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## The two dimensional motion of a particle in an inverse square potential: Classical and quantum aspects

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The classical 2D dynamics of a particle moving under an inverse square potential,  $-k/r^2$ , is analysed. We show that such problem is an example of a *geometric system* since its negative energy orbits are equivalent to free motion on a certain hypersurface. We then solve in momentum space, the corresponding unrenormalized quantum problem showing that there is no discrete energy spectrum and, particularly, no ground state. © 2013 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4804356>]

### I. INTRODUCTION

The motion of a particle under an attractive inverse square potential has been discussed for years.<sup>1–23</sup> The problem has been investigated from a quantum point of view because it is useful for describing electron scattering off polar molecules,<sup>3</sup> and has shown to provide a simple realization of a quantum anomaly in molecular physics.<sup>4</sup> Besides, it serves to calculate the critical dipole moment in polar molecules and in nanowires,<sup>6</sup> and to deal with the so-called “fall-to-the-center” behavior.<sup>7,8</sup> Furthermore, it can be regarded as equivalent to the Calogero model but with no bounding term.<sup>9,12,13</sup> It also shows properties which can be traced back to the non-self-adjointness of its quantum Hamiltonian.<sup>5,9,10,14</sup> An analysis of such problem was recently presented using advanced techniques<sup>14</sup> in which we proved that the classical 1D system is geometric, i.e., is equivalent to certain free motions on a hypersurface in phase space, we also proved that some of the features of the 1D quantum problem can be explained by the action of a superselection rule.

In this work, we analyse some aspects of the classical and then of the unrenormalized quantum 2D dynamics of a particle with mass  $m$  interacting with an inverse square potential. We show the equivalence of its classical dynamics to geodesic motion on a noncompact hypersurface, establishing the non-existence of bound orbits in the classical negative-energy case. We exhibit that its supposedly bound motions are canonically equivalent to free motions. The procedure used to exhibit such equivalence may be also regarded as a regularization.

The equivalence of classical motion under the inverse square potential to free motion is the most important result of this work since, to our knowledge, the only other problem in which an equivalence of this sort has been proved is Kepler’s.<sup>16</sup> Besides this feature, as in the Coulomb or hydrogen atom case, may be found useful in various situations.<sup>15,24</sup> We next exhibit that the negative energy case of the unrenormalized quantum problem does not possess a discrete energy spectrum and so neither a ground state. This last feature may be thought as a quantum manifestation of the classical equivalence to free motion. We use the term bound state in the sense of a normalizable, negative-energy solution, belonging to the discrete part of the spectrum of a quantum system.

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We pinpoint again that we always work with the problem described with the basic quantum Hamiltonian of the problem [Eq. (3) below] never with its self-adjoint extensions nor with the renormalized versions. This is to be contrasted with the bound states found in the literature that mostly are understood as states of the *renormalized (or self-adjoint extended)* inverse square potential.<sup>4,9</sup> In this work, we **never** analyse such version of the problem. Our main purpose is to exhibit the geometric nature, in the sense of Boya *et al.* and of Moser,<sup>15,16</sup> of the classical problem and to pinpoint possible quantum manifestations of such property.

## II. THE CLASSICAL PROBLEM AND THE EQUIVALENCE TO GEODESIC MOTION

We first prove that the classical case of the problem is equivalent to free motion on a hyperbolic hypersurface. Let us start with one particle of mass  $m$  moving under the potential  $V(x, y) = -k/(x^2 + y^2)$  ( $k$  being a positive constant), with the Lagrangian

$$L = \frac{1}{2}m\|\mathbf{v}\|^2 + \frac{k}{\|\mathbf{r}\|^2}. \quad (1)$$

Lagrangian (1) describes a scale invariant system which is equivalent to free motion on a hyperboloidal surface of phase space.<sup>14–16</sup> The singularity at  $r = 0$  makes system (1) a good candidate for regularization—as the one we manage to perform in the following.

Using polar coordinates  $r$  and  $\theta$ ,  $x = r\cos(\theta)$ ,  $y = r\sin(\theta)$ , the Lagrangian of the system becomes  $L = (m/2)(\dot{r}^2 + r^2\dot{\theta}^2) + k/r^2$ . The angular momentum  $\ell = mr^2\dot{\theta}$  is clearly a constant of motion. Thus, we can write

$$L = \frac{1}{2}m\dot{r}^2 + \frac{(k + \ell^2/2m)}{r^2}. \quad (2)$$

The 2D radial Hamiltonian is, therefore,

$$H = \frac{p^2}{2m} - \frac{\beta}{r^2}, \quad (3)$$

where  $p = m\dot{r}$  and we have defined the constant  $\beta \equiv k - \ell^2/2m$ . Hamiltonian (3), together with  $\dot{\theta} = \ell/(mr^2)$  encompass completely the 2D dynamics of the problem. There are 2 obvious constants of motion in the problem, the energy  $E$  and the 2D angular momentum  $\ell$ .

Classical Hamiltonian (3) is scale invariant. Any change  $r \rightarrow \lambda r$  and  $p \rightarrow p/\lambda$  leaves the equations of motion unchanged if the energy is at the same time rescaled as  $E \rightarrow E/\lambda^2$ . This exhibits that the problem has no characteristic energy scale at the classical level, i.e., the classical description of the motion of a particle in an inverse square potential is invariant under dilations.

Our first step to establish the equivalence with geodesic motion is to perform a  $-\pi/2$  rotation in phase space,  $p \rightarrow r$  and  $r \rightarrow -p$ , which transforms (3) into

$$\frac{r^2}{2m} - \frac{\beta}{p^2} = E = -\epsilon, \quad (4)$$

where  $\epsilon(p, r) \equiv \beta/p^2 - r^2/(2m)$  is an explicit function of  $p$  and  $r$  which could be regarded as positive when analyzing negative energies. Then Eq. (4) becomes

$$\left(1 + \frac{r^2}{2m\epsilon(p, r)}\right)p^2 = \frac{\beta}{\epsilon(p, r)}, \quad (5)$$

which suggests defining a new momentum as

$$P = p\sqrt{1 + \frac{r^2}{2m\epsilon}}. \quad (6)$$

A generating function<sup>25</sup> leading to the momentum  $P$  above, Eq. (6), is

$$F(r, P) = \sqrt{2m\beta} \log\left(2Pr + 2\sqrt{2m\beta + P^2r^2}\right). \quad (7)$$

$F$  also generates a new coordinate  $Q$  as

$$Q = \frac{\partial F}{\partial P} = r \sqrt{1 - \frac{p^2 r^2}{2m\beta}}. \quad (8)$$

Clearly,  $Q$  and  $P$  are canonical coordinates as they follow from the generating function  $F(r, P)$ . The transformed Hamiltonian is

$$H' = \frac{P^2}{2M}, \quad (9)$$

where  $M \equiv \beta/2$ . We have thus transformed the Hamiltonian of the inverse square problem to a free particle form and thus we also managed to regularize the problem in the process—i.e., no trace of the singularity at  $r = 0$  remains. Notice that if we use the alternative—noncanonical—coordinates  $\xi = \operatorname{arcsinh}(r/\sqrt{2m\epsilon(p, r)})$  and  $p_\xi = p \cosh(\xi)$ , Hamiltonian (4) is also converted to a free particle form. That is, the particle may be considered as moving on a branch of a hyperbola, which is a region in the reduced phase-space and thus the problem can be termed geometric.<sup>16</sup> The 2D motion under an inverse square potential is equivalent to free motion on an phase-space hyperboloid (a non-compact manifold) as can be ascertained because we still may rotate the plane of the hyperbola branch by any angle whatsoever, as follows from the canonical transformation that stem from the constancy of  $\ell$ . From this result, we may see that the symmetry algebra of the classical problem is  $O(2) \times O(1, 1)$ —which is isomorphic to  $SO(2, 1)$  the known commutator algebra of the quantum problem.<sup>30</sup>

Now to return to the canonical equivalence we proved before. The equivalence between a negative energy region of phase space with the unbounded hyperbola arch should not be surprising since there are no bound orbits in the classical problem. This can be seen simply realizing that the inverse squared potential has the same functional form as the centrifugal potential, or by solving explicitly its equations of motion. From Eqs. (2) or (3), we get the radial equation

$$m\ddot{r}(t) = -\frac{2\beta}{r^3}, \quad (10)$$

where  $\beta$  is the constant in Eqs. (2) or (3). The solution of this equation, both for  $\beta > 0$  or for  $\beta < 0$ , is

$$r(t) = \sqrt{(R + tV)^2 + \frac{2\beta t^2}{mR^2}}, \quad (11)$$

where  $R = r(0)$  is the initial radial position and  $V = \dot{r}(0)$ , the initial radial velocity. It is to be noted that the behavior of the solution does not change if the sign of the constant  $k$  is changed, it remains of the form given in (11). How can it be possible that a strongly attractive potential has unbounded solutions as the solutions to the corresponding repulsive potential? We may explain the reason just noting that in the effective potential [Eq. (3)]  $V_{\text{eff}} = -\beta/r^2$  we are introducing, albeit implicitly, an effective angular momentum through  $\ell_{\text{eff}}^2 = \ell^2/2m - k$  in terms of which the equation of motion of the problem takes the form of a classical problem with no interaction—in spite of the  $-k/r^2$  one. Hence, there are no bound orbits in the classical problem. Thus, the sign of  $k$  is of no importance whatsoever for the non-existence of bound motions in the system. However, there is a further point worth mentioning. When  $\beta > 0$ , at the times  $t_1 = -(R/V)(1 - (\sqrt{2\beta}/RV))^{-1}$  and  $t_2 = -(R/V)(1 + (\sqrt{2\beta}/RV))^{-1}$ , the  $r$ -coordinate vanishes causing the potential energy term to blow up. This behavior should have no consequences for the dynamics, in exactly the same way as the vanishing of  $r$  has no consequences whatsoever for a free radial problem described with the help of a centrifugal potential. The behavior is also no trouble to our geometrization because, as we also mentioned, such procedure amounts to a regularization of the inverse square problem.

We have canonically transformed the negative energy motions to motions on a branch of a hyperbola—a noncompact manifold—in which all motions are necessarily unbounded. To see if this feature has any relevance in the quantum case, in Sec. III, we analyse the quantum version of the problem. The conclusion we obtain is that the quantum version of the problem does not admit

negative energy normalizable discrete states. So, there are no surprises, as the classical negative-energy orbits are canonically equivalent to unbound ones we could not expect the corresponding quantum system to admit a discrete energy spectrum. For a general feature of the quantum systems with a discrete energy spectrum is that the corresponding classical motion needs to be confined into a compact region of configuration space for such energy spectrum to exist.<sup>7,14,19</sup>

### III. THE QUANTUM PROBLEM AND THE NONEXISTENCE OF A GROUND STATE

The scale invariance of the classical problem can be shown to be valid also for the quantum case, as the scaling of the coordinates  $x_i \rightarrow \lambda x_i$ ,  $i = 1, 2$ , would leave the Schrödinger equation unchanged if, at the same time, the energy is rescaled as  $E \rightarrow E/\lambda^2$ . In quantum mechanics such invariance would mean that there is no way of determining the energy spectrum of the problem. This last feature is known to occur in the  $N$ -dimensional general case.<sup>5</sup> Here, we establish the property for the 2D problem and argue that it can be regarded as a quantum manifestation of the classical equivalence to motion on an unbounded region of phase space. Also recall that for an interaction as the  $-k/r^2$  one, self-adjoint extensions and renormalization methods are not equivalent with renormalization acting as sort of selector of a preferred self-adjoint extension and as a regulator of the unbounded Hamiltonian, as has been proved in Ref. 26.

If the radial Hamiltonian (3) is interpreted as a quantum operator, it can be factored as<sup>10</sup>

$$H = -\frac{\hbar^2}{2m} \left( \frac{d}{dr} + \frac{b}{r} \right) \left( \frac{d}{dr} - \frac{b}{r} \right), \quad (12)$$

where  $b(1 - b) = \alpha$  and, for the sake of compactness, we defined  $\alpha \equiv 2m\beta/\hbar^2$ . This exhibits that the mean value,  $\langle E \rangle$ , of the energy in any state,  $\psi$ ,

$$\langle E \rangle = \frac{\hbar^2}{2m} \langle \psi | \left( \frac{d}{dr} - \frac{b^*}{r} \right) \left( \frac{d}{dr} - \frac{b}{r} \right) | \psi \rangle = \frac{\hbar^2}{2m} \int_0^\infty \left| \left( \frac{d\psi}{dr} - \frac{b}{r} \psi \right) \right|^2 dr, \quad (13)$$

has to be a strictly positive quantity and hence can be no bound states if we assume, as we did for obtaining the right hand side of the above equation, that  $b$  is real. Contrarywise, we must conclude that  $\alpha$  has to be less than 1/4 for bound states to exist. Hence,  $\alpha_c = 1/4$  plays the role of a critical value. Even so  $H$  may still be required of renormalization for producing bound eigenstates.<sup>10,14</sup>

The above feature is only a particular instance of the property valid in any scale-invariant quantum theory, the strength of particle interactions cannot depend on the energy involved. This should also be clear in our problem, for no combination of the dimensional parameters describing the system (i.e.,  $\hbar$ ,  $m$ ,  $k$ ), may produce a quantity with the dimensions of energy. Hence, there is no way of determining a formula for an energy spectrum. Besides, if we assume that any state with energy  $E_0 < 0$  could exist then there would necessarily exist another state with an energy  $E_1 = a^2 E_0 < 0$  where  $a$  is any number, i.e., given any negative energy state, the spectrum would give rise to a sort of ultraviolet catastrophe. This can be proved as follows, assume you could find one bound state  $\psi(r)$  with eigenenergy  $E$ , if now you change  $r$  to  $ar$  then you can easily show that  $\psi(ar)$  is also a solution with eigenenergy  $a^2 E$ , hence no discrete energy spectrum could be found. In particular, the inverse square potential could not admit a ground state. If we insist in determining a ground state, we would need to renormalize the system but this would break the scale invariance of the problem.<sup>4,5,14</sup>

It should also be noted that the singular Hamiltonian (3) is an example of those operators where the notion of Hermiticity cannot be taken to guarantee the more stringent requirement of self-adjointness, as is required to obtain unambiguous physical conclusions. It is usually recognized that the main problem caused by the singular nature of the  $1/r^2$  problem lies in that its Hamiltonian, being Hermitian but not self-adjoint, admits self-adjoint extensions.<sup>5,17,27</sup> Let us remind the reader that an operator is self-adjoint if the domain of definition of the operator and the domain of definition of its Hermitian conjugate are the same. That is, an operator  $H$  with domain of definition  $D(H)$  is said to be Hermitian (a *symmetric operator* in standard mathematical terminology) if for all functions  $\phi$ ,

$\psi \in D(H)$ , we have  $(H\phi, \psi) = (\phi, H\psi)$ , that is,  $H = H^\dagger$ ; but, if additionally the domain of  $H$  and the domain of  $H^\dagger$  coincide, i.e., if  $D(H) = D(H^\dagger)$ , then  $H$  is called self-adjoint.<sup>27</sup>

The non-existence of a discrete energy spectrum can be explicitly proved in the process of obtaining the quantum solution as is done in the following. For the classical equivalence to motion on a certain hypersurface we used canonical transformations to a sort of “momentum representation” to reduce the classical problem<sup>14,15</sup> to free motion on a hyperboloid. Such consideration suggested us a momentum space approach for the corresponding quantum problem. Thus, we transform the radial Schrödinger equation of the problem, based on Hamiltonian (3), to the momentum representation to get

$$\int_{-\infty}^p \int_{-\infty}^{p'} \phi(p'') dp'' dp' = -\frac{\hbar^2}{2m\beta} (p^2 + 2m\epsilon) \phi(p), \quad (14)$$

where  $\phi(p)$  is the momentum space radial wave function. To obtain (14) we use the operator correspondence<sup>28</sup>

$$\hat{r}^{-1} \rightarrow i \int_{-\infty}^p \dots dp'. \quad (15)$$

In writing (14), we are implicitly assuming that the corresponding  $r$ -representation radial wave function,  $\psi(r)$ , vanishes at the origin  $\psi(0) = 0$ . The necessity of such condition follows from the superselection rule we proved to exist in the 1D problem<sup>14</sup>—in any straight line passing through the origin (hence, with  $\ell = 0$ ) in our 2D problem a strict separation of one of the sides of the origin from the other should exist. Therefore,  $\psi(0)$  must necessarily vanish. This is also one of the boundary conditions on  $\psi(r)$  required for Hamiltonian (3) to be self-adjoint.<sup>9,14,29</sup> The system would also need of renormalization for a proper derivation of its quantum properties but this would provoke a breaking of its scale invariance as shown in Ref. 18.

To solve (14), we derive it twice to get

$$2p\phi'(p) + \frac{1}{2} (p^2 + 2m\epsilon) \phi''(p) = \left( \frac{m\alpha}{\hbar^2} - 1 \right) \phi(p), \quad (16)$$

the solutions to such equation<sup>21</sup> are linear combinations of the hypergeometric functions  ${}_2F_1[u_-, u_+, 1/2, -|p|^2/2m\epsilon]$  and  ${}_2F_1[u_-, u_+, 1/2, -|p|^2/2m\epsilon]p$ , where  $p = |p|$  is the modulus of the linear momentum, and we have also introduced  $\chi = \sqrt{1/4 - \alpha}$ ,  $u_\pm = (3 \pm \chi)/4$  and  $v_\pm = (5 \pm \chi)/4$ , these functions are the negative energy components of the unrenormalized radial wave functions in the 1D  $p$ -representation.<sup>14</sup> Note that such feature limits the values the modulus of the momentum can take in any negative energy state to  $-\sqrt{2m\epsilon} \leq p \leq \sqrt{2m\epsilon}$ .

As one may infer from transformed Hamiltonian (9), the quantum system obtained by directly quantizing it has eigenfunctions with no discrete energy levels. This happens basically because there is no way to quantize the energy if the corresponding classical system moves in an unbound region with no singularities. The energy levels should be thus continuous. Besides, given any single state with negative energy, we can found infinitely more with lower energies—as we have argued from scaling considerations.<sup>14</sup> A discrete energy spectrum does not exist because no further condition may be imposed on the solutions of the problem, thus there are no limitation on its possible energy values. Energy is not quantized as the absence of bounded orbits in the classical case suggests, a result that corroborates what is known about the  $-1/r^2$  interaction in quantum theory,<sup>4,14</sup> a result that can be regarded as an alternative proof of the non-existence of a critical value for the electric dipole moment in 2D. Worst of all, the system has no proper ground state making it unstable unless we renormalize it. In conclusion, the non-renormalized quantum inverse square problem has no discrete energy levels and no ground state.

It is to be noted also that the parameter  $\chi$  becomes imaginary when  $\alpha$  is greater than  $1/4$ , so we again found this value to act as a critical value,  $\alpha_c$ , separating the two regimes we described above, one with no bound states ( $\alpha > \alpha_c$ ) and other where bound states may exist ( $\alpha \leq \alpha_c$ ) in 2D. In fact, in 1D and 3D it has been found that there exist a single renormalized bound state.<sup>10,14,29</sup> On the other hand, we have found that in 2D  $\alpha_c$  divides the problem according to its  $\alpha$  value. Namely,

1. if  $\alpha \leq \alpha_c$ , the problem has to be renormalized and a single renormalized bound state can be found after such renormalization.<sup>5,10,29</sup>
2. if  $\alpha > \alpha_c$ , the problem cannot support bound states even after renormalization.<sup>5,10,29</sup>

We conclude then that in the 2D inverse square interaction problem, the unrenormalized (or non-self-adjoint extended) system has no discrete energy spectrum and hence no ground state but after renormalization an arbitrary-energy bound state is expected to appear.<sup>4,14,22</sup>

#### IV. CONCLUSIONS

In summary, we have analysed the 2D inverse squared problem in classical mechanics and found that the problem is equivalent to free motion on a hypersurface of phase space, this is a property we have also proved in the 1D classical case.<sup>14</sup> The negative-energy classical orbits of the system can be canonically transformed into geodesic orbits on a phase-space noncompact hypersurface. This means that they are unbounded motions. Such property is reflected in the non-renormalized quantum problem as the non-existence of a discrete bound energy spectrum. A possible explanation to such peculiar feature can stem from the fact that both the classical and the quantum Hamiltonians may be understood as free Hamiltonians but with a redefined angular momenta. Take, for example, the classical case where we implicitly introduce a new “angular momentum” through  $\ell'^2 \rightarrow \ell^2 + 2mk$  in terms of which the equation of motion of the problem may be regarded as a classical problem with all the appearance of a system with no interaction in spite of the  $-k/r^2$  one. The 2D classical  $-k/r^2$  problem is thus geometrical, that is, the flow on the aforementioned hypersurface can be viewed as a fibration on it—in the sense used by Moser<sup>16</sup> for the classical Kepler’s problem, that is, the energy surface of the problem is equivalent to the unit tangent bundle of a hyperboloidal surface in phase space and the integral curves of the Hamiltonian belong to the set of geodesics on that hypersurface. Notice that as a part of the proof of the equivalence we also regularized the problem. Classical motion avoids approaching the origin as the phase portrait in Ref. 14 exhibits—the conclusion, obtained from a 1D phase portrait, is only applicable to the radial motions with  $\ell = 0$  of the present problem, but this case suffices for establishing our result.

The scaling properties of the inverse square potential are important in determining the quantum properties of the physical dipole potential since most of its scale and other symmetries are inherited by the full-fledged electric dipole potential<sup>4,29</sup> needed to model interactions with polar molecules.<sup>3,4,29</sup> In 3D electron binding occurs only for a sufficiently strong dipole moment, i.e., a quantum mechanical symmetry breaking ensues.<sup>4,14,20</sup> The breaking of the scale symmetry of the 3D problem has been regarded as a manifestation of a quantum anomaly. Such anomaly is manifested by the formation of anions through electron capture by polar molecules with supercritical dipole moments. Such behavior represents one of the simplest realizations of a symmetry breaking in a physical system.<sup>3,4,14</sup>

We have found that the 2D problem has a  $SO(2) \times SO(1, 1) \sim SO(2, 1)$  symmetry algebra.<sup>30</sup> We also solved the quantum problem in the momentum representation showing that such representation is rather convenient for its study. We exhibited that there is a strong-coupling regime, for which a quantum-mechanical breaking of symmetry takes place and we mention that through renormalization a single bound state may appear. Let us point out again that the inverse square problem serves to model quantum point-dipole interactions,<sup>3</sup> and that it is relevant in polymer studies.<sup>31</sup> In addition to its remarkable similarities with the properties of a 2D  $\delta$ -function potential<sup>32</sup> and that it provides an example of a system in which its classical conformal symmetry can be anomalously broken in quantum theory.<sup>22</sup>

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