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Quantum Mechanics of Rectilinear Orbits of the Coulomb-Kepler Problem (II.)

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Abstract

As compared to the wave function ψ adopted previously (Adv. Stud. in Theor. Phys. Vol.11, 2017, p.365), the new ansatz for ψ fulfills now energy conservation rigorously with respect to a curve parameter $w \geq 0$. The symmetry of ψ implies that the mean position and mean velocity are parallel or anti-parallel, always. The model describes the scattering of a wave packet by the Coulomb potential over a finite time range, where in the mean only forward and back scattering is possible. The decisive point is to elaborate the definition interval of w as a time equivalent curve parameter. The mean initial position and velocity are built into ψ and form a two-dimensional parameter space P. As it turns out, within a subspace $A \subset P$, curve parameter w and time t are in 1-1 correspondence for all $t \geq 0$; moreover, one observes mean forward scattering when the mean initial velocity is directed towards the force center: the mean trajectory "tunnels" through the Coulomb singularity. On the other hand, in the parameter space complementary to A, the definition domain of the curve parameter is limited and ends before the singularity is reached, which means that forward or backscattering cannot be predicted by the given model where the time dependent Schrödinger equation is not generally solved.

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1 Introduction

This work is to supplement the previous article [20] on the quantum mechanics of rectilinear orbits. Essentially, energy conservation will be implemented rigorously, which liberates us from resorting to an asymptotic approximation. This means that we do not have any more restrictions on the magnitude parameter κ, which in the classical limit equals $2mX_0V_0/\hbar$; X_0 and V_0 denote the mean initial position and velocity, respectively, with X_0 taken from the force center. We can consider now also non-relativistic microscopic models for head-on collisions, in principle. By the definition of a rectilinear orbit, the mean initial vectors $\mathbf{x}_0$ and $\mathbf{v}_0$ are parallel or antiparallel which we describe by

$$\mathbf{x}_0 = X_0\{1,0,0\}, \quad \mathbf{v}_0 = \sigma V_0\{1,0,0\}, \quad \sigma = \pm 1, \quad X_0 > 0,\, V_0 > 0. \tag{1}$$

As in related studies on the quantum mechanics of the Coulomb-Kepler problem, see [8, 16, 17, 18, 20] the wave function lives, at first, in the four-dimensional Kustaanheimo-Stiefel space $\mathbf{u} \in \mathbf{R}^4$ [14], abbreviated KS,

$$\Psi_w = C\prod_{j=1}^{4} S_j, \quad S_j = \exp\left[a_j(w)u_j - \Gamma(w)u_j^2/2\right], \tag{2}$$

where S_j essentially is a coherent state of the reversed harmonic oscillator, [2, 7, 16, 19]; C denotes the normalization constant. The complex number a_j corresponds to the complex quantum number of a coherent state, often denoted by z. The parameter space $\mathbf{a}(0) \in \mathbf{C}^4$ is sufficient to implement the mean values of position and velocity, $\mathbf{x}_0$ and $\mathbf{v}_0$, at time $t = 0$ or $w = 0$; $w \geq 0$ is a curve parameter which describes the evolution of the mean rectilinear orbit. The connection between the KS and the ordinary three-dimensional configuration space is described by [6, 16]

$$\begin{array}{ll} u_1 = \sqrt{r}\cos(\theta/2)\cos(\varphi - \Phi); & u_2 = \sqrt{r}\cos(\theta/2)\sin(\varphi - \Phi); \\ u_3 = \sqrt{r}\sin(\theta/2)\cos(\Phi); & u_4 = \sqrt{r}\sin(\theta/2)\sin(\Phi), \end{array} \tag{3}$$

where

$$r > 0, \quad 0 < \theta < \pi, \quad 0 \leq \varphi < 2\pi, \quad \text{and} \quad 0 \leq \Phi < 2\pi; \tag{4}$$

the KS phase Φ describes the extension to the fourth dimension. Eventually, in physical 3D space, the wave function ψ_w is obtained by projecting out the phase Φ as

$$\psi_w = \int_0^{2\pi} \mathrm{d}\Phi\, \Psi_w(\Phi). \tag{5}$$

The curve parameter w is inherited from the time dependence of the basic coherent harmonic oscillator states. In the classical limit of elliptic orbits, w is the eccentric anomaly. The question is, how far into the quantum region

w remains a time-equivalent curve parameter. As a matter of fact, the study on quantum corrections to Kepler's equation [18] predicted a finite definition domain of w. Similarly, the asymptotically calculated mean rectilinear orbits [20] were defined over a finite interval only, which, in particular, did not cover the neighborhood of the Coulomb (gravitational) singularity. The motivation for the present paper was that, if energy conservation is taken into account rigorously, then the definition domain of w can be extended, possibly into the region where the potential is singular, a hope which came true partially.

Energy conservation with respect to the curve parameter w is a necessary requirement for the assumption that time t enters only via w. If it is fulfilled, then we can profit from the mean value relation $\mathrm{d}\langle x\rangle/\mathrm{d}t = \langle v_x\rangle$, or

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}w}\,\frac{\mathrm{d}w}{\mathrm{d}t} = \langle v_x\rangle, \tag{6}$$

which is an ordinary differential equation for $w(t)$. In order that w is a time equivalent curve parameter, the definition interval is determined by the monotonicity property $\mathrm{d}w/\mathrm{d}t > 0$, more precisely

$$w \in \{0,\, w_c\}, \quad w_c > 0, \quad \frac{\mathrm{d}w}{\mathrm{d}t} > 0, \quad \text{for } 0 \le w < w_c; \tag{7}$$

w_c is either the first zero or the first singular point of $\mathrm{d}w/\mathrm{d}t$.

Clearly, the mean value relation (6) is not equivalent to the time dependent Schrödinger equation. We have to concede that within the given model the strict fulfillment of energy conservation with respect to w in many cases still leads to a finite time interval where the orbits are well defined. This is in particular true if $\sigma = -1$, i.e., when the initial velocity is in the direction of the force singularity. An exceptional parameter region, the "funnel domain", is shown in Fig. 1. where the mean trajectories are defined without restriction on w and time t .

On the other hand, when the initial velocity points away from the force center, i.e., if $\sigma = +1$, and when simultaneously the mean initial energy is positive, then, as is rigorously proved in [24], the trajectories asymptotically escape to infinity, a property which appears to be physically evident.

We have pondered on alternatives to describe the time dependence. In [18], we briefly discussed selected literature on the time dependent Green function [22, 10, 11, 3, 4, 12, 13, 21]. As to our opinion, corresponding results are not feasible to analytically calculate mean values over finite rather than asymptotically large time spans.

As a further possible tool, we explicitly derive in Appendix A time dependent solutions of the transformed Hamiltonian in KS space, which produce, at first, the discrete energy eigenvalues of the hydrogen atom. The latter were also derived within the KS scheme e.g. in [5] and [8], however, without mentioning

the problem with the corresponding eigenfunctions which are not orthogonal to each other: The solutions for different principal quantum numbers n turn out to belong to different Hamiltonians of harmonic oscillator type, so we do not have the discrete spectrum in the usual sense. This situation is consistent with the fact that the eigenfunctions of the discrete energy eigenvalues of the hydrogen atom, though orthogonal, are, nevertheless, not complete.

Another possibility could be the direct numerical integration of the Schrödinger equation. The method, certainly, will not amount to a routine task, mainly due the presence of the Coulomb singularity. In [20] we mentioned that a regularized version [15] predicts an orbit which tunnels through the singularity rather than correctly describing backscattering. In addition, in the classical limit, the order of magnitudes differ extremely when the scales of a mean orbit and its quantum fluctuations are compared.

Main results are formulated in Section (V.) by the Statements (I.) and (II.), see subsection "Rigorous results", by Statement (III.) in subsection "Numerical Analysis", and by Statement (IV.) in subsection "Asymptotic approximation".

2 Mean values of position, velocity, and potential energy

In [20], these mean values were rigorously calculated, without asymptotic approximation. Thus, the results reported below are valid for all parameters

$$\kappa = 2mX_0V_0/\hbar\,[1+\mathcal{O}(1/\kappa)]\,. \tag{8}$$

A more precise definition of κ is given below. We use the abbreviations

$$\begin{aligned} \kappa_0 &= \gamma_0\sigma\sinh(2w), \quad \kappa_1 = \cosh(w)^2+\gamma_0^2\sinh(w)^2, \\ K &= \kappa/\kappa_1, \quad I_\kappa = I_0(\kappa)/I_1(\kappa), \quad \sigma=\pm1, \quad M = 2+K\kappa_0+\kappa\, I_\kappa, \end{aligned} \tag{9}$$

where I_n denotes the modified Bessel function of order n. As compared to [20], we have set the disposable number $\nu = 1$. From [20], we write down the mean values as follows (we make use of the property $K\kappa_1 = \kappa$):

$$\langle x\rangle = r_0\,\left[4\kappa_0+(3\kappa_1+2\kappa\kappa_0)I_\kappa+K\kappa_0^2+\kappa\kappa_1)\right]M^{-1}, \tag{10}$$

$$\langle v_x\rangle = (\hbar K\kappa)/(4mr_0\gamma_0)\left[2\gamma_0\sigma\cosh(2w)+I_\kappa(1+\gamma_0^2)\sinh(2w)\right]M^{-1}, \tag{11}$$

$$E_{pot} = \alpha\langle 1/r\rangle = (\alpha/r_0)KM^{-1}. \tag{12}$$

The parameter γ_0 is disposable for energy conservation.

At $w=0$, the mean initial value $X_0 = \langle x\rangle_{w=0}$ has to be implemented which amounts to fixing the parameter r_0. After the substitutions $w=0$ with $K=\kappa$, one gets from (10)

$$X_0 = r_0\,\frac{\kappa+3I_\kappa}{2+\kappa\, I_\kappa}, \quad \text{or} \quad r_0 = X_0\,\frac{2+\kappa\, I_\kappa}{\kappa+3I_\kappa}. \tag{13}$$

For large κ, since $I_\kappa = 1 + \mathcal{O}(1/\kappa)$, we get

$$r_0 = X_0(1 + \mathcal{O}(1/\kappa)) \tag{14}$$

Furthermore, the mean initial velocity component $V_0 = \sigma\langle v_x\rangle_{w=0}$ results from (11) as

$$V_0 = v_0\kappa^2(\kappa + 3I_\kappa)/(2 + \kappa I_\kappa)^2, \quad v_0 = \hbar/(2mX_0), \tag{15}$$

which allows for fixing the width parameter κ in terms of the initial data X_0 and V_0. For large κ, one obtains

$$V_0 = \frac{\hbar\kappa}{2mX_0}(1 + \mathcal{O}(1/\kappa)) \quad \text{or} \quad \kappa = \zeta(1 + \mathcal{O}(1/\zeta)), \quad \zeta = 2mV_0X_0/\hbar, \tag{16}$$

which is consistent with (8). As it is noticed, v_0 has the dimension of a velocity whereas ζ and κ are dimensionless.

3 Energy conservation

3.1 The overall energy

The mean kinetic energy, E_{kin}, is calculated in Appendix B. Whereas the mean value of a single component, $(m/2)\langle v_i^2\rangle$, could be simplified previously up to an integral expression and then evaluated approximately only [16, 20], the calculation of the full kinetic energy includes favorable compensations and allows for a compact expression. In the formulas to follow, the symbols F_j, $j = 0, 1, 2, 3$ denote factors which do not depend on the curve parameter w.

$$\begin{aligned} E_{kin} &= F_0N_w/D_w, \quad F_0 = hq^2\kappa^2\left[3 + \kappa I_\kappa\right]^2\left[16mX_0^2\gamma_0^2(\kappa + 2I_\kappa)^2\right]^{-1}, \\ N_w &= M_1(2 + \kappa I_\kappa) + 2\kappa\kappa_0, \quad M_1 = -1 + \gamma_0^2 + (1 + \gamma_0^2)\cosh(2w), \\ D_w &= \kappa_1(\kappa I_\kappa + 2) + \kappa\kappa_0. \end{aligned} \tag{17}$$

We add the potential energy according to (12). It is convenient to replace the coupling constant α by the dimensionless number δ as follows

$$\alpha = (\hbar^2\kappa^2)/(8mX_0)\,\delta, \tag{18}$$

which takes into account that the mean energy has the order of magnitude κ^2. After straightforward simplifications, we obtain

$$\begin{aligned} E &\equiv E_{kin} + E_{pot} = F_1E_{num}/E_{den}, \quad F_1 = \hbar^2/(16mX_0^2), \\ E_{num} &= \kappa^2(3 + I_\kappa\kappa)\left[M_1(6 + 5I_\kappa\kappa + I_\kappa^2\kappa^2) + 2\kappa(2I_\kappa\gamma_0^2\delta + \gamma_0^2\delta\kappa + \right. \\ &\quad \left. 3\kappa_0 + I_\kappa\kappa\kappa_0)\right], \quad E_{den} = \gamma_0^2(\kappa + 2I_\kappa)^2\left[(2 + \kappa I_\kappa)\kappa_1 + \kappa\kappa_0\right]. \end{aligned} \tag{19}$$

By setting $w = 0$, the mean initial energy results as

$$E_0 \equiv E(w=0) = 2F_1F_2\left(\kappa^2(3+\kappa I_\kappa)\right)\left[(\kappa+2I_\kappa)^2(2+\kappa I_\kappa)\right]^{-1}. \tag{20}$$

with

$$F_2 = 6 + \delta\kappa^2 + (5+2\delta)\kappa I_\kappa + \kappa^2 I_\kappa^2). \tag{21}$$

3.2 Condition for energy conservation

We require that the difference $\Delta E = E - E_0$ vanishes identically. With the help of the Mathematica [23] commands Factor[...] and Simplify[...], the following factorization is achieved:

$$\begin{aligned} \Delta E &= F_1F_3G_w/E_{den}, \\ F_3 &= -6 + \gamma_0^2(6+\delta\kappa^2) + \left[-5+\gamma_0^2(5+2\delta)\right]\kappa I_\kappa + (-1+\gamma_0^2)\kappa^2 I_\kappa^2, \\ G_w &= -2\kappa^2(3+\kappa I_\kappa)\left\{(1+\gamma_0^2)(\kappa I_\kappa+2)\sinh(w)^2 + \kappa\kappa_0\right\}. \end{aligned} \tag{22}$$

Obviously, $\Delta E = 0$, if $F_3 = 0$. Solving for γ_0^2, we find the following condition on γ_0, which guarantees energy conservation:

$$\gamma_0^2 = F_2^{-1}\,(2+\kappa I_\kappa)(3+\kappa I_\kappa). \tag{23}$$

Remarkably, γ_0^2 does not depend on the curve parameter w.

From (20), it is noticed that $E_0 = 0$, if $F_2 = 0$. Considering δ as the control parameter, the zero of F_2 is at

$$\delta_\kappa = -(2+\kappa I_\kappa)(3+\kappa I_\kappa)\left[\kappa(\kappa+2I_\kappa)\right]^{-1}. \tag{24}$$

The factor F_2, which depends linearly on δ, changes sign at $\delta = \delta_\kappa$. The parameter δ_κ separates, thus, positive and negative mean initial energies E_0, this means domains where unbounded and bounded mean orbits are expected. Consistent with this, γ_0^2 is positive and negative, respectively; in the latter case γ_0 is purely imaginary which implies that the curve parameter w has be analytically continued to a purely imaginary one, $w \to \tilde{w}$:

$$w = \mathbf{i}\,\tilde{w}. \tag{25}$$

Correspondingly, the hyperbolic functions which appear in the expressions of the mean values, change to trigonometric functions which are bounded as a function of $\tilde{w}$.

The function δ_κ is monotonically increasing with $\kappa > 0$ and covers the interval $-\infty < \delta_\kappa < -1$ with the limit $\delta_\infty = -1$, see dotted line of Fig. 1. Clearly, E_0 can vanish or become negative only for an attractive potential with the coupling constant $\alpha < 0$.

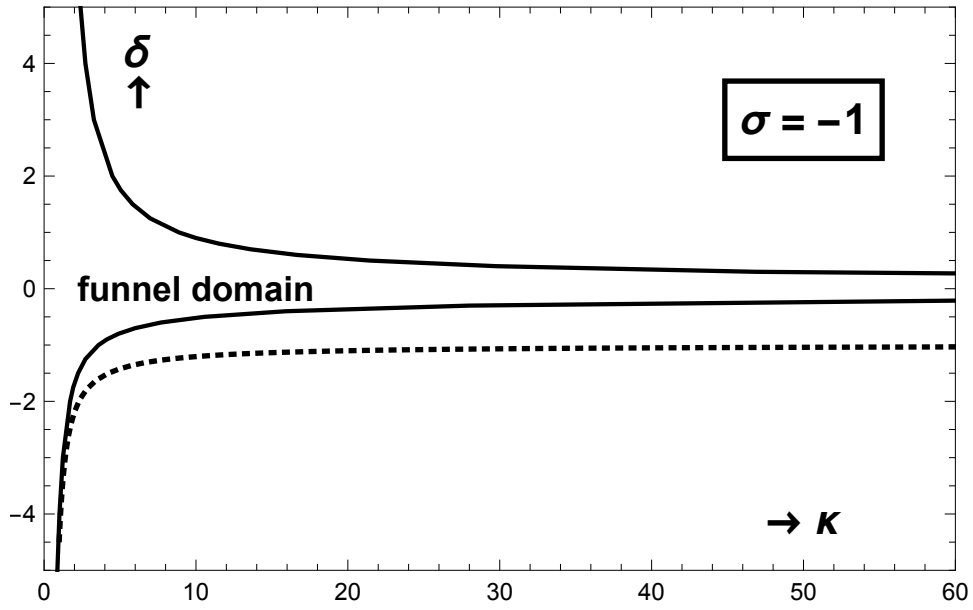

Figure 1: Domains of bounded and unbounded trajectories, below and above the dotted line, respectively. Within the "funnel domain" which has the shape of a lying funnel, the curve parameter w is in 1-1 correspondence with time t for $t \geq 0$, without restriction. In the complementary domain, w has a limited definition interval and, thus, limits the applicability of the wave function used in the given work. Note that the figure refers to the case $\sigma = -1$ where the mean initial velocity points toward the force center. If the mean initial values X_0 and V_0 are varied independently, then κ and δ are independent parameters.

To finish this subsection, we connect δ to the mean values of the initial energy. From (12) and (17), one derives

$$D(\kappa) \equiv E^{(0)}_{pot}/E^{(0)}_{kin} = \delta/|\delta_\kappa| \quad \text{or} \quad \delta = |\delta_\kappa| D(\kappa). \tag{26}$$

As a check, if $E_0 = 0$, then $E^{(0)}_{pot} = -E^{(0)}_{kin}$ which implies $D(\kappa) = -1$ and, thus, $\delta = -|\delta_\kappa| = \delta_\kappa$.

3.3 The energy constant E_0

In the limit $\kappa \to \infty$, the mean initial energy E_0, given in (20), attains the classical form of the total initial energy

$$E_0 \to (1/2)mV_0^2 + \alpha/X_0. \tag{27}$$

To see this, we use the property that $\lim_{\kappa\to\infty} I_\kappa = 1$ and obtain

$$E_0 \to 2F_1\kappa^2(1+\delta)(1+\mathcal{O}(1/\kappa)). \tag{28}$$

With the aid of the asymptotic relation $\hbar\kappa = 2mX_0V_0$, see (16), and in view of (18), we can express δ as follows:

$$\delta = (\alpha/X_0) \,/\, \big(V_0^2 m/2\big) \equiv \Big(E^{(0)}_{pot}/E^{(0)}_{kin}\Big)_{asymp}, \tag{29}$$

which, with $2F_1\kappa^2 \equiv \hbar^2\kappa^2/(8mX_0^2) = (m/2)V_0^2$, leads to the result (27).

It should be noted that, due to the independence of the initial values X_0 and V_0, the parameters δ and κ are independent variables. By (15) and (16), $\kappa = \kappa(\zeta)$ is a monotonous function of $\zeta = 2mX_0V_0/\hbar$, whereas, by the definition (18), $\delta = 2\alpha/(mX_0V_0^2) \equiv 4\alpha/(\zeta\, V_0)$. The functional determinant is

$$\det\left(\frac{\partial(\delta,\kappa)}{\partial(X_0,V_0)}\right) = \frac{4\alpha}{\hbar X_0V_0^2}\,\frac{\mathrm{d}\kappa}{\mathrm{d}\zeta} \neq 0. \tag{30}$$

4 Time dependence

For the given Hamiltonian, the commutator relation $\mathrm{d}x/(\mathrm{d}t) \equiv (\mathbf{i}\,/\hbar)[H,x] = p_x/m = v_x$ implies the necessary condition

$$\mathrm{d}\langle x\rangle/(\mathrm{d}t) = \langle v_x\rangle, \tag{31}$$

which holds true for any initial state which evolves by the operator $\exp[-\mathbf{i}\,Ht/\hbar]$. As a consequence of (31), one obtains the following first order differential equation for $w(t)$:

$$\partial_t w \;\equiv F(w) = \langle v_x\rangle/(\partial_w\,\langle x\rangle). \tag{32}$$

In order that w and t are in 1-1 relation, we require that

$$\partial_t w > 0 \quad \text{for} \quad w \in (0,\, w_c), \quad w_c > 0. \tag{33}$$

The critical interval limit, w_c, is determined by the property that $\partial_t w$ changes sign or gets singular the first time for $w > 0$

Let us heuristically discuss the case of positive initial energy, $E_0 > 0$, and $\sigma = -1$ where the mass point initially moves towards the Coulomb singularity. If the mean (rectilinear) trajectory overcomes the singularity and escapes asymptotically to arbitrary negative values $\langle X\rangle$, then both $\partial_w\langle X\rangle < 0$ and $\langle V_x\rangle < 0$, throughout, with the consequence that, by the definition (32), $F(w) > 0$ for $w > 0$. In this case, w would be a well defined time equivalent in the infinite interval $w \geq 0$. As another scenario, the mean value $\langle X\rangle$ decreases to a minimum value at $w = w_x$, which, classically, would imply sign inversion of the velocity component. If sign inversion of $\langle V_x\rangle$ simultaneously occurs at the extremum of $\langle X\rangle$, at the curve parameter w_x, then $\partial_t w > 0$ in the neighborhood of w_x and the definition domain of w covers the backscattering process. However, as it will turn out, the minimum position w_x differs,

in general, from the instant w_v where sign reversion of $\langle V_x\rangle$ is observed. For a classical rectilinear trajectory, on the other hand, $w_x = w_v$ always. In quantum mechanics where we are dealing with mean values rather than with a sharp trajectory, the two inversion points do not coincide, in general.

In the given model, when $w_x \neq w_v$, then the definition domain of the curve parameter is limited either by $w_c = w_x$ or by $w_c = w_v$, depending on which value comes first. The decisive point for the limitation of the present model are the quantum fluctuations of the orbit which prevent, in general, that the inversion points of position and velocity coincide as in the classical case.

5 Analysis of mean orbits

5.1 Rigorous results

For positive mean values of the energy, $E_0 > 0$, the mean values of an orbit $\{\langle x\rangle, \langle v_x\rangle\}$, are stated in (10) and (11). We prefer using the dimensionless magnitudes X and V_x, instead, as follows

$$\langle X\rangle = \langle x\rangle/r_0, \quad \langle V_x\rangle = \langle v_x\rangle(4mr_0)/(\hbar\kappa), \tag{34}$$

to write

$$\begin{aligned} \langle X\rangle &= \left[4\kappa_0 + K\kappa_0^2 + \kappa\kappa_1 + (3\kappa_1 + 2\kappa\kappa_0)I_\kappa\right] M^{-1}, & (35)\\ \langle V_x\rangle &= K\,\left[2\gamma_0\sigma\cosh(2w) + (1+\gamma_0^2)\sinh(2w)\,I_\kappa\right][\gamma_0 M]^{-1}, & (36)\end{aligned}$$

where the functions κ_0, κ_1, K, M are defined in (9).

If $E_0 < 0$, then the formulas for the mean orbit are obtained by means of the analytical continuation

$$w \to \mathbf{i}\,\tilde{w}, \quad \gamma_0 \to -\mathbf{i}\,\tilde{\gamma}_0, \quad \tilde{\gamma}_0 > 0,\ \tilde{w} \geq 0, \tag{37}$$

which implies the replacements

$$\begin{aligned} \kappa_0 &\to \tilde{\kappa}_0 = \tilde{\gamma}_0\sigma\,\sin(2\tilde{w}), \quad K \to \tilde{K} = \kappa/[\cos(\tilde{w})^2 + \tilde{\gamma}_0^2\sin(\tilde{w})^2],\\ \kappa_1 &\to \tilde{\kappa}_1 = \kappa/\tilde{K}, \quad M \to \tilde{M} = 2 + \kappa I_\kappa + \tilde{K}\tilde{\kappa}_0, \end{aligned} \tag{38}$$

and gives rise to

$$\begin{aligned} \langle\tilde{X}\rangle &= \left[4\tilde{\kappa}_0 + \tilde{K}\tilde{\kappa}_0^2 + \kappa\tilde{\kappa}_1 + (3\tilde{\kappa}_1 + 2\kappa\tilde{\kappa}_0)I_\kappa\right]\tilde{M}^{-1}, & (39)\\ \langle\tilde{V}_x\rangle &= \tilde{K}\,\left[2\tilde{\gamma}_0\sigma\cos(2\tilde{w}) + (\tilde{\gamma}_0^2 - 1)\sin(2\tilde{w})\,I_\kappa\right]\left[\tilde{\gamma}_0\tilde{M}\right]^{-1}. & (40)\end{aligned}$$

We have the following two rigorous properties:

Statement (I.) For any finite value of the curve parameter $w \geq 0$, the orbits are finite. This is true for both values $\sigma = \pm 1$ and all mean values of the initial energy $-\infty < E_0 < \infty$.

Statement (II.) If the initial velocity is positive ($\sigma = +1$) and the initial energy $E_0 > 0$, then the curve parameter w is in 1-1 correspondence with time t for all $w \geq 0$.

Property (I.) appears to be in contradiction to the classical limit $\kappa \to \infty$ for $\sigma = -1$, where according to Eq.(42) of [20], the mean velocity becomes infinite at the instant of backscattering. However, we meet a finite definition interval of $w \in (0, w_c)$ for most values of the control parameters κ and δ: the definition domain then ends before back scattering takes place.

To prove (I.), one first verifies that the numerators of the mean coordinates are bounded in any closed interval of $w, \tilde{w}, \kappa, \delta$. So, the main task consists in showing that the denominators $M(w)$ and $\tilde{M}(\tilde{w})$ cannot vanish. The proofs are given in Appendix C.

Property (II.) is physically obvious. The mean coordinate $\langle X \rangle$ increases away from the force center to escape to infinity. As a consequence, $\partial_w \langle X \rangle > 0$ together with $\langle V_x \rangle > 0$, and, thus, by (32) $\partial_t w > 0$. However intuitive this may appear, to be true, w has to be a proper time parameter with $\partial_t w > 0$ for all $w > 0$. By (36), the mean velocity component, $\langle v_x \rangle$, is positively definite for $\sigma = +1$ and, therefore, does not change its sign. The remaining proof that in addition $\partial_w \langle x \rangle > 0$, is recorded in [24].

5.2 Numerical evaluations

This subsection deals with the numerical elaboration of the funnel domain of Fig. 1. In the corresponding parameter space with $\delta \in \mathbf{R}$, $\kappa \geq 0$, and $\sigma = -1$, the definition domain of the curve parameter is infinite with $w \geq 0$. Outside the domain, however, w is a faithful time equivalent in a finite interval only. This means, the wave function adopted fails to describe the full time evolution. In other words, the assumption, that the time evolution exclusively is through $w = w(t)$, cannot be maintained outside the funnel domain. We remind that for $\sigma = +1$, when the mean initial velocity points away from the force center, and if $E_0 > 0$, then the curve parameter w has an infinite definition domain.

In the case $\sigma = -1$, the funnel domain is relatively broad for small values of κ, where the wave packet is relatively extended, so the Coulomb singularity has a comparatively weak effect. With increasing κ, the funnel gets narrower, and its width shrinks to zero proportional to $1/\kappa^\mu$ with $\mu \approx 1/4$. As a consequence, if $\sigma = -1$, then, in order to get to the classical limit $\kappa \to \infty$, the only safe path is along the line $\delta = 0$, which by (26) corresponds either to an infinitely large kinetic initial energy or the potential free case with $\alpha = 0$.

We have the following numerically established property:

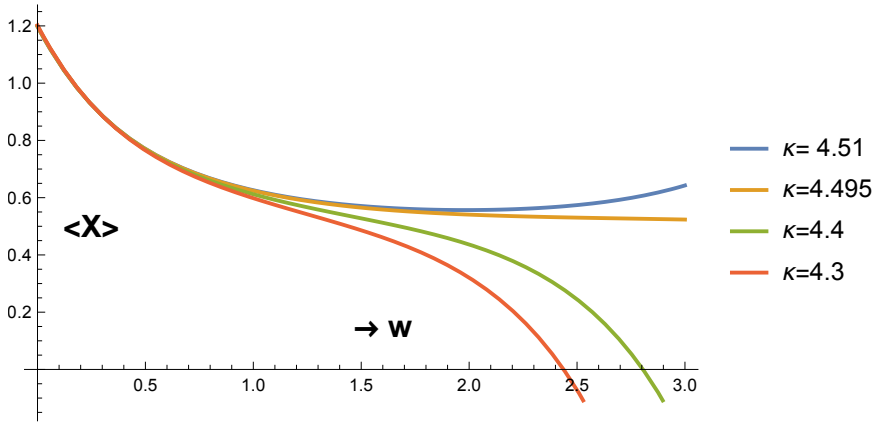

Figure 2: Illustration of the graphical analysis adopted to generate the funnel domain of Fig.1. The parameters are $\delta = 2$ (positive energy), $\sigma = -1$, and four values of κ. For the lowest two κ values, the curves of $\langle X\rangle(w)$ have no minimum and move with increasing curve parameter w to minus infinity, whereas the mean velocity component $\langle V_x\rangle$ turns out (not shown) to stay negative for all four values of κ. At $\kappa = 4.495$, the X curve is just before bending upwards. At $\kappa = 4.51$, the existence of a minimum is manifest.

Statement (III.) For parameters within the funnel domain, the mean orbits are not backscattered by the singularity, but rather go through and eventually escape to $\langle X\rangle$ = minus infinity.

The contours of the funnel domain were produced from a set of discrete data points $(\delta_j,\, \kappa_j)$, $j = 1, \ldots, 58$, which were joined by the plot program used. Each point was inferred graphically by plotting a family of curves of $\langle X\rangle$ as a function of w, as is illustrated in Fig. 2. If $\langle X\rangle$ has a minimum, then by (34), $\partial_t w$ becomes singular. Furthermore, the first zero of $\langle V_x\rangle$, at $w = w_v$, causes $\partial_t w = 0$ and limits the definition domain of w; unless both w positions coincide, which, however, appears remote. In the next subsection, we show analytically that for large κ the minimum of $\langle X\rangle$ and the zero of $\langle V_x\rangle$ are at different w points.

5.3 Asymptotic approximation for $\sigma = -1$

In the following, it is shown that for sufficiently large κ the definition domain of the curve parameter w is finite. To this end, the minimum position $w = w_X$ of $\langle X\rangle$ is determined together with the first zero position $w = w_V$ of $\langle V_x\rangle$. Asymptotically in κ, both values are finite with $w_X \neq w_V$. As a consequence, $w_c = \mathrm{Min}(w_X, w_V)$, and w is a faithful time parameter in the finite interval $w \in (0,\, w_c)$.

It is convenient to replace the constant δ by the real parameters λ or $\tilde{\lambda}$, as

follows:

$$\lambda = 1/\sqrt{1+\delta}, \quad \text{if} \quad \delta > -1 \quad \text{and} \quad \lambda = -\mathbf{i}\,\tilde{\lambda}, \quad \text{if} \quad \delta < -1. \tag{41}$$

We have to pay attention to the different signs of the potential. We remind that $\delta < 0$ for an attractive potential, and $\delta > 0$ for a repellent one. Accordingly,

$$E_0 > 0: \quad 0 \le \lambda < 1 \quad \text{if} \quad \delta > 0 \quad \text{and} \quad \lambda > 1 \quad \text{if} \quad -1 < \delta < 0, \tag{42}$$

$$E_0 < 0: \quad \tilde{\lambda} > 0 \quad \text{with} \quad \delta < -1. \tag{43}$$

As mentioned above, the line $\delta = 0$, or equivalently $\lambda = 1$, is contained in the funnel domain where the definition domain of w is infinite. As a matter of fact, the asymptotic formulas to follow become singular at $\lambda = 1$. Therefore, we keep us sufficiently far away from this singular point, which means that we exclude mean values of the initial energy, where by (26) the kinetic part is much larger than the absolute magnitude of the potential part.

The asymptotic expressions are obtained by means of Taylor expansion with respect to $\epsilon \equiv 1/\kappa$ near $\epsilon = 0$. They are obtained in an analytical form with the aid of Mathematica [23].

5.3.1 $E_0 > 0$

We confine ourself, exemplarily, to the case $\lambda > 1$, where the mean initial energy, E_0, is positive and the potential is attractive. The minimum position of $\langle X \rangle$ and the zero position of $\langle V_x \rangle$ attain the following asymptotic forms

$$w_X = w_X^{(0)} + w_X^{(1)}\epsilon + \mathcal{O}(\epsilon^2), \quad w_V = w_V^{(0)} + w_V^{(1)}\epsilon + \mathcal{O}(\epsilon^2), \quad \epsilon = 1/\kappa. \tag{44}$$

One finds straightforwardly for $\lambda > 1$, $E_0 > 0$, and $\sigma = -1$

$$\begin{aligned} w_X^{(0)} &= \tanh^{-1}(1/\lambda), \quad w_X^{(1)} = \lambda\frac{61 - 77\lambda^2 + 46\lambda^4}{46(\lambda^2-1)^2}, \\ w_V^{(0)} &= \tanh^{-1}(1/\lambda), \quad w_V^{(1)} = \lambda\frac{3 - 3\lambda^2 + 2\lambda^4}{2(\lambda^2-1)^2}. \end{aligned} \tag{45}$$

The leading part, $w_X^{(0)} = w_V^{(0)} = \tanh^{-1}(1/\lambda)$, agrees with the results in [20] for the classical limit, see there Eqs.(35), (42), and (53).

We ask for the value of the curve parameter w, where $\partial_t w$ changes sign, or becomes singular, the first time. If λ is sufficiently far away from the value 1 and if $\epsilon \equiv 1/\kappa$ is sufficiently small, then

$$w_X - w_V = -(4/23)\lambda(1+\lambda^2)/(\lambda^2-1)^2\,\epsilon + \mathcal{O}(\epsilon^2), \quad \lambda > 1. \tag{46}$$

This means that asymptotically $w_X < w_V$, so the definition domain of w is limited by w_X. As a consequence, we have the following:

Statement (IV.): For negative initial velocity with $\sigma = -1$ and positive energy, $E_0 > 0$ with $\lambda > 1$, $\partial_t w$ asymptotically becomes singular at the minimum $w = w_X$ of $\langle X \rangle$. For small $\epsilon \equiv 1/\kappa$, the minimum is near $w_X = \tanh^{-1}(1/\lambda) + \mathcal{O}(\epsilon)$ provided λ is sufficiently far away from the value 1.

For illustration of a macroscopic example, see Fig. 3. As a technical remark, the task for Mathematica to analytically calculate the Taylor expansions of the mean values was subdivided by considering numerator and denominator of the mean values separately; each part was expanded up to order two in ϵ, before the quotient was expanded to the same order, and the following approximation of the Bessel function quotient I_κ was used:

$$I_\kappa^{(2)} = 1 - 1/(2\kappa) - 1/(8\kappa^2). \tag{47}$$

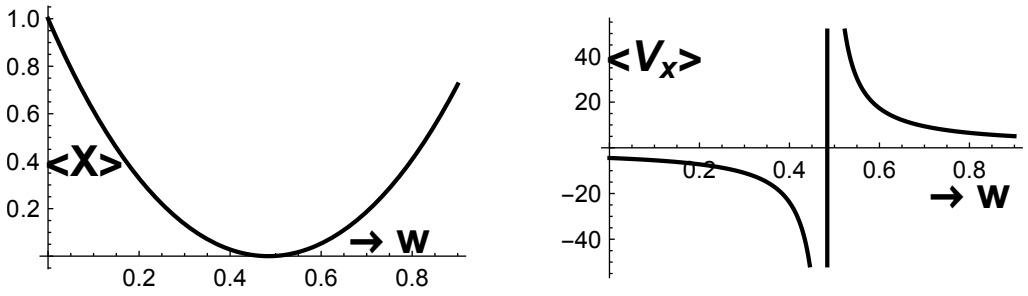

Figure 3: Macroscopic example with orbiter mass $m = 1000\,kg$, central mass $M = 6\times10^{24}kg$, $X_0 = 4\times10^7 m$, $V_0 = 5000\,m/s$ which gives rise to $\kappa = 4\times10^{48}$ and $\lambda = 2.2247$. The minimum of $\langle X \rangle$ is near $w_X \approx \tanh^{-1}(1/\lambda) \approx 0.48407....$ By the asymptotic theory, the sign change of $\langle V_x \rangle$ occurs at $w_V = w_X + 3.7 \times 10^{-50}$, which is later in a principal mathematical sense. At $w = w_V$ the slope of $\langle V_x \rangle$ is steep but, by statement (I.), not singular; so there exists a zero near $w_V \approx \tanh^{-1}(1/\lambda) \approx 0.48407$.

5.3.2 Negative energy

As it turns out, the first minimum position $\tilde{w}_x$ of $\langle \tilde{X} \rangle$, and zero position $\tilde{w}_v$ of $\langle \tilde{V}_x \rangle$, can simply be obtained from (45) by means of the analytical continuation (37) and (41). We find for $\sigma = -1,\ \tilde{\lambda} > 0$

$$\tilde{w}_x^{(0)} = \tilde{w}_v^{(0)} = \arctan(1/\tilde{\lambda}), \quad \tilde{w}_x^{(1)} = -\tilde{\lambda}\frac{61 + 77\tilde{\lambda}^2 + 46\tilde{\lambda}^4}{46(1+\tilde{\lambda}^2)^2},$$
$$\tilde{w}_v^{(1)} = -\tilde{\lambda}\frac{3 + 3\tilde{\lambda}^2 + 2\tilde{\lambda}^4}{2(1+\tilde{\lambda}^2)^2}; \quad \tilde{w}_x - \tilde{w}_v = \epsilon\frac{4\tilde{\lambda}(1-\tilde{\lambda}^2)}{23(\tilde{\lambda}^2+1)^2} + \mathcal{O}(\epsilon^2). \tag{48}$$

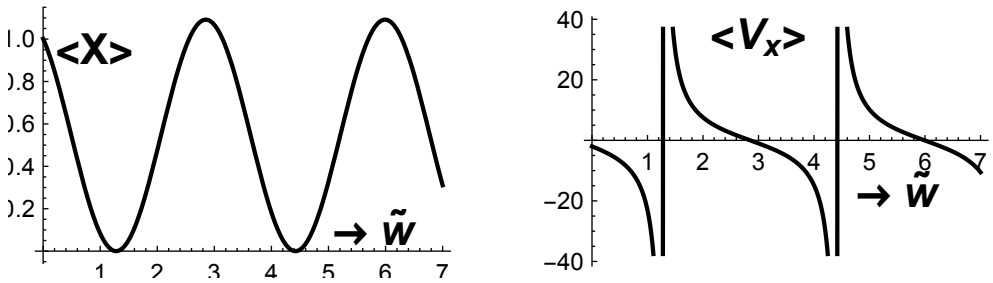

Figure 4: Illustration of the case of negative mean energy, $E_0 < 0$, and negative mean initial velocity ($\sigma = -1$). The parameters are $\kappa = 1000$ and $\delta = -12$ with $\tilde{\lambda} = 0.301511$. Formerly, the mean values are periodic with respect to the curve parameter $\tilde{w}$, but the definition domain is limited by the first zero of $\langle V_x \rangle$ which is close to the first minimum of $\langle X \rangle$ at $w_c \approx 1.27795$. The slopes of $\langle V_x \rangle$ near the points of sign inversion are steep, but not infinite.

The crucial point is that the two positions differ and give rise to either $\partial_t w = \infty$ or $\partial_t w = 0$ at finite values close to $w = \arctan(1/\tilde{\lambda})$. From (48), we formulate the following:

Statement (V.): If $0 < \tilde{\lambda} < 1$, then the definition interval of the curve parameter $\tilde{w}$ is limited by $w_c = \tilde{w}_v$, the first zero of $\langle V_x \rangle$. Else, if $\tilde{\lambda} > 1$, then $w_c = \tilde{w}_x$, the first minimum position of $\langle X \rangle$. The interval is finite with $w_c = \arctan(1/\tilde{\lambda}) + \mathcal{O}(\epsilon)$.

6 Conclusions

With the wave function adopted, the rectilinear trajectory of a wave packet is described by means of a curve parameter w. Within the "funnel domain" of Fig. 1, the curve parameter is in 1-1 correspondence with time t without restriction. In particular, in the case of a head-on collision with positive initial energy, the trajectory tunnels through the Coulomb singularity; there is no backscattering. Outside the funnel domain, in the case of a head-on configuration, the curve parameter w has a limited definition range which does not allow to predict forward or backscattering. The two-dimensional parameter space is formed by the mean initial position $\langle X_0 \rangle$ and the the mean initial velocity $\langle V_0 \rangle$, which are generally built into the wave function.

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A Special solutions of the Schrödinger equation in KS space

The transformed time dependent Schrödinger equation reads (for the stationary version, see, e.g., [5, 8])

$$-\frac{\hbar}{\mathbf{i}}\frac{\partial}{\partial t}\psi = H\psi, \quad H = \frac{1}{u^2}\left[-\frac{\hbar^2}{8\mu}\Delta_u + \alpha\right], \quad u^2 = u_1^2 + u_2^2 + u_3^2 + u_4^2, \quad \text{(A1)}$$

where Δ_u denotes the 4D Laplacian. For a dimensionless form, we introduce the dimensionless variables ζ_j for u_j, τ for t, and β for α:

$$\zeta_j = \frac{u_j}{\sqrt{\xi_0}}, \quad \xi_0 = \frac{1}{\Gamma_0}; \quad \tau = \frac{t}{T_0}, \quad T_0 = \frac{8\mu}{\hbar\Gamma_0^2}; \quad \beta = \frac{\alpha}{r_0 E_0} \quad E_0 = \frac{\hbar^2\Gamma_0}{8\mu r_0}; \quad \text{(A2)}$$

and obtain

$$\mathbf{i}\,\frac{\partial}{\partial\tau}(\zeta^2\psi) = \left[-\sum_{j=1}^{4}\frac{\partial^2}{\partial\zeta_j^2} + \beta\right]\psi, \quad \zeta^2 = \sum_{j=1}^{4}\zeta_j^2. \quad \text{(A3)}$$

Let us first consider the one-dimensional case, with $\zeta_1 \to \zeta$,

$$\mathbf{i}\,\frac{\partial}{\partial\tau}(\zeta^2\psi) = \left[-\frac{\partial^2}{\partial\zeta^2} + \beta\right]\psi \quad \text{(A4)}$$

and try to solve it by means of the separation ansatz

$$\psi = F(\tau)\,G(\zeta). \quad \text{(A5)}$$

We divide the equation by $F(\tau)$ to obtain

$$+\mathbf{i}\,\frac{F'(\tau)}{F(\tau)}\,\zeta^2 G = \left[-\frac{\partial^2}{\partial\zeta^2} + \beta\right]G(\zeta). \quad \text{(A6)}$$

Since the right hand side is a function of ζ only, the F part must be a constant:

$$\mathbf{i}\,F'(\tau)/F(\tau) = A = const. \quad \text{or} \quad F(\tau) = F(0)\exp[-\mathbf{i}\,A\,\tau]. \quad \text{(A7)}$$

So we have to solve the differential equation

$$0 = \left[-A\,\zeta^2 - \frac{\partial^2}{\partial\zeta^2} + \beta\right]G(\zeta). \quad \text{(A8)}$$

The general solutions of (A8) are parabolic cylinder functions, which generally are not normalizable, see sections 9.24 - 9.25 in [9], except for the eigenfunctions of the harmonic oscillator. In order to obtain such solutions, we scale

$\zeta \to \xi$ with $\zeta = s\,\xi$ and choose the constants A and s such that we get the dimensionless eigenvalue equation of the harmonic oscillator

$$\left[-\frac{\partial^2}{\partial\xi^2} + \xi^2 - (2n+1)\right]\tilde{G}(\xi) = 0, \quad n = 0, 1, 2, \ldots . \tag{A9}$$

To achieve the above equation, we have to stipulate

$$A < 0; \quad \beta < 0; \qquad s^2 = (-A)^{-1/2}; \quad s^2 = -(1+2n)/\beta. \tag{A10}$$

Since $\beta < 0$, our separation ansatz is possible only for an attractive potential. By (A10), the constants s and A become n dependent:

$$s \to s_n = \sqrt{(2n+1)/(-\beta)}, \quad A \to A_n = A_n = -\beta^2/(1+2n)^2. \tag{A11}$$

The normalizable solution of (A9) is given in terms of the n-th order Hermite polynomial $(He)_n$

$$G_n(\xi) = C(He)_n(\xi)\exp[-\xi^2/2], \tag{A12}$$

where C is a normalization constant.

Now comes the crucial point: the coordinate ξ is actually n-dependent and with it the Hamiltonian in (A9):

$$\xi = \zeta/s_n, \quad H(\xi)\tilde{G}(\xi) = (2n+1)\tilde{G(\xi)} \quad \to \quad H_n G(\zeta) = (2n+1)G(\zeta) \tag{A13}$$

with

$$H_n = -s_n^2\frac{\partial^2}{\partial\zeta^2} + \frac{1}{s_n^2}\zeta^2. \tag{A14}$$

Simultaneously, in the original ζ space the eigenfunctions read

$$G_n(\zeta) = C_n(He)_n(\zeta/s_n))\exp[-\zeta^2/(2s_n^2)], \tag{A15}$$

which implies that eigenfunctions belonging to different quantum numbers n and n' are not any more orthogonal. Moreover, we cannot speak of the spectrum of a Hamiltonian; rather, we have a family of Hamiltonians.

The extension to four dimension is readily obtained. Instead of (A8), one has to consider

$$0 = \left[-\sum_{j=1}^{4}\left(A\,\zeta_j^2 - \frac{\partial^2}{\partial\zeta_j^2}\right) + \beta\right] G(\zeta_1, \zeta_2, \zeta_3, \zeta_4) \tag{A16}$$

With the separation ansatz $G = \prod_{j=1}^{4} G_j(\zeta_j)$, one finds after division by G

$$0 = \sum_{j=1}^{4} Z_j + \beta, \quad Z_j = \frac{1}{G_j}\left[-A\,\zeta_j^2 - \frac{\partial^2}{\partial\zeta_j^2}\right] G_j. \tag{A17}$$

Since Z_j must be constant, we get for each j the previous differential equation (A8), and to obtain eigenfunctions of the harmonic oscillator, we introduce once more the scaling $\zeta_j = s\,\xi_j$ (with s independ of j),

$$s^2 Z_j = 2n_j + 1, \quad n_j = 0, 1, 2, \ldots, \quad A = -1/s^4. \tag{A18}$$

The constraint $\sum_{j=1}^{4} Z_j + \beta = 0$ leads to

$$s^2 = (-1/\beta)\sum_{j=1}^{4}(2n_j+1) = (-2/\beta)(n+2), \quad n = n_1 + ...n_4, \quad n_j = 0, 1, 2, \ldots. \tag{A19}$$

For A, which up to a constant is an eigenvalue of the KS Hamiltonian, we get

$$A \to A_{\mathbf{n}} = -(1/4)\frac{\beta^2}{(n+2)^2}, \quad \mathbf{n} = \{n_1, n_2, n_3, n_4\}. \tag{A20}$$

As it turns out, the projection of the KS space into the physical space allows for even numbers n_j only; so with $n_j = 2k_j$, $k_j = 0, 1, 2, \ldots$ and abbreviating $k := k_1 + k_2 + k_3 + k_4$, we arrive at

$$A_{\mathbf{k}} = -(1/16)\beta^2/(k+1)^2, \quad k = 0, 1, 2, .., \tag{A21}$$

which somehow miraculously coincides with the discrete spectrum of the hydrogen atom with respect to the principal quantum number $N = k + 1$, $N = 1, 2, ...$ Once more, different quantum numbers k belong to different Hamiltonians.

B Mean kinetic energy

According to [17], the velocity observables in $\mathbf{u}$ space read

$$v_j = \hbar/(\mathbf{i}\,m)\,D_j, \quad j = x, y, z, \tag{B1}$$

with

$$\begin{aligned} D_x &= (1/(2u^2))\left[u_3\partial_{u_1} - u_4\partial_{u_2} + u_1\partial_{u_3} - u_2\partial_{u_4}\right], \\ D_y &= (1/(2u^2))\left[u_4\partial_{u_1} + u_3\partial_{u_2} + u_2\partial_{u_3} + u_1\partial_{u_4}\right], \\ D_z &= (1/(2u^2))\left[u_1\partial_{u_1} + u_2\partial_{u_2} - u_3\partial_{u_3} - u_4\partial_{u_4}\right]. \end{aligned} \tag{B2}$$

In calculating the mean value $\langle v_i^2\rangle$, we shift one operator to the left hand wave function which produces a minus sign:

$$\begin{aligned} \langle v_i^2\rangle &= (F/2)\int_0^{2\pi} \mathrm{d}\phi \int \mathrm{d}u_1 \ldots \mathrm{d}u_4 (8u^2)\left[D_i\psi^*\right]\left[D_i\psi\right] \\ &= F\int_0^{2\pi} \mathrm{d}\phi \int (1/u^2)\,\mathrm{d}u_1 \ldots \mathrm{d}u_4 Q_i \exp\left[\mathbf{A}\cdot\mathbf{u} - \Gamma_R u^2\right] \\ F &= 2\hbar^2 C^2/m^2, \end{aligned} \tag{B3}$$

In view of (B3), the kinetic energy reads, with $Q = Q_x + Q_y + Q_z$,

$$E_{kin} = (mF/2) \int_0^{2\pi} \mathrm{d}\phi \int \mathrm{d}u_1 \ldots \mathrm{d}u_4 \left[Q/u^2\right] \exp\left[\mathbf{A}\cdot\mathbf{u} - \Gamma_R u^2\right], \qquad \text{(B4)}$$

After some ordering efforts, the following form of Q is achieved

$$\begin{aligned}
Q/u^2 &= \left[q_0/u^2 + q_1 + q_2 u^2\right], \quad u^2 = u_1^2 + u_2^2 + u_3^2 + u_4^2, \\
q_0 &= -(a_2u_1 - a_1u_2 - a_4u_3 + a_3u_4)(a_2^*u_1 - a_1^*u_2 - a_4^*u_3 + a_3^*u_4), \\
q_1 &= a_1a_1^* + a_2a_2^* + a_3a_3^* + a_4a_4^* - \\
&\quad \Gamma_R\left[(a_1 + a_1^*)u_1 + (a2 + a_2^*)u_2 + (a_3 + a_3^*)u_3 + (a_4 + a_4^*)u_4\right] + \\
&\quad \mathbf{i}\,\Gamma_I\left[(a_1 - a_1^*)u_1 + (a_2 - a_2^*)u_2 + (a_3 - a_3^*)u_3 + (a_4 - a_4^*)u_4\right], \\
q_2 &= \Gamma_R^2 + \Gamma_I^2. \qquad \text{(B5)}
\end{aligned}$$

The factors $1/u^2$ and u^2 in (Q/u^2) are taken care by means of parameter integration and differentiation, respectively. To this end, the parameter Γ_R in the exponent of the integrand is replaced by the variable g:

$$E_{kin} = (mF/2) \int_0^{2\pi} \mathrm{d}\phi \left[q_0 \int_{\Gamma_R}^{\infty} \mathrm{d}g \; + q_1 + q_2\partial_g\right] I_A(g) \qquad \text{(B6)}$$

The polynomials q_i are expanded and each factor u_k generated by differentiation with respect to A_k. Then, the u-integrals are carried out which leads to the generating function I_A:

$$\begin{aligned}
I_A(g) &\equiv \int \mathrm{d}u_1 \ldots \mathrm{d}u_4 \exp\left[\mathbf{A}\cdot\mathbf{u} - g\,u^2\right] = (\pi^2/g^2)\exp\left[(\mathbf{A}\cdot\mathbf{A})/(4g)\right] \qquad \text{(B7a)} \\
&= (\pi^2/g^2)\exp\left[(r_0\Gamma_R^2/g)\,(\kappa_0 + \kappa_1\cos(\phi))\right] \qquad \text{(B7b)} \\
&= (\pi^2 s^2/\Gamma_R^2)\exp\left[sK\,(\kappa_0 + \kappa_1\cos(\phi))\right], \quad \phi = \Phi - \Phi', \qquad \text{(B7c)}
\end{aligned}$$

where in (B7c) we substituted $g = \Gamma_R/s$. The differential operators $q_i(\{\partial_{A_k}\})$ are applied to I_A, in the form (B7a).

We will use the following relations, see [20]:

$$\begin{aligned}
f(w) &= \cosh(w) - \mathbf{i}\,\gamma_0\sinh(w), \quad K = \kappa/\left[f(w)f^*(w)\right] = \kappa/\kappa_1, \\
\Gamma_R &= K/r_0, \quad \Gamma_I = -(K/r_0)\sinh(2w)\,(1 + \gamma_0^2)/(2\gamma_0), \\
2\kappa &= K\,\left[1 - \gamma_0^2 + (1 + \gamma_0^2)\cosh(2w)\right], \quad \rho_0 = \Gamma_0\sqrt{r_0/2}; \qquad \text{(B8)}
\end{aligned}$$

furthermore, the symmetry

$$a_1(w,\Phi) = a_3(w,\Phi), \quad a_2(w,\Phi) = -a_4(w,\Phi); \quad A_1 = A_3, \quad A_2 = -A_4, \qquad \text{(B9)}$$

and the normalization condition

$$1/C^2 = 2(2\pi r_0/K)^3\exp(K\,\kappa_0)I_0(\kappa)\left[\kappa\,I_\kappa + 2 + K\gamma_0\sigma\sinh(w)\right]. \qquad \text{(B10)}$$

The evaluation of q_2 leads to the expression

$$q_2 \equiv \Gamma_I^2 + \Gamma_R^2 = K^2/(4r_0^2\gamma_0^2)\left[4\gamma_0^2 + (1+\gamma_0^2)^2\sinh(2w)^2\right]. \tag{B11}$$

Evaluation of q_1 gives rise to the following forms:

$$\begin{aligned} q_1 &= -K\sigma(\gamma_0^2-1)\left[(\Gamma_I + \mathbf{i}\,\Gamma_R)f(w)^2 + (\Gamma_I - \mathbf{i}\,\Gamma_R)f^*(w)^2\right] \\ &= -K^2/(2r_0\gamma_0)\sigma(\gamma_0^2-1)\sinh(2w)\left[1-\gamma_0^2+(1+\gamma_0^2)\cosh(2w)\right] \\ &= -2\kappa\,K/(2r_0\gamma_0)\sigma(\gamma_0^2-1)\sinh(2w). \end{aligned} \tag{B12}$$

The contribution of q_0 will vanish identically after the integration over the KS phase ϕ. In the following, we will show this in some detail.

$$\begin{aligned} q_0 &= -(1/g^2)\left[A_1^2a_2a_2^* - A_1A_2(a_1^*a_2 + a_1a_2^*) + a_2a_2^*g + a_1a_1^*(A_2^2+g)\right] \\ &= r_0\Gamma_0^2\left[-g\cos(\phi)/\kappa_1 + r_0\Gamma_0^2\sin(\phi)^2\right]\left[g^{-2}\kappa_1\right], \end{aligned} \tag{B13}$$

where $\phi = \Phi - \Phi'$. We introduce the variable transformation $g \to s = \Gamma_R/g$ and use the relation $\Gamma_R = \Gamma_0\kappa_1 = (\kappa\kappa_1/r_0)$ to obtain

$$q_0 = (1/2)\left[s^2\kappa^2 - 2s\kappa\cos(\phi) - s^2\kappa^2\cos(2\phi)\right]. \tag{B14}$$

For the ϕ integration of the q_0 term, we use the form (B7c) and write

$$\begin{aligned} Q_0 :\; &= \int_0^{2\pi} \mathrm{d}\phi\, q_0 I_A(g) = \exp\left[sK(\kappa_0 + \kappa_1\cos(\phi))\right] \times \\ &\quad \pi^2 s^2/(2\Gamma_R^2)\int_0^{2\pi}\mathrm{d}\phi\,\left[s^2\kappa^2 - 2s\kappa\cos(\phi) - s^2\kappa^2\cos(2\phi)\right]. \end{aligned} \tag{B15}$$

The phase integrals amount to modified Bessel functions, I_n,

$$\int_0^{2\pi}\mathrm{d}\phi\,\cos(n\phi)\exp[\cos(z\phi)] = 2\pi I_n(z), \quad n = 0,1,2. \tag{B16}$$

With the aid of the I_n, we can write using the the relation $K\kappa_1 = \kappa$

$$Q_0 = (\pi^3 s^2/\Gamma_R^2)\exp[sK\kappa_0]\left[s^2\kappa^2 I_0(s\kappa) - 2s\kappa I_1(s\kappa) - s^2\kappa^2 I_2(s\kappa)\right]. \tag{B17}$$

Eventually, we make use of the recurrence relation

$$I_2(s\kappa) = -2/(s\kappa)I_1(s\kappa) + I_0(s\kappa), \tag{B18}$$

to make evident that the square bracket factor of Q_0 is identically zero.

We are left with the contributions of q_1 and q_2. Restoring the factor $F = 2\hbar^2C^2/m^2$, where C is the normalization constant, we have to consider

$$E_{kin} = (\hbar^2C^2/m)\int_0^{2\pi}\mathrm{d}\phi\,\left[q_1 + q_2\partial_g\right]I_A(g) \tag{B19}$$

with I_A defined in (B7c) (not to be confused with Bessel function). The q_2 term, essential amounts to the normalization integral and we find

$$\begin{aligned} Q_2: &= (\hbar^2 C^2/m)\int_0^{2\pi} \mathrm{d}\phi\, q_2 \partial_g I_A(g) \\ &= \hbar^2 K^2 \left[4\gamma_0^2 + (1+\gamma_0^2)^2 \sinh(2w)^2)\right]/(32 m r_0^2 \gamma_0^2). \end{aligned} \tag{B20}$$

The contribution of q_1 gives rise to

$$Q_1 := (\hbar^2 C^2/m)\int_0^{2\pi} \mathrm{d}\phi\, q_1 I_A(g) = -\frac{\hbar^2 K^2(\gamma_0^2-1)\kappa\kappa_0}{8 m r_0^2 \gamma_0^2 (2+\kappa I_\kappa + K\kappa_0)}. \tag{B21}$$

With the aid of the renormalization $r_0 \to X_0$, where X_0 is the mean initial x coordinate,

$$r_0 = X_0(2+\kappa I_\kappa)/(\kappa + 3I_\kappa) \tag{B22}$$

one arrives at the expression for E_{kin}, as claimed in (17). As a check, for $w=0$ and in the macroscopic limit $\kappa \to \infty$, one finds that

$$\lim_{\kappa\to\infty} E_{kin}(w=0) = \frac{\hbar^2\kappa^2}{8 m X_0^2)}\left[1+\mathcal{O}(1/\kappa)\right] = \frac{m}{2}V_0^2\left[1+\mathcal{O}(1/\kappa)\right] \tag{B23}$$

with $\sigma V_0 = \langle v_x\rangle(w=0) = \hbar\kappa\sigma/(2mX_0)\left[1+\mathcal{O}(1/\kappa)\right]$.

C Proof for the non vanishing of M and $\tilde{M}$

The functions M and $\tilde{M}$ are defined in (12) and (38), respectively. We introduce the auxiliary functions F and $\tilde{F}$ as follows

$$M = 2+\kappa I_\kappa + \kappa\sigma F(w), \quad \tilde{M} = 2+\kappa I_\kappa + \kappa\sigma \tilde{F}(\tilde{w}) \tag{C1}$$

with

$$F = \frac{2\gamma_0 \cosh(w)\sinh(w)}{\cosh(w)^2 + \gamma_0^2 \sinh(w)^2}, \quad \gamma_0 > 0; \quad \tilde{F} = \frac{2\tilde{\gamma_0}\cos(\tilde{w})\sin(\tilde{w})}{\cos(\tilde{w})^2 + \tilde{\gamma_0}^2\sin(\tilde{w})^2}, \quad \tilde{\gamma_0} > 0. \tag{C2}$$

With the aid of the substitutions $w \to z$ and $\tilde{w} \to \tilde{z}$ with $z = \sinh(w)$ and $\tilde{z} = \sin(\tilde{w})$, one easily finds

$$0 \le F \le \frac{2\gamma_0}{1+\gamma_0^2} \le 1 \quad \text{for} \quad 0 \le \gamma_0 < 1; \quad 0 \le F \le 1 \quad \text{for} \quad \gamma_0 \ge 1; \tag{C3}$$

$$-1 \le \tilde{F} \le 1 \quad \text{for} \quad \tilde{\gamma_0} > 0. \tag{C4}$$

Hence, both $M \ge M_0$ and $\tilde{M} \ge M_0$ with

$$M_0 = 2+\kappa I_\kappa - \kappa > 1.39, \tag{C5}$$

where the latter inequality is established numerically; the minimum of M_0 is at $\kappa \approx 1.70238$; asymptotically, for $\kappa \to \infty$, since $I_\kappa \to 1$, one gets $M_0 = 2$. In any case, the denominators M and $\tilde{M}$ are larger 1, which proves Statement (I.)

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