mean-motion ground state can be as small as 58%, demonstrating the significance of the effect of the phase hop. For the rapidly scanning optical tweezers (4) we find

\[ p_{0,m}^{OT} = \frac{1}{2m!} \left( \frac{\omega_{\text{ref}}}{\omega} \right)^{2m} e^{-\frac{1}{2} \left( \frac{\omega_{\text{ref}}}{\omega} \right)^2}. \]

As p0,0 → 1 for ω → ∞, the effect of the phase hop becomes negligible for too large ω. However, Fig. 3 shows that for ω = ωref the effect of the phase hop is still significant.

For weakly interacting bosonic quantum gases, p0,0 could be determined by measuring the number of atoms that remain in a Bose-Einstein condensate [3], provided that the measurement is performed immediately after the phase hop before a rethermalisation takes place. For an atomic gas of degenerate fermions, phase hops (cf. Eq. (13)) could offer a tool to more quickly increase the energy and thus, after thermalization, the temperature in a controlled way [3] without having to change or to switch off-and-back-on the trapping potential and to instead await an expansion of the gas [25].

The manipulation by phase hops can be made more effective by inducing several phase hops successively. Figure 3 shows the transition probability p0,0 for two successively induced phase hops of size ∆φ = π as a function of their time delay. Although the effects of the two phase hops on the particle’s (2π-periodic) Hamiltonian can cancel each other, their effects on the particle’s mean-motion do not necessarily cancel and can even be more significant as in the case of a single phase hop.

To countercheck our theoretical predictions, we per-
FIG. 4: (Color online) Time-evolution of the rms-deviation ∆x for a particle in the Paul-trap (3) which initially is in the mean-motion ground state, affected by a phase hop of different sizes ∆ϕ (normalized to the theoretically predicted initial mean-motion value ∆xy,eff = √ℏ/(2mΩ)). Solid (red) curves: results of numerical simulations, dashed (black) curves: theoretical mean-motion prediction. Driving frequency: ω = 70 Ω.

In this article we have presented a quantum mechanical treatment of the effect of phase hops in ROPs on a single trapped particle. We have computed the particle’s mean-motion wave function for all times and the resulting consequences on its mean-motion observables. We have calculated the transition probabilities between stationary mean-motion states and we have shown that the particle’s mean-energy can in general be both increased and decreased, except if it is in a stationary mean-motion state, then the mean-energy can only be increased. In particular we have shown that the effect of a phase hop can be very strong.

Both for classical and for quantum particles, the induction of phase hops provides a powerful tool for particle manipulation. Besides its strong effect it has the following further appealing properties: firstly, its experimental implementation would be very simple and would not even require a change of an existing setup. Secondly, its application would be a controlled operation since a phase hop does not have an influence on the effective trapping potential, because that is independent of the phase of the ROP. Finally, it could be applied to any kind of trapable particles, because its mechanism is simply based on changes of the ROP and does thus not rely on particular internal properties of the particles as do laser-based manipulation methods.

In this article we have restricted our considerations to a single particle. Our main goal was to obtain analytical results, as these directly apply to a widely used and studied experimental system, the single ion in a Paul-trap [1, 2]. Due to the experimentally achievable pureness of this system, it can be used to precisely investigate phase hops and their possible applications experimentally. One of such possible applications could be to decelerate a single ion, which we here showed to be possible also in the quantum regime.

For future research, it will be interesting to study the effect of phase hops on ensembles of (interacting) particles. The extension of single particle effects in time-periodic systems [23–25] to multi-particle systems is an active field of theoretical and experimental physics [29, 30]. An experimental investigation of the schemes proposed in this manuscript could be performed with cold ion clouds stored in a Paul-trap [3] or ultracold neutral atoms stored in a TOP-trap [3] or in rapidly scanning optical tweezers [2, 3]. In the field of degenerate Fermi gases, phase hops could offer a convenient way to realize controlled heating [24].

V. CONCLUSION

The results presented in this article must be consistent with the classical results of Ref. [30]. To countercheck this we calculated Δ(TE) for the case that the mean-motion of a quantum particle in the Paul-trap potential is in a coherent state [3, 6], and showed that its classical limit equals the corresponding classical result (see appendix).

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APPENDIX: EFFECT OF A PHASE HOP ON COHERENT MEAN-MOTION STATES

Let the mean-motion of a quantum particle in the Pauli-trap potential (3) be in a coherent state. This is a quantum state which describes a wave packet that follows the motion of a classical particle in a harmonic oscillator potential while retaining its shape (thus also referred to as quasiclassical state). As the effective potential of the Pauli-trap is harmonic, the particle’s mean-motion possesses coherent states which are given by

$$\phi_{CS}(x) = \left(\frac{m\Omega}{\pi \hbar}\right)^{\frac{1}{4}} e^{\frac{i}{\hbar} \bar{p} x} e^{-\frac{m\Omega}{2\hbar} (x - \langle x \rangle)^2}, \quad (22)$$

where Eq. (22) describes a quantum particle with mean-position $\langle x \rangle$, mean-momentum $\bar{p}$ and mean-energy $\langle E_{CS} \rangle = \langle \phi_{CS}|\hat{p}^2|\phi_{CS}\rangle/(2m) + \langle \phi_{CS}|V_{eff}(x)|\phi_{CS}\rangle$. When a phase hop is induced, $\langle E_{CS} \rangle$ changes according to Eq. (14) by

$$\Delta \langle E_{CS} \rangle = \sqrt{2\Omega} \langle x \rangle \langle \hat{p} \rangle \delta + m\Omega^2 \langle \phi_{CS}|\hat{x}^2|\phi_{CS}\rangle \delta^2, \quad (23)$$

where $\delta = \sin(\tau_{ph} + \Delta \varphi) - \sin(\tau_{ph})$. A classical particle with mean-position $\bar{x}$, mean-momentum $\bar{p}$ and mean-energy $\overline{E}_{class} = \bar{p}^2/(2m) + V_{eff}(\bar{x})$ would, in the case of the phase hop, change its mean-energy by $\Delta \overline{E}_{class} = \sqrt{2\Omega} \langle x \rangle \langle \hat{p} \rangle \delta + m\Omega^2 \langle \phi_{CS}|\hat{x}^2|\phi_{CS}\rangle \delta^2$ [24], which is the classical limit of Eq. (23) (since it is $\lim_{\hbar \rightarrow 0} \langle x \rangle = \bar{x}$, $\lim_{\hbar \rightarrow 0} \langle \hat{p} \rangle = \bar{p}$, $\lim_{\hbar \rightarrow 0} \langle \phi_{CS}|\hat{x}^2|\phi_{CS}\rangle = \lim_{\hbar \rightarrow 0} \langle \phi_{CS}|\hat{x}|\phi_{CS}\rangle^2 = \bar{x}^2$ and $\lim_{\hbar \rightarrow 0} \langle \phi_{CS}|\hat{p}^2|\phi_{CS}\rangle = \lim_{\hbar \rightarrow 0} \langle \phi_{CS}|\hat{p}|\phi_{CS}\rangle^2 = \bar{p}^2$). This demonstrates that the quantum mechanical results presented in this article are consistent with the classical results of Ref. [24]. In particular it shows that in the quantum regime as well as in the classical regime the particle’s mean-energy can in general be both increased and decreased by inducing a phase hop (cf. Eq. (14)).

[21] A more rigorous treatment shows that $F$ is an operator [10] which can be expanded in powers of $\omega^{-1}$. The leading-order term is the function considered here.
[22] This analogy only approximately holds for the particle’s real motion, since the particle’s micromotion is affected differently by a phase hop than by a collision: A phase hop induces a change of phase of the oscillating phase factor $e^{-i\Omega \tau}$ of $\psi$ and thus instantaneously changes the phase of the particle’s micromotion, whereas a collision does not.
[23] A stationary mean-motion state obeys the relation $\phi_n(x, t_{ph})^* \phi_n(x, t_{ph}) = \phi_n(x, t_{ph})^* \phi_n(x, t_{ph})$, because as an eigenstate of a time-independent Hamiltonian it can be written in the form $\phi_n(x, t) = \xi_n(t) \exp(-iE_n t/\hbar)$. Thus, one has $\phi_n(x, t) = \xi_n(t) \exp(-iE_n t/\hbar)$ and thus $\phi_n(x, t_{ph})^* \phi_n(x, t_{ph}) = \xi_n(t)^* \xi_n(t) \phi_n(x, t_{ph}) = \phi_n(x, t_{ph})^* \phi_n(x, t_{ph})$.
[26] In most experimental setups it is possible to generate such small timescales, although the period of the ROP is already very small.
[28] E. Kierig, U. Schnorrberger, A. Schietinger, J. Tomkovic,

