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Center-of-mass properties of composite systems subject to nonlinear external interactions

James A. Lock

If two bound nonrelativistic quantum particles are each subject to a nonlinear external potential, their Schrödinger equation does not separate in relative and center-of-mass coordinates. For this case, the details of internal state of the composite affect its center-of-mass properties. The extent of this internal state influence is examined for an exactly soluble one-dimensional model system.

INTRODUCTION

In the classical and nonrelativistic quantum-mechanical treatments of a two-particle system with internal and external interactions, the transformation to relative and center-of-mass coordinates allows the two-body problem to be analytically soluble for a large class of physically interesting interactions. In these situations, the equations of motion for the two particles decouple into an equation of motion which describes the average or overall motion of the system and an equation of motion which describes the relative or internal motion. However, it occasionally happens that for a situation of interest, the equation of motion for a two-particle system does not decouple via the relative and

center-of-mass coordinate transformation. In the nonrelativistic quantum-mechanical domain, well-known examples of this are hydrogen in very strong magnetic fields¹ and the homonuclear diatomic molecule.²

In the standard solution of both of these problems, a particular physically motivated point of view is adopted. Since $\omega_{\text{internal}}^{-1}$ is much shorter than times characteristic of the motion of the center of mass, it is assumed that the center-of-mass configuration appears static as viewed by the internal system. As a result, the center-of-mass–relative coupling terms describe the influence of the center-of-mass configuration on the internal state of the system and the internal state does not influence the center-of-mass motion. The physical motivation for this “one-way influence” as-

sumption is well founded for both of the above examples.

However, from a mathematical point of view, the presence of center-of-mass–relative coupling terms in the Schrödinger equation may be the result of an influence on the center-of-mass motion produced by the details of the internal state just as easily as it could be associated with the influence on the internal state of the system produced by the center-of-mass configuration. In this paper we study this converse possibility in the context of an exactly soluble model problem. Specifically we prepare a free composite (and thus separable) system with the internal state $\psi_j(\mathbf{r}, t)$ and with a given amount of localization present in the center-of-mass wave packet $\Pi(\mathbf{R}, t)$. We suddenly switch on a nonlinear external potential at $t = 0$. For $t > 0$, assuming that the nonlinear external potential acts on each of the constituent particles (but possibly with unequal strengths), the Schrödinger equation is not separable in relative and center-of-mass coordinates. The subsequent time evolution of the expectation values of the various center-of-mass observables then may depend on the initial internal state j in a dramatic or easily observable manner. We explore this possibility in the present study.

To turn the problem around, one could infer that a quantum-mechanical object was a composite system, rather than being elementary, by placing it in a nonlinear external potential, measuring the center-of-mass attributes of the object, and observing that these attributes behave differently than the corresponding attributes of a structureless particle in the same external potential. This is similar in spirit to the way in which the anomalous magnetic moments of the proton and neutron signal that they are composites rather than elementary systems.

MODEL PROBLEM

Our model problem is that of two particles of masses m_1 and m_2 nonrelativistically bound to each other by a one-dimensional harmonic oscillator potential of strength k . At $t = 0$, an external harmonic oscillator interaction acting on each of the constituent masses is suddenly switched on. The strengths of the external couplings are K_1 and K_2 , respectively. Assuming the additivity of the external interaction, the Hamiltonian for this system for $t \geq 0$ is

$$H = \frac{-\hbar^2}{2m_1} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2} \frac{\partial^2}{\partial x_2^2} + \frac{k}{2} (x_1 - x_2)^2 + \frac{K_1}{2} x_1^2 + \frac{K_2}{2} x_2^2. \quad (2.1)$$

When this Hamiltonian is transformed to relative and center-of-mass coordinates

$$r \equiv x_1 - x_2 \quad (2.2)$$

and

$$R \equiv (m_1 x_1 + m_2 x_2) / (m_1 + m_2), \quad (2.3)$$

we obtain

$$H = \frac{-\hbar^2}{2M} \frac{\partial^2}{\partial R^2} - \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + \frac{K_1 + K_2}{2} R^2 + \frac{1}{2} \left(k + \frac{m_1^2}{M^2} K_2 + \frac{m_2^2}{M^2} K_1 \right) r^2 + \left(\frac{K_1 m_2 - K_2 m_1}{M} \right) R r, \quad (2.4)$$

where

$$M \equiv m_1 + m_2 \quad (2.5)$$

and

$$\mu \equiv m_1 m_2 / M, \quad (2.6)$$

and which is nonseparable in these coordinates for

$$K_1 m_2 \neq K_2 m_1. \quad (2.7)$$

At this point, a number of comments concerning the assumptions inherent in this model problem are pertinent. First, the question of whether external interactions on the constituents of a composite system are additive has been examined in the relativistic situation for the case of external electromagnetic interactions.^{3,4} It has been found that the total fully relativistic external interaction is well approximated by the sum of the individual fully relativistic external interactions of the constituents. However, when the total fully relativistic interaction is replaced by its nonrelativistic Foldy–Wouthuysen reduction, the question of whether the reductions of the constituent interactions are additive depends on whether the relativistic or nonrelativistic versions of the center-of-mass and relative coordinates are employed. If the relativistic version is used, the reduced interactions are additive.⁵ If the nonrelativistic version is used, the interactions are nonadditive to within a term describing the Thomas precession of the orbital angular momentum.^{3,4} Thus, for nonrelativistic situations in which the velocities of the constituents remain small, any v^2/c^2 corrective terms to either additivity or to the definitions of the center-of-mass and relative variables are negligible, and additivity of the external interactions is expected to be a reasonable approximation.

The present model problem is also closely related to, but possesses important differences from, nuclear shell models. In shell model Hamiltonians for a free nucleus, it is customary to replace the individual nucleon–nucleon interactions by the sum of a model interaction of each nucleon with the center of the nucleus plus a residual constituent–constituent interaction which is treated in perturbation theory.^{6–8} The model nucleon–center interaction is mathematically equivalent to our interaction of the constituents with the external potential. However, for equal mass nucleons coupling equally strongly to the external harmonic oscillator force center, the inequality (2.7) is not satisfied and the nuclear shell model Hamiltonian is separable when expressed in relative and center-of-mass coordinates. This separability is the source of the utility of such models in nuclear physics. In the present study, we effectively consider the same model situation but are interested only in the case where the inequality (2.7) is satisfied and the model is not separable when relative and center-of-mass coordinates are employed.

Finally, our nonrelativistic one-dimensional harmonic oscillator model problem is admittedly very specialized. Thus the direct applicability of our results to a number of interesting physical problems is limited by this artificiality. In our model, the center-of-mass–relative coupling vanishes for $m_1 K_2 = m_2 K_1$. This special behavior may not in general occur for systems with more arbitrary external interactions. Such a more general interaction in a three-dimensional relativistic context would be required if one were to adopt our point of view for systems with equal mass constituents such as hadrons comprised of up and down quarks. Our present formalism could in principle be

used to describe the center-of-mass properties of hadrons containing a single charmed or bottom quark. However, the short lifetimes of these composites hinder the detailed observation of any of the center-of-mass attributes calculated in Sec. III. Further, the idealization of suddenly switching on the external interaction is physically difficult to realize in the tight-binding limit where the angular frequency of the internal motion is very large.

Nonetheless, our model possesses one overriding pedagogic virtue. It is analytically soluble and thus easily allows one to assess the importance of the influence of the internal dynamics on the center-of-mass motion for any strength external coupling. For more general external interactions, a perturbation theory approach could be employed in the tight-internal-binding limit. However, as the strength of the external interaction is increased, this method loses its relevancy. On the other hand, for any strength coupling, a Faddeev expansion approach could be adopted. However, the calculational complexity of such a program makes detailed quantitative results very expensive and time consuming to obtain. The present calculation with our exactly soluble model avoids these difficulties.

Returning to the solution of our model problem, it is well-known that the Hamiltonian of Eq. (2.1) separates when the transformation to normal mode coordinates

$$u = (m_1 \gamma x_1 + m_2 x_2)/M \quad (2.8)$$

and

$$v = x_1 - \gamma x_2 \quad (2.9)$$

is made, where

$$\gamma = \frac{1}{2k} \left(k \left(1 - \frac{m_2}{m_1} \right) + K_2 - \frac{m_2}{m_1} K_1 \right) + \left\{ \left[k \left(1 - \frac{m_2}{m_1} \right) + K_2 - \frac{m_2}{m_1} K_1 \right]^2 + \frac{4m_2}{m_1} k^2 \right\}^{1/2}. \quad (2.10)$$

In the limit of very tight internal binding or a very weak external interaction, $k \gg K_1$, $k \gg K_2$, and

$$\lim_{K/k \rightarrow 0} \gamma = 1. \quad (2.11)$$

In the normal mode coordinates, the model Hamiltonian of Eq. (2.1) reduces to two independent harmonic-oscillator Schrödinger equations

$$-\frac{\hbar^2}{2m_u} \frac{\partial^2 \Phi(u)}{\partial u^2} + \frac{k_u}{2} u^2 \Phi(u) = E_u \Phi(u) \quad (2.12)$$

and

$$-\frac{\hbar^2}{2m_v} \frac{\partial^2 \phi(v)}{\partial v^2} + \frac{k_v}{2} v^2 \phi(v) = E_v \phi(v), \quad (2.13)$$

where

$$m_u \equiv M^2 / (\gamma^2 m_1 + m_2), \quad (2.14)$$

$$k_u \equiv [M / (\gamma^2 m_1 + m_2)]^2 [K_1 \gamma^2 + K_2 + k(1 - \gamma^2)], \quad (2.15)$$

$$m_v \equiv m_1 m_2 / (\gamma^2 m_1 + m_2), \quad (2.16)$$

and

$$k_v \equiv [1 / (\gamma^2 m_1 + m_2)]^2 \times [K_1 m_2^2 + K_2 m_1^2 \gamma^2 + k(\gamma m_1 + m_2)^2]. \quad (2.17)$$

For reasons apparent in Sec. III, the harmonic-oscillator

wave functions $\Phi(u, t)$ and $\phi(v, t)$ are each chosen to be normalized to the square root of the Jacobian of the transformation connecting u and v to r and R , $[(\gamma^2 m_1 + m_2)/M]^{1/2}$, rather than to unity.

We consider the situation where the external harmonic-oscillator potential is suddenly switched on at $t = 0$. For $t < 0$, the wave function of the internally interacting system is the product of the center-of-mass free-particle wave packet and the relative harmonic-oscillator wave function

$$\Psi(x_1, x_2, t) = \Pi(R, t) \psi_j(r, t). \quad (2.18)$$

The wave function for $t \geq 0$ may be expressed as

$$\Psi(x_1, x_2, t) = \sum_{Nn} a_{Nn} \Phi_N(u, t) \phi_n(v, t). \quad (2.19)$$

In the sudden approximation, the continuity of the wave function at $t = 0$ requires that

$$a_{Nn} = \frac{M}{\gamma^2 m_1 + m_2} \int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} dv \Pi(R(u, v), 0) \times \psi_j(r(u, v), 0) \Phi_N(u, 0) \phi_n(v, 0). \quad (2.20)$$

CENTER-OF-MASS OBSERVABLES

One way in which to demonstrate the influence of the details of the internal structure on the center-of-mass motion is to observe the expectation value of the position of the center of mass

$$\langle R(t) \rangle = \frac{M}{\gamma^2 m_1 + m_2} \int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} dv \sum_{Mm} a_{Mm}^* a_{Nn} \times \Phi_M^*(u, t) \phi_m^*(v, t) R \Phi_N(u, t) \phi_n(v, t). \quad (3.1)$$

Using the transformation connecting the normal mode coordinates to the relative and center-of-mass coordinates, the properties of harmonic-oscillator matrix elements, and the equality of Eqs. (2.18) and (2.19) at $t = 0$, we obtain for $t \geq 0$,

$$\begin{aligned} \langle R(t) \rangle = & \langle \Pi(R, 0) | R | \Pi(R, 0) \rangle \left(\frac{A^2}{A^2 - BC} \cos \omega_u t \right. \\ & \left. - \frac{BC}{A^2 - BC} \cos \omega_v t \right) \\ & - \langle \psi_j(r, 0) | r | \psi_j(r, 0) \rangle \frac{AB}{A^2 - BC} (\cos \omega_u t \\ & - \cos \omega_v t) \\ & + \langle \Pi(R, 0) | P_R | \Pi(R, 0) \rangle \left(\frac{A^2}{(k_u m_u)^{1/2}} \sin \omega_u t \right. \\ & \left. + \frac{B^2}{(k_v m_v)^{1/2}} \sin \omega_v t \right) \\ & + \langle \psi_j(r, 0) | p_r | \psi_j(r, 0) \rangle \left(\frac{AC}{(k_u m_u)^{1/2}} \sin \omega_u t \right. \\ & \left. + \frac{AB}{(k_v m_v)^{1/2}} \sin \omega_v t \right), \end{aligned} \quad (3.2)$$

where

$$P_R = -i\hbar \frac{\partial}{\partial R}, \quad p_r = -i\hbar \frac{\partial}{\partial r}, \quad \omega_u = \left(\frac{k_u}{m_u} \right)^{1/2},$$

$$\omega_v = \left(\frac{k_v}{m_v} \right)^{1/2}, \quad A = \frac{\gamma m_1 + m_2}{\gamma^2 m_1 + m_2},$$

$$B = \frac{m_1 m_2}{M} \left(\frac{1 - \gamma}{\gamma^2 m_1 + m_2} \right), \quad C = -M \left(\frac{1 - \gamma}{\gamma^2 m_1 + m_2} \right).$$

In comparison, for a structureless particle of mass M whose wave function is identical to the center-of-mass wave packet of the structured system before the interaction is switched on at $t = 0$, and which couples to the external interaction with the strength K , we have

$$\langle R(t) \rangle = \langle \Pi(R, 0) | R | \Pi(R, 0) \rangle \cos \omega t + (KM)^{-1/2} \langle \Pi(R, 0) | P_R | \Pi(R, 0) \rangle \sin \omega t \quad (3.3)$$

with

$$\omega = (K/M)^{1/2}. \quad (3.4)$$

The comparison of Eq. (3.2) with Eq. (3.3) contains a number of interesting features. In the tight-binding limit, the expectation value of the center-of-mass motion consists of a sinusoidal component with the slow frequency

$$\omega_u \approx [(K_1 + K_2)/M]^{1/2} \quad (3.5)$$

superimposed on a small-amplitude, high-frequency oscillation of frequency

$$\omega_v \approx (k/\mu)^{1/2}. \quad (3.6)$$

The presence of this high-frequency oscillation of the center-of-mass expectation value is one indication that the system is composite rather than elementary and that the existence of an internal dynamics is influencing the center-of-mass motion through the matrix elements of ψ_j in Eq. (3.2).

The way in which the details of the initial internal state affect the behavior of $\langle R(t) \rangle$ is intimately connected with the parity of the internal state ψ_j . If ψ_j is either an even or odd eigenstate of parity, then

$$\langle \psi_j(r, 0) | r | \psi_j(r, 0) \rangle = \langle \psi_j(r, 0) | p_r | \psi_j(r, 0) \rangle = 0. \quad (3.7)$$

In this case, while the expectation value of the center-of-mass position betrays the fact that the system possesses an internal structure, it is independent of the details of the quantum state of the internal system. On the other hand, if the internal state is of mixed parity, i.e.,

$$\psi_j(r, t) = \alpha \psi_{\text{even}} + \beta \psi_{\text{odd}} \quad (3.8)$$

with

$$\alpha^* \alpha + \beta^* \beta = 1, \quad (3.9)$$

then $\langle \psi_j(r, 0) | r | \psi_j(r, 0) \rangle$ and $\langle \psi_j(r, 0) | p_r | \psi_j(r, 0) \rangle$ are nonzero functions of α and β . Assuming the high-frequency oscillations are too rapid to be detected in the tight-binding limit for the mixed-parity case, Eq. (3.2) assumes the form

$$\langle R(t) \rangle \approx F(\alpha, \beta) \cos \omega_u t + G(\alpha, \beta) \sin \omega_u t, \quad (3.10)$$

where F and G are functions of α and β . The various different combinations of the even-parity and odd-parity makeup of the initial internal state influence the expectation value of the center-of-mass motion by producing an effective small phase change and amplitude change in the approximately simple harmonic motion of $\langle R(t) \rangle$ for $t > 0$.

In a manner similar to the calculations leading from Eq. (3.1) to Eq. (3.2) we may obtain the expectation values of additional center-of-mass properties, such as $\langle R^2(t) \rangle$ and $\langle P_R^2(t) \rangle$. The calculation of these two expectation values is straightforward but tedious and, due to the length of the results, these matrix elements are not given here. However,

the important result of their calculation is that, contrary to the structureless situation, no energy-like constant of the motion can be constructed from a linear combination of them. However, in the tight-binding limit, if we again assume that the high-frequency oscillations are too rapid to be observed, we may obtain a quantity ξ which is approximately constant for times long in comparison with ω_v^{-1} . Specifically,

$$\xi \equiv \frac{-\hbar^2 (A^2 - BC)^2}{2m_u} \langle P_R^2(t) \rangle + \frac{k_u}{2A^2} \langle R^2(t) \rangle$$

$$\approx \sum_{Nn} |a_{Nn}|^2 (N + \frac{1}{2}) \hbar \omega_u$$

$$+ \frac{1}{2} \left(\frac{B^2 k_u}{A^2 k_v} + \frac{C^2 m_v}{A^2 m_u} \right) \sum_{Nn} |a_{Nn}|^2 (n + \frac{1}{2}) \hbar \omega_v. \quad (3.11)$$

The value of ξ is sensitive to the makeup of the initial internal state of the system ψ_j since the a_{Nn} which appear in Eq. (3.11) depend on j through Eq. (2.20).

DISCUSSION

Equations (3.2), (3.10), and (3.11) detail a few of the ways in which the initial internal state j of our model system affects the time evolution of its center-of-mass observables. From these equations, one gets the impression that, especially in the tight-binding limit for times large compared with ω_v^{-1} , the center-of-mass time evolution resembles a harmonic oscillator with an effective natural frequency

$$\omega_{\text{eff}} = \omega_u, \quad (4.1)$$

having an effective mass

$$M_{\text{eff}} = m_u A^2 / (A^2 - BC)^2, \quad (4.2)$$

and with the external force having the effective coupling strength

$$K_{\text{eff}} = k_u / A^2. \quad (4.3)$$

If the object under consideration were structureless, then

$$Z_{\text{eff}} \equiv \omega_{\text{eff}}^2 M_{\text{eff}} / K_{\text{eff}} = 1. \quad (4.4)$$

However for our composite system, due to the existence of an internal dynamics the effective center-of-mass harmonic-oscillator parameters are incompatible, i.e.,

$$Z_{\text{eff}} = \left(\frac{(\gamma m_1 + m_2)^2}{M(\gamma^2 m_1 + m_2)} \right)^2$$

$$\approx 1 - \frac{2m_1 m_2}{M^2} \left(\frac{m_1 K_2 - m_2 K_1}{Mk} \right)^2 + O\left(\frac{K_i^3}{k^3}\right). \quad (4.5)$$

This resulting incompatibility of the center-of-mass parameters is only of the order of the square of the strength of the external interaction coupling divided by the square of the strength of the internal interaction coupling. For the usual perturbative problems such as atomic or molecular systems in laboratory-strength magnetic fields or hadrons in nonuniform external electric fields, this influence of the internal structure on the center-of-mass motion is unmeasurably small. Thus Eq. (4.5) justifies the usual "one-way influence" assumption discussed in Sec. I.

However, the center-of-mass observables of Eq. (3.2) and of the calculations leading to Eq. (3.11) are exact for all values of the coupling strengths and thus serve to continuously connect this perturbative limit to the situation where the internal coupling strength and the external coupling

strength are comparable. In the latter case the resulting influences of the relative and center-of-mass motions on each other are so great that the separation of the system into a readily identifiable internal part and a readily identifiable overall part is not at all clear cut. In this limit the internal and center-of-mass motions completely lose their individual identities and it is often deemed fruitful to consider both of them together as internal motions in Faddeev calculations for the larger composite system formed by the original particles and the external force center. The pedagogic virtue of present study is that its exact results for our model serve as a bridge calculation continuously connecting the extent of the influence of the relative motion on the center-of-mass motion from this one type of limiting be-

havior to the other without having to rely on perturbation-theory calculations in the one limit and Faddeev-type calculations in the other.

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